

read_screen_result_middle

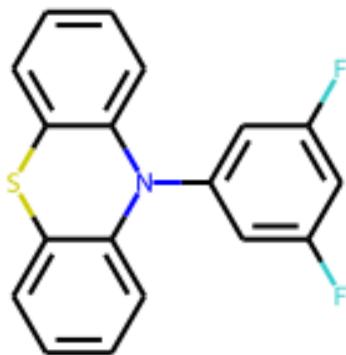
May 10, 2022

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[6]: import pickle
from rdkit import Chem

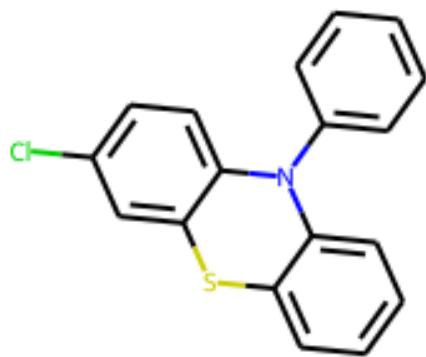
with open('screen_middle_70%.pkl', 'rb') as f:
    result_middle = pickle.load(f)

for i, v in enumerate(result_middle):
    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: Fc1cc(F)cc(N2c3cccc3Sc3cccc32)c1
prob: 0.92



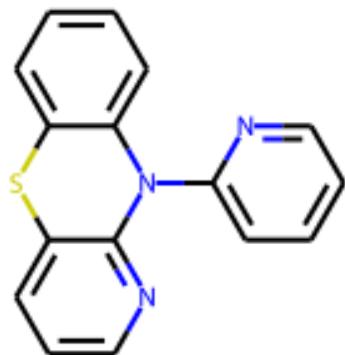
No.2
SMILES: Clc1ccc2c(c1)Sc1ccccc1N2c1ccccc1
prob: 0.92



No.3

SMILES: c1ccc(N2c3ccccc3Sc3cccnc32)nc1

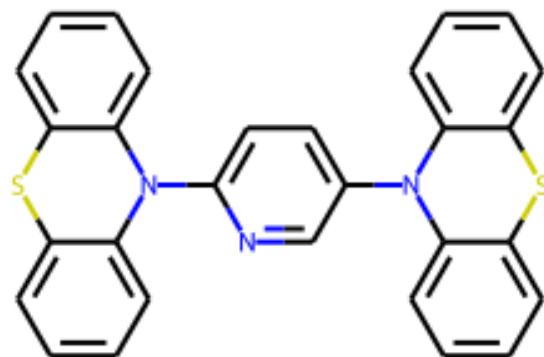
prob: 0.89



No.4

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(N2c3ccccc3Sc3cccc32)nc1

prob: 0.89



No.5

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cnccn1

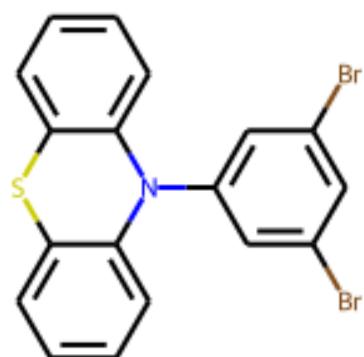
prob: 0.88



No.6

SMILES: Brc1cc(Br)cc(N2c3ccccc3Sc3ccccc32)c1

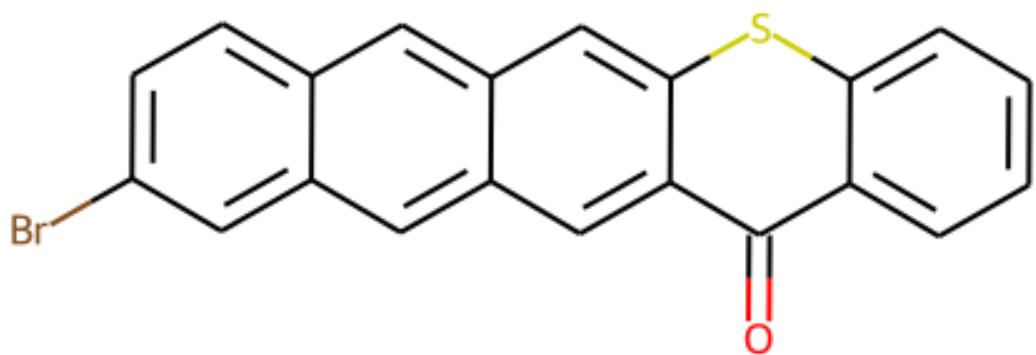
prob: 0.87



No.7

SMILES: O=c1c2ccccc2sc2cc3cc4ccc(Br)cc4cc3cc12

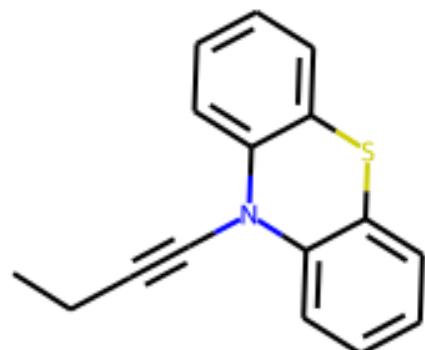
prob: 0.87



No.8

SMILES: CCC#CN1c2ccccc2Sc2ccccc21

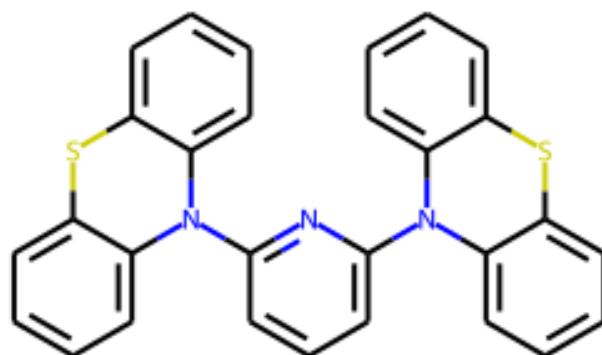
prob: 0.87



No.9

SMILES: c1cc(N2c3ccccc3Sc3ccccc32)nc(N2c3ccccc3Sc3ccccc32)c1

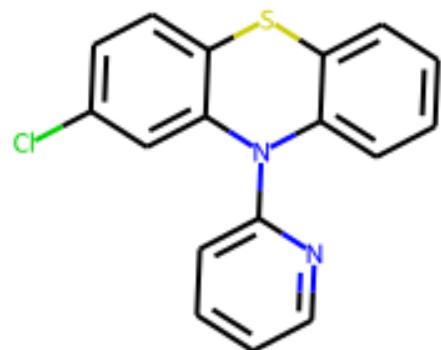
prob: 0.87



No.10

SMILES: Clc1ccc2c(c1)N(c1cccn1)c1ccccc1S2

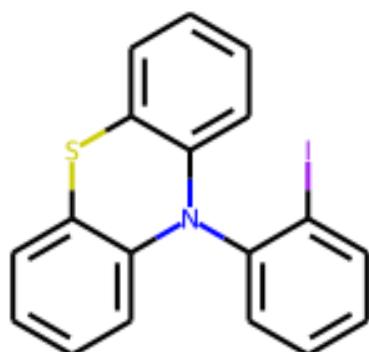
prob: 0.87



No.11

SMILES: Ic1ccccc1N1c2ccccc2Sc2ccccc21

prob: 0.86

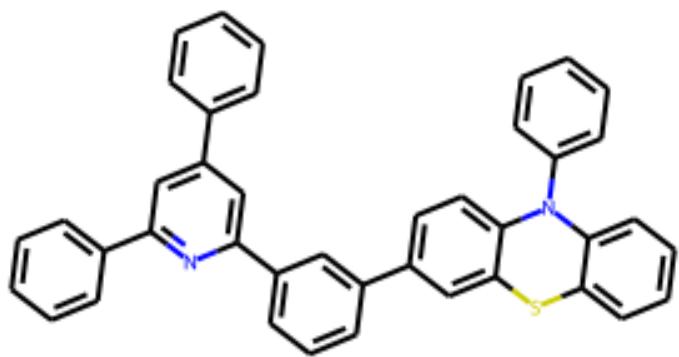


No.12

SMILES:

c1ccc(-c2cc(-c3ccccc3)nc(-c3cccc(-c4ccc5c(c4)Sc4ccccc4N5c4ccccc4)c3)c2)cc1

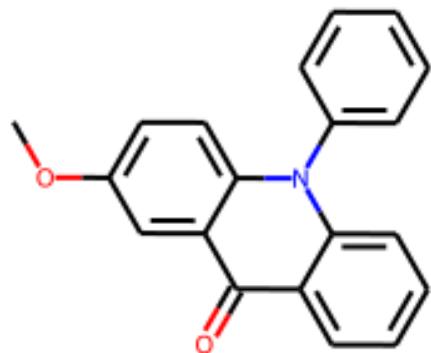
prob: 0.86



No.13

SMILES: C0c1ccc2c(c1)c(=O)c1ccccc1n2-c1ccccc1

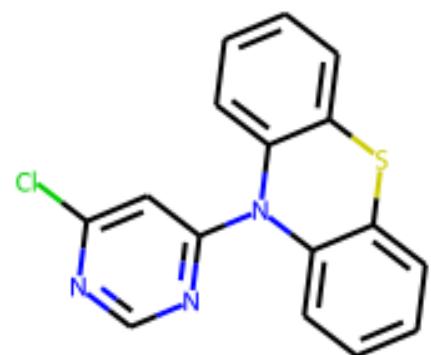
prob: 0.86



No.14

SMILES: Clc1cc(N2c3ccccc3Sc3ccccc32)ncn1

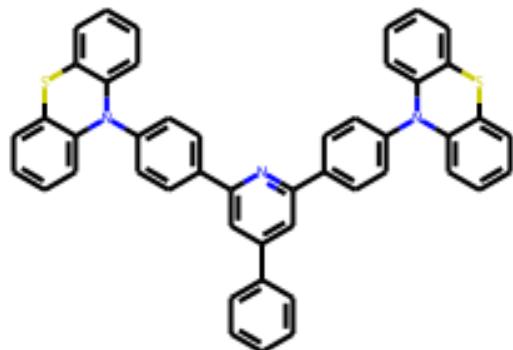
prob: 0.85



No.15

SMILES: c1ccc(-c2cc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)nc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)c2)cc1

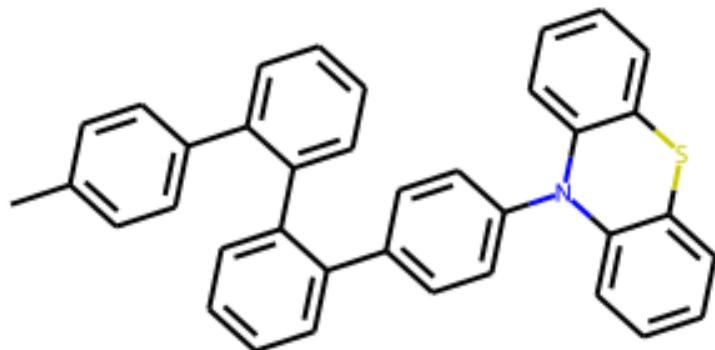
prob: 0.85



No.16

SMILES: Cc1ccc(-c2ccccc2-c2ccccc2-c2ccc(N3c4cccc4Sc4cccc43)cc2)cc1

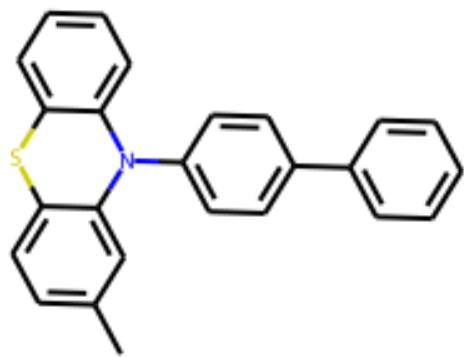
prob: 0.85



No.17

SMILES: Cc1ccc2c(c1)N(c1ccc(-c3ccccc3)cc1)c1ccccc1S2

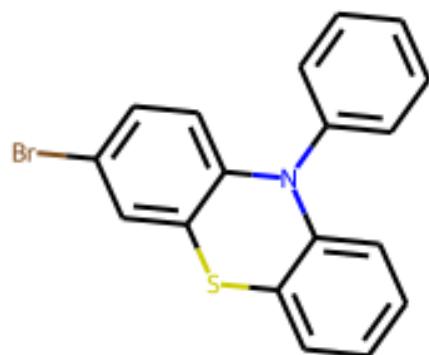
prob: 0.85



No.18

SMILES: Brcc1ccc2c(c1)Sc1ccccc1N2c1ccccc1

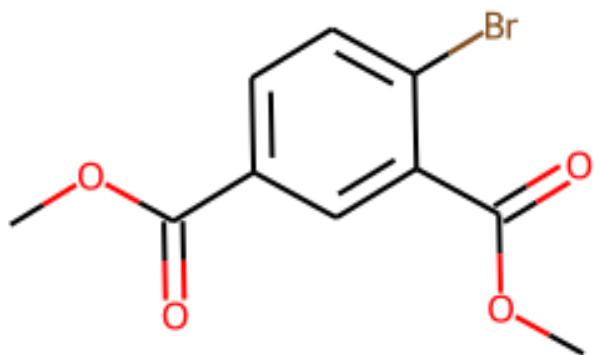
prob: 0.85



No.19

SMILES: COC(=O)c1ccc(Br)c(C(=O)OC)c1

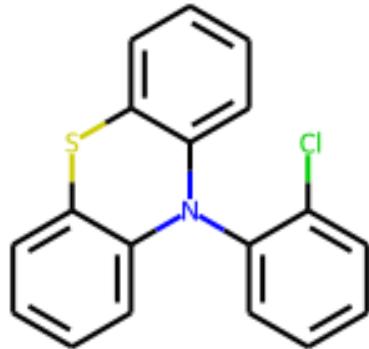
prob: 0.85



No.20

SMILES: Clc1ccccc1N1c2ccccc2Sc2ccccc21

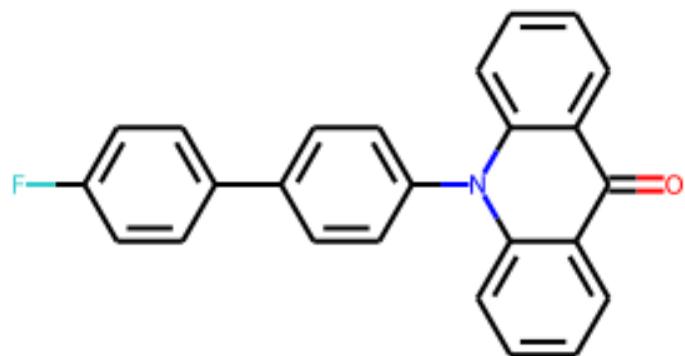
prob: 0.85



No.21

SMILES: O=c1c2ccccc2n(-c2ccc(-c3ccc(F)cc3)cc2)c2ccccc12

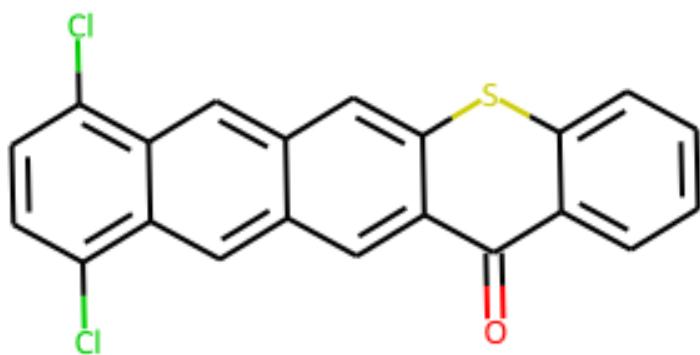
prob: 0.85



No.22

SMILES: O=c1c2ccccc2sc2cc3cc4c(Cl)ccc(Cl)c4cc3cc12

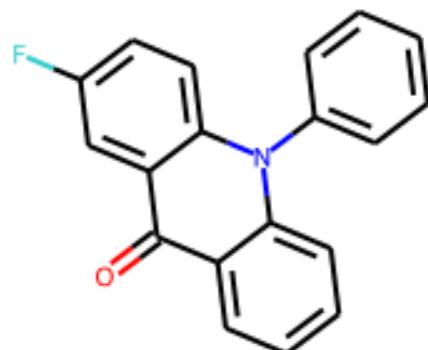
prob: 0.85



No. 23

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2ccc(F)cc12

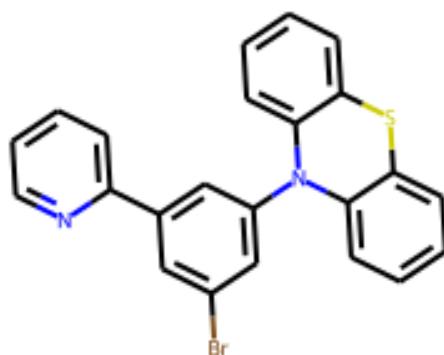
prob: 0.85



No. 24

SMILES: Brc1cc(-c2cccn2)cc(N2c3cccc3Sc3cccc32)c1

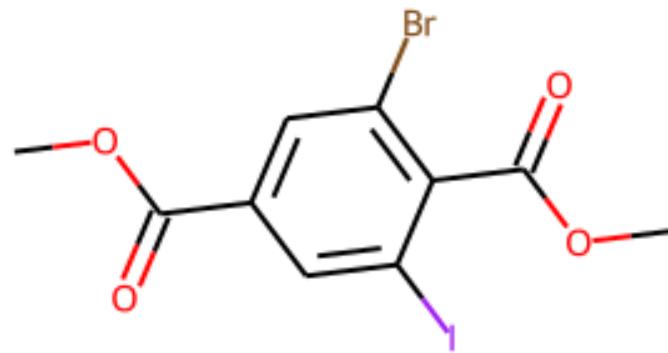
prob: 0.84



No.25

SMILES: COC(=O)c1cc(Br)c(C(=O)OC)c(I)c1

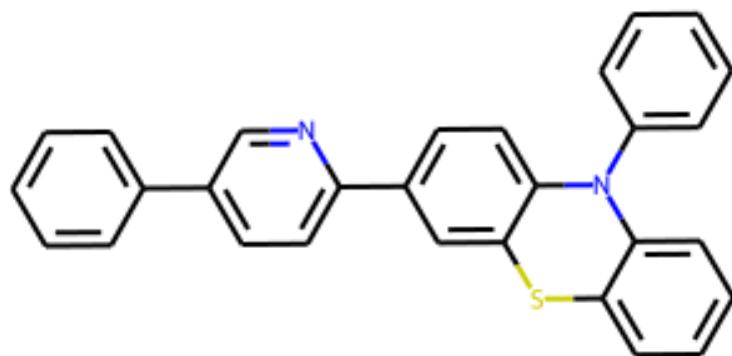
prob: 0.84



No.26

SMILES: c1ccc(-c2ccc(-c3ccc4c(c3)Sc3cccc3N4c3cccc3)nc2)cc1

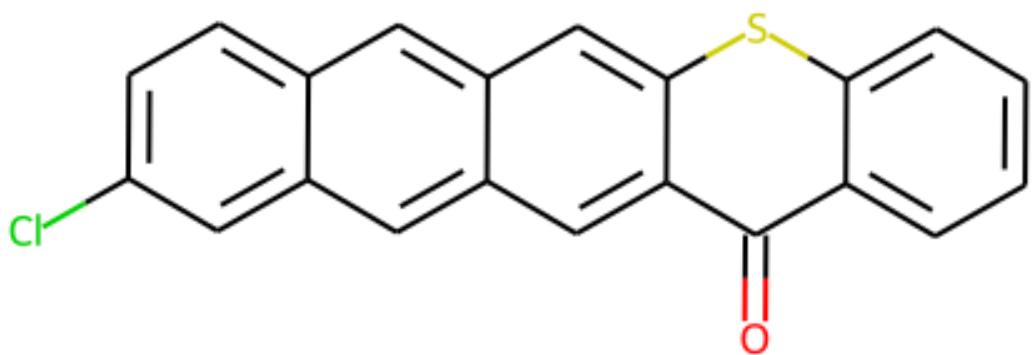
prob: 0.84



No.27

SMILES: O=c1c2ccccc2sc2cc3cc4ccc(Cl)cc4cc3cc12

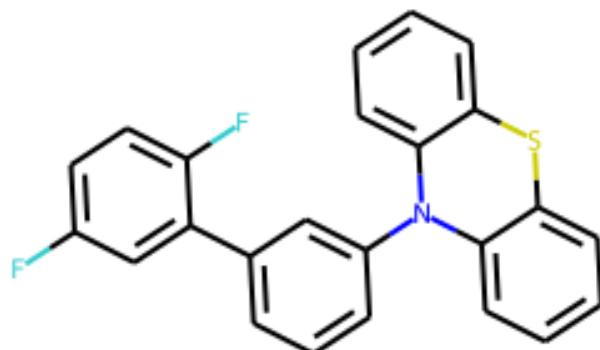
prob: 0.84



No. 28

SMILES: Fc1ccc(F)c(-c2cccc(N3c4ccccc4Sc4ccccc43)c2)c1

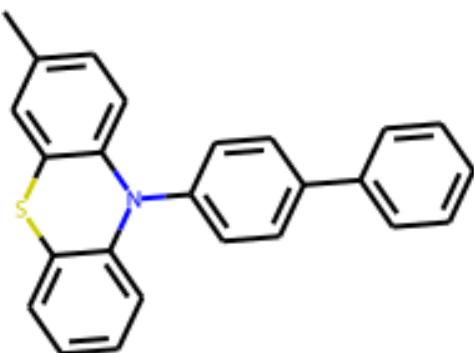
prob: 0.84



No. 29

SMILES: Cc1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2ccccc2)cc1

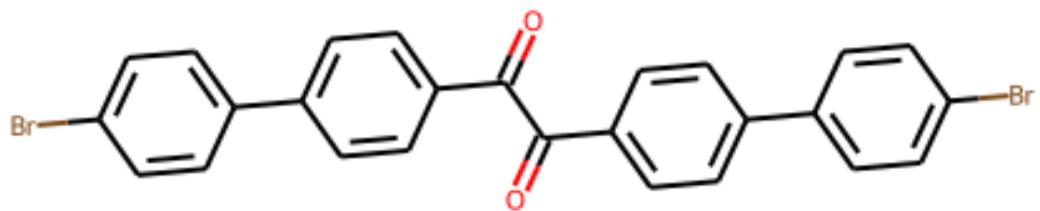
prob: 0.84



No.30

SMILES: O=C(C(=O)c1ccc(-c2ccc(Br)cc2)cc1)c1ccc(-c2ccc(Br)cc2)cc1

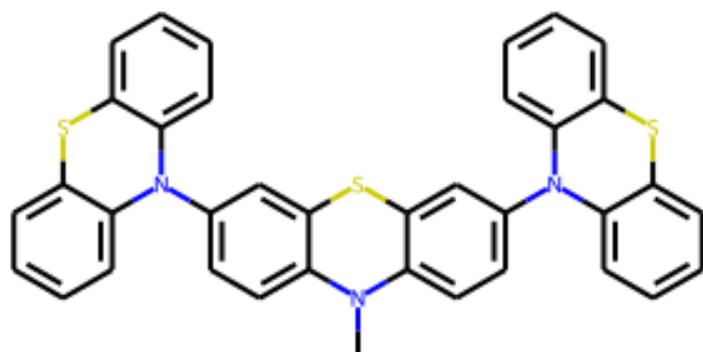
prob: 0.84



No.31

SMILES: CN1c2ccc(N3c4cccc4Sc4cccc43)cc2Sc2cc(N3c4cccc4Sc4cccc43)ccc21

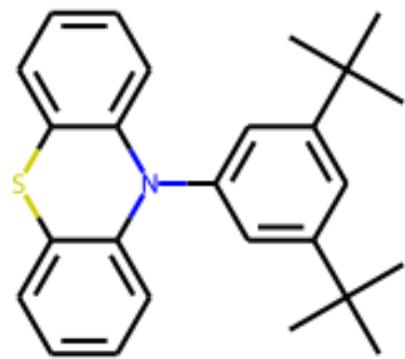
prob: 0.84



No.32

SMILES: CC(C)(C)c1cc(N2c3cccc3Sc3cccc32)cc(C(C)(C)C)c1

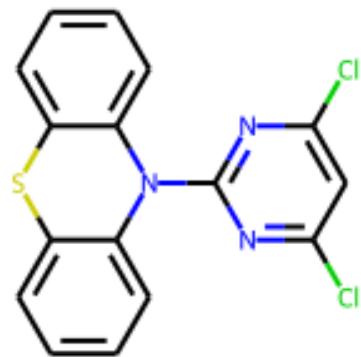
prob: 0.84



No.33

SMILES: Clc1cc(Cl)nc(N2c3cccc3Sc3cccc32)n1

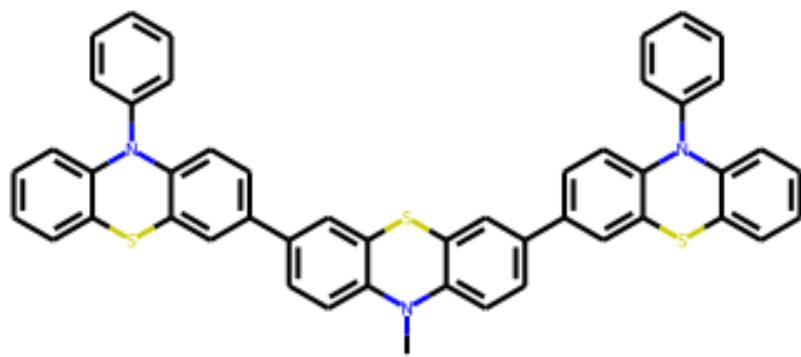
prob: 0.84



No.34

SMILES: CN1c2ccc(-c3ccc4c(c3)Sc3cccc3N4c3cccc3)cc2Sc2cc(-c3ccc4c(c3)Sc3cccc3N4c3cccc3)ccc21

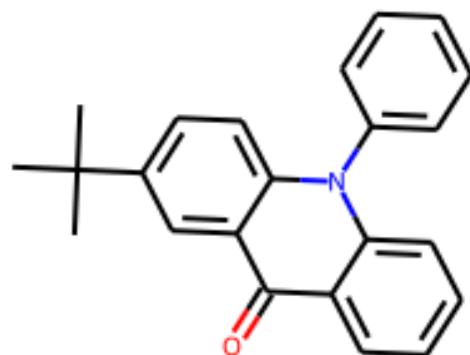
prob: 0.83



No.35

SMILES: CC(C)(C)c1ccc2c(c1)c(=O)c1ccccc1n2-c1ccccc1

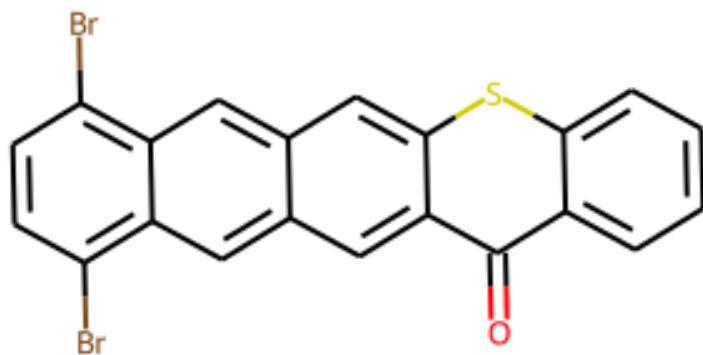
prob: 0.83



No.36

SMILES: O=c1c2ccccc2sc2cc3cc4c(Br)ccc(Br)c4cc3cc12

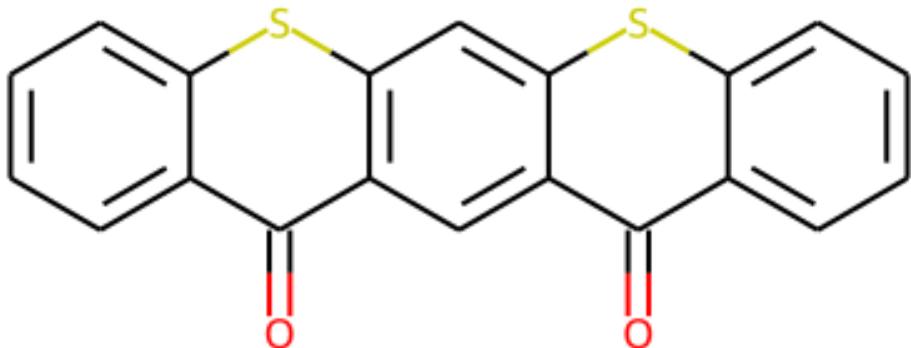
prob: 0.83



No.37

SMILES: O=c1c2ccccc2sc2cc3sc4ccccc4c(=O)c3cc12

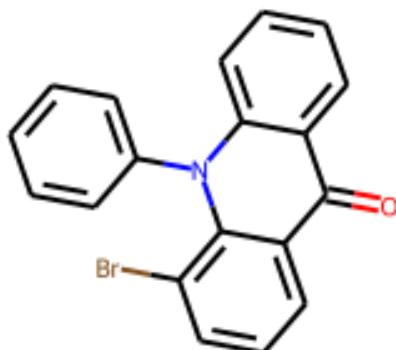
prob: 0.83



No.38

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2c(Br)cccc12

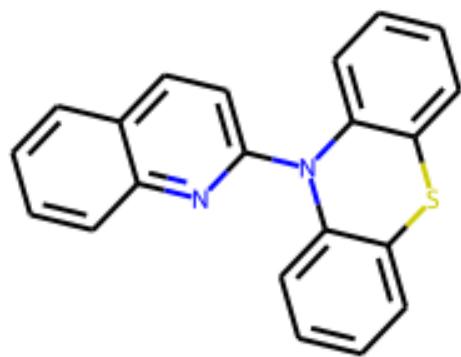
prob: 0.83



No.39

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2ccccc2n1

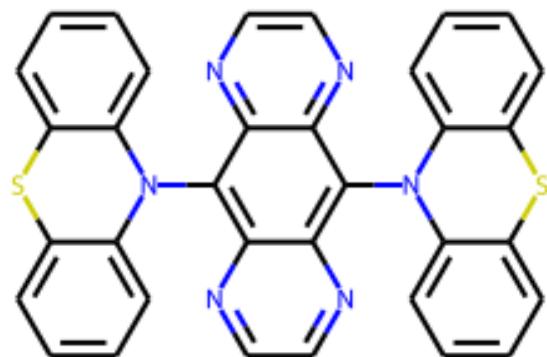
prob: 0.83



No.40

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1c2nccnc2c(N2c3cccc3Sc3cccc32)c2nccnc12

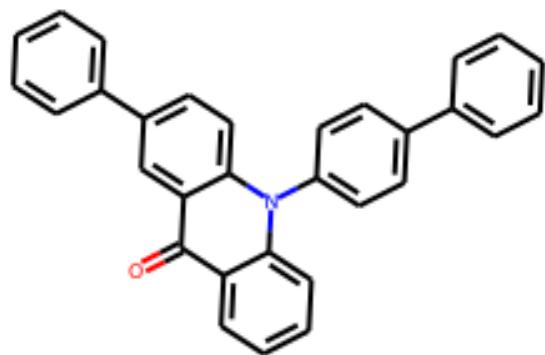
prob: 0.83



No.41

SMILES: O=c1c2ccccc2n(-c2ccc(-c3cccc3)cc2)c2ccc(-c3cccc3)cc12

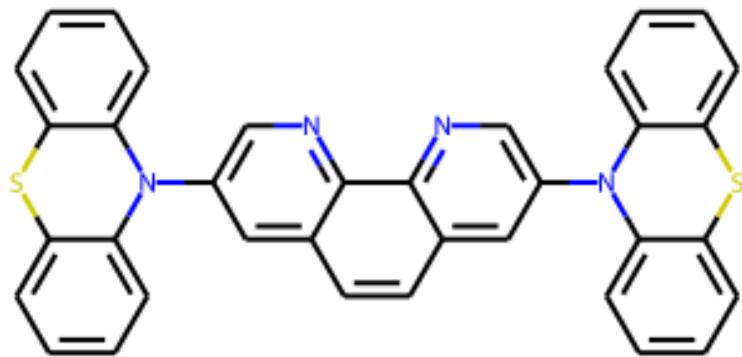
prob: 0.83



No.42

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cnc2c(ccc3cc(N4c5ccccc5Sc5ccccc54)cnc32)c1

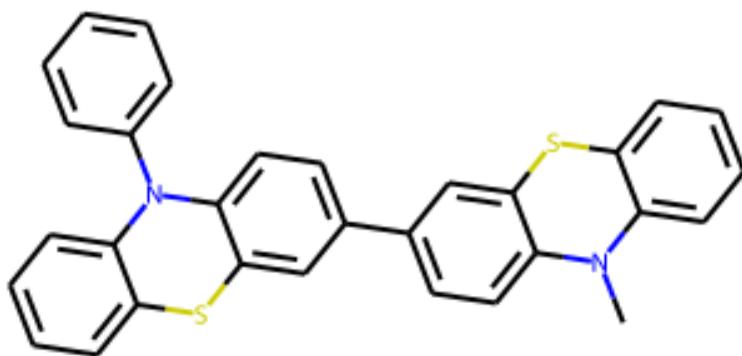
prob: 0.83



No.43

SMILES: CN1c2ccccc2Sc2cc(-c3ccc4c(c3)Sc3ccccc3N4c3ccccc3)ccc21

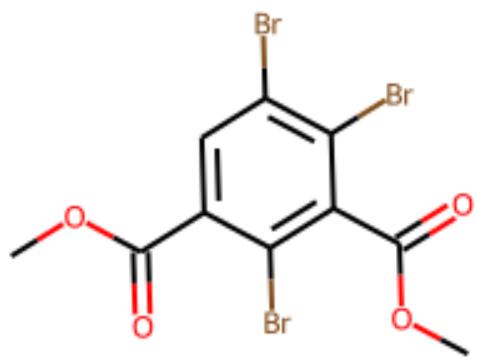
prob: 0.83



No.44

SMILES: COC(=O)c1cc(Br)c(Br)c(C(=O)OC)c1Br

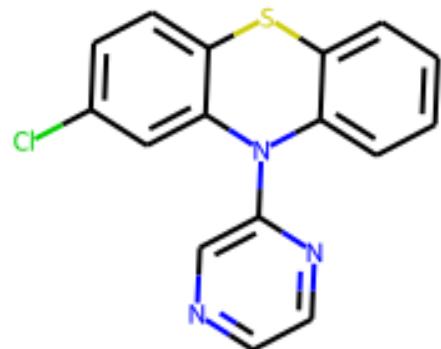
prob: 0.83



No.45

SMILES: Clc1ccc2c(c1)N(c1nccn1)c1ccccc1S2

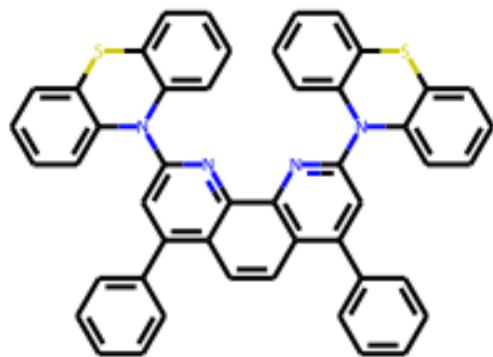
prob: 0.82



No.46

SMILES: c1ccc(-c2cc(N3c4ccccc4Sc4ccccc43)nc3c2ccc2c(-c4ccccc4)cc(N4c5ccccc5Sc5ccc54)nc23)cc1

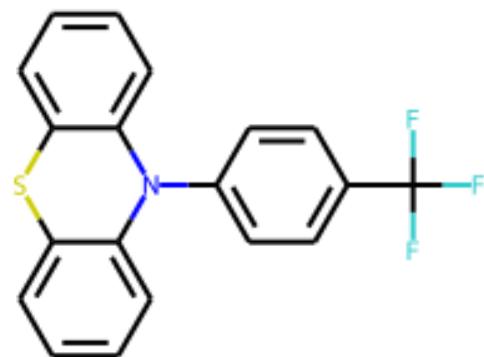
prob: 0.82



No.47

SMILES: FC(F)(F)c1ccc(N2c3ccccc3Sc3ccccc32)cc1

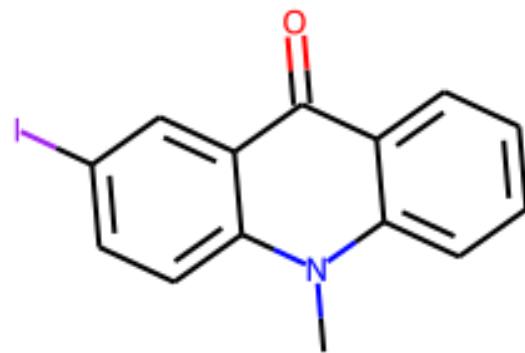
prob: 0.82



No.48

SMILES: Cn1c2ccccc2c(=O)c2cc(I)ccc21

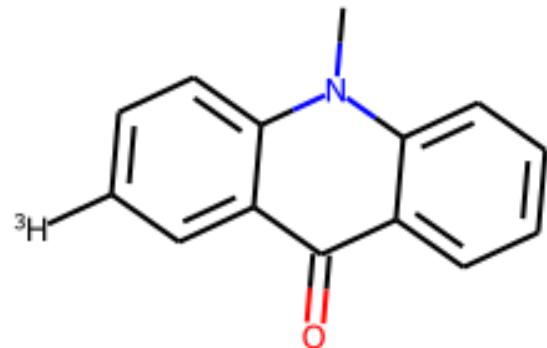
prob: 0.82



No.49

SMILES: [3H]c1ccc2c(c1)c(=O)c1ccccc1n2C

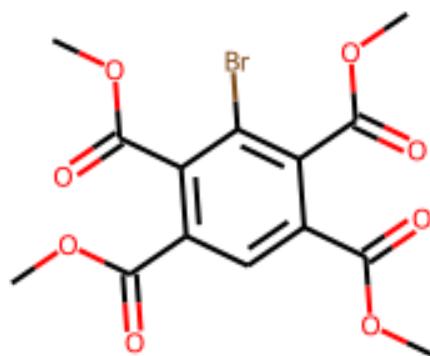
prob: 0.82



No.50

SMILES: COC(=O)c1cc(C(=O)OC)c(C(=O)OC)c(Br)c1C(=O)OC

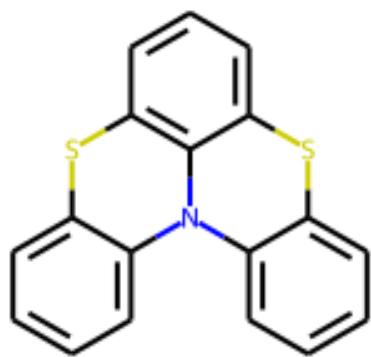
prob: 0.82



No.51

SMILES: c1ccc2c(c1)Sc1ccccc3c1N2c1ccccc1S3

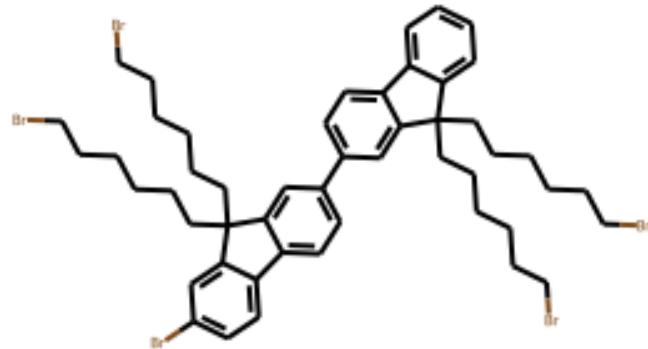
prob: 0.82



No.52

SMILES: BrCCCCCCC1(CCCCCCBr)c2ccccc2-c2ccc(-c3ccc4c(c3)C(CCCCCCBr)(CCCCCCBr)c3cc(Br)ccc3-4)cc21

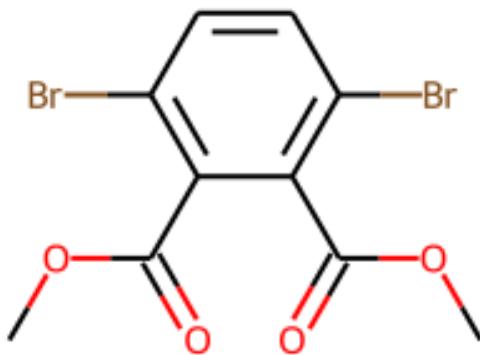
prob: 0.82



No.53

SMILES: COC(=O)c1c(Br)ccc(Br)c1C(=O)OC

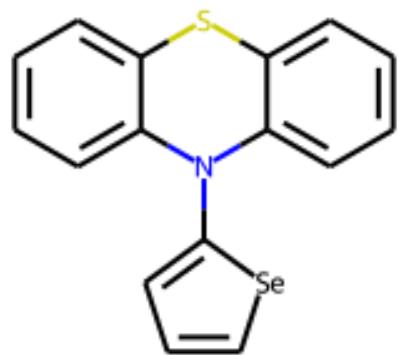
prob: 0.82



No.54

SMILES: c1c[se]c(N2c3ccccc3Sc3ccccc32)c1

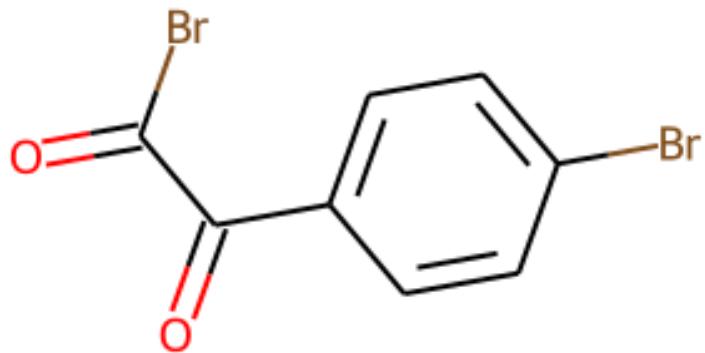
prob: 0.82



No.55

SMILES: O=C(Br)C(=O)c1ccc(Br)cc1

prob: 0.82

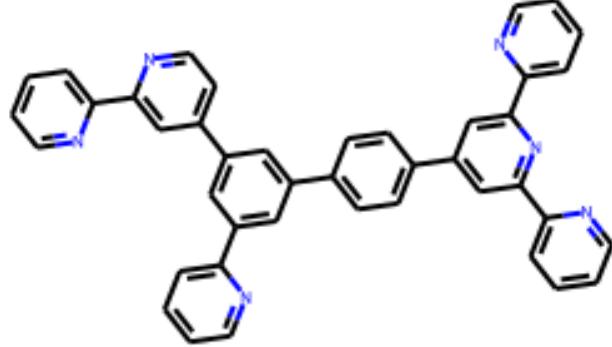


No.56

SMILES: c1ccc(-c2cc(-c3ccc(-c4cc(-c5cccn5)nc(-c5cccn5)c4)cc3)cc(-c3ccnc(-c4ccc

cn4)c3)c2)nc1

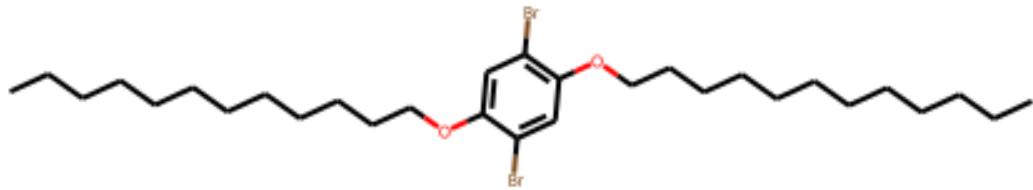
prob: 0.82



No.57

SMILES: CCCCCCCCCCCC0c1cc(Br)c(OCCCCCC)cc1Br

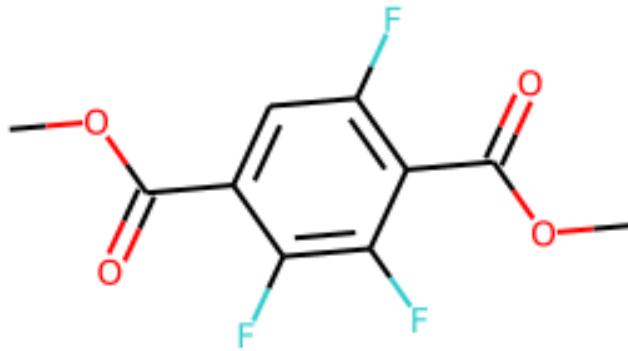
prob: 0.81



No.58

SMILES: COC(=O)c1cc(F)c(C(=O)OC)c(F)c1F

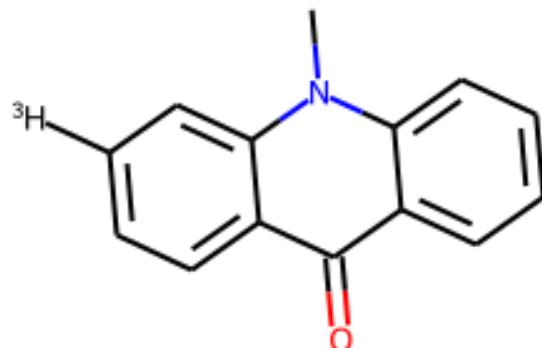
prob: 0.81



No.59

SMILES: [3H]c1ccc2c(=O)c3ccccc3n(C)c2c1

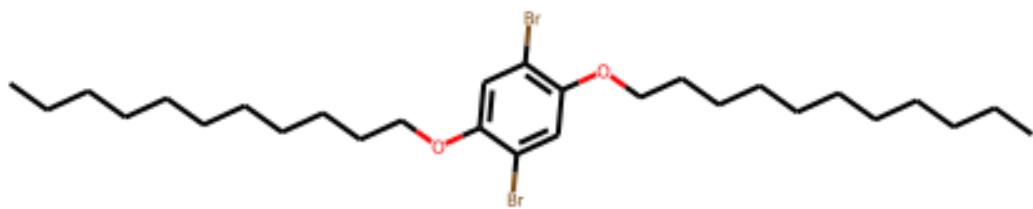
prob: 0.81



No.60

SMILES: CCCCCCCCCCCCc1cc(Br)c(OCCCCCC)cc1Br

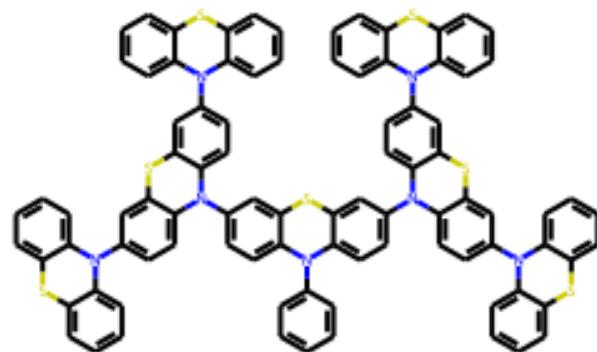
prob: 0.81



No. 61

SMILES: c1ccc(N2c3ccc(N4c5ccc(N6c7cccc7Sc7cccc76)cc5Sc5cc(N6c7cccc7Sc7cccc76)ccc54)cc3Sc3cc(N4c5ccc(N6c7cccc7Sc7cccc76)cc5Sc5cc(N6c7cccc7Sc7cccc76)ccc54)ccc32)cc1

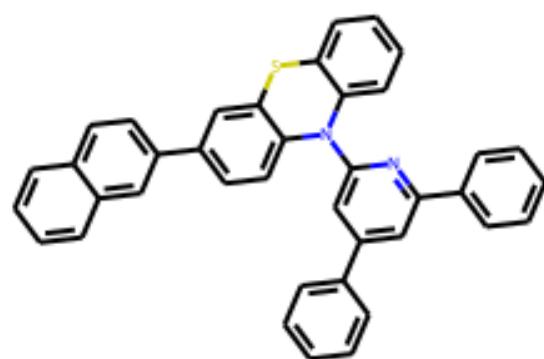
prob: 0.81



No. 62

SMILES: c1ccc(-c2cc(-c3cccc3)nc(N3c4cccc4Sc4cc(-c5ccc6cccc6c5)ccc43)c2)cc1

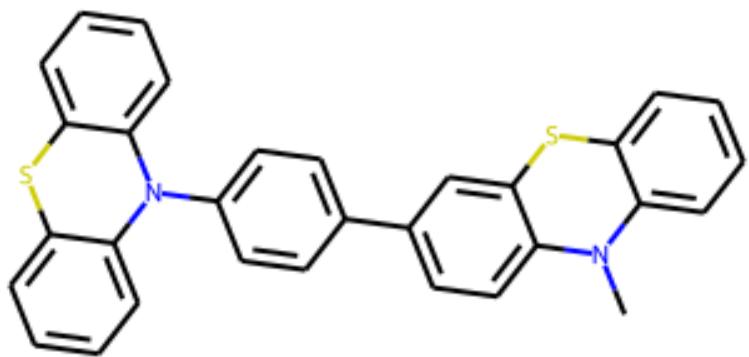
prob: 0.81



No. 63

SMILES: CN1c2cccc2Sc2cc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)ccc21

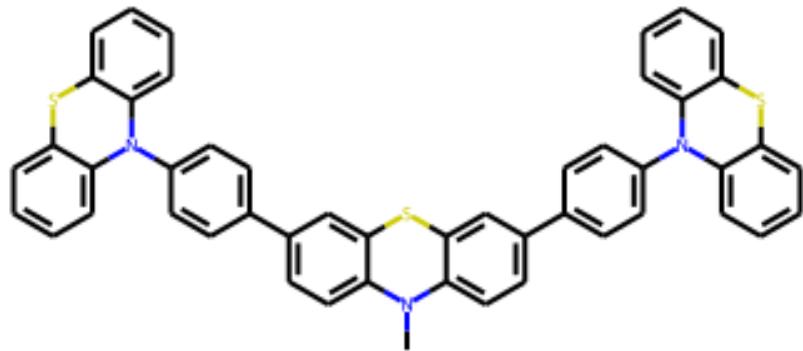
prob: 0.81



No. 64

SMILES: CN1c2ccc(-c3ccc(N4c5cccc5Sc5ccccc54)cc3)cc2Sc2cc(-c3ccc(N4c5cccc5Sc5ccc54)cc3)ccc21

prob: 0.81



No. 65

SMILES: CCCCCCCC0c1cc(I)c(OCCCCCC)cc1Br

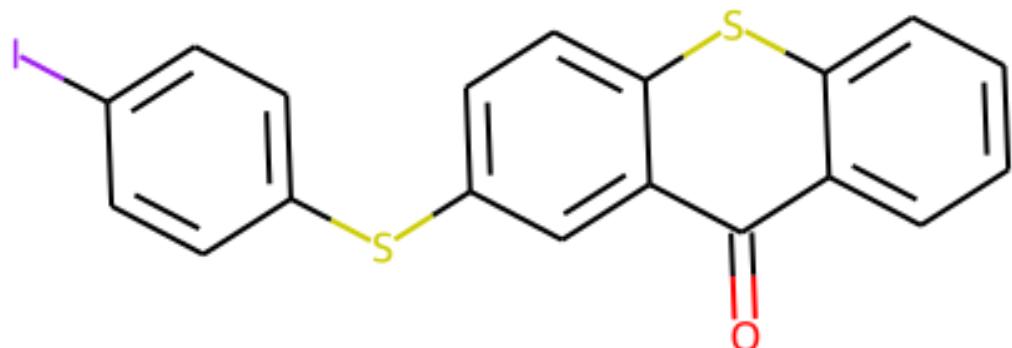
prob: 0.81



No. 66

SMILES: O=c1c2ccccc2sc2ccc(Sc3ccc(I)cc3)cc12

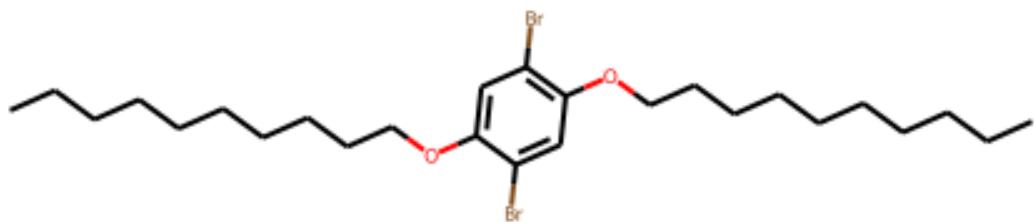
prob: 0.81



No. 67

SMILES: CCCCCCCCCCOC1cc(Br)c(OCCCCCC)cc1Br

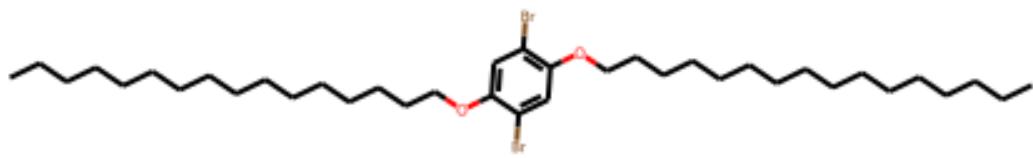
prob: 0.81



No. 68

SMILES: CCCCCCCCCCCCCCCC0c1cc(Br)c(OCCCCCC)cc1Br

prob: 0.81

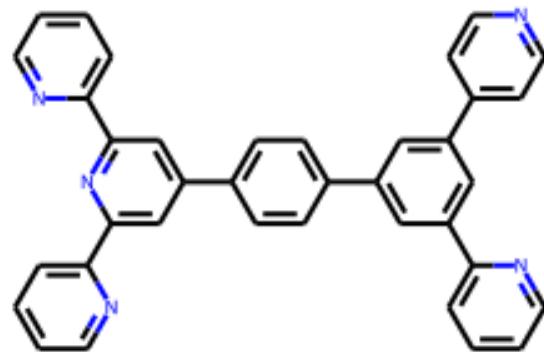


No. 69

SMILES:

c1ccc(-c2cc(-c3ccncc3)cc(-c3ccc(-c4cc(-c5cccn5)nc(-c5cccn5)c4)cc3)c2)nc1

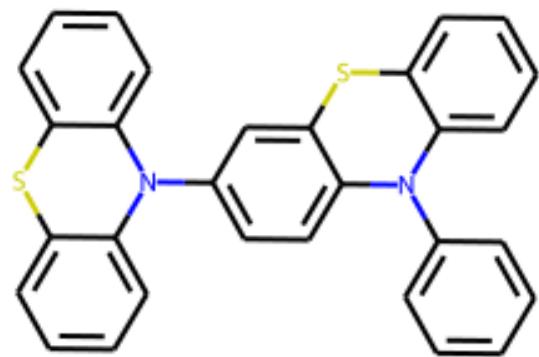
prob: 0.81



No. 70

SMILES: c1ccc(N2c3cccc3Sc3cc(N4c5ccccc5Sc5ccccc54)ccc32)cc1

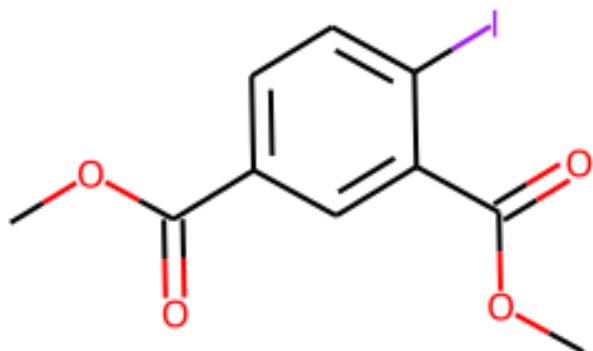
prob: 0.81



No.71

SMILES: COC(=O)c1ccc(I)c(C(=O)OC)c1

prob: 0.81

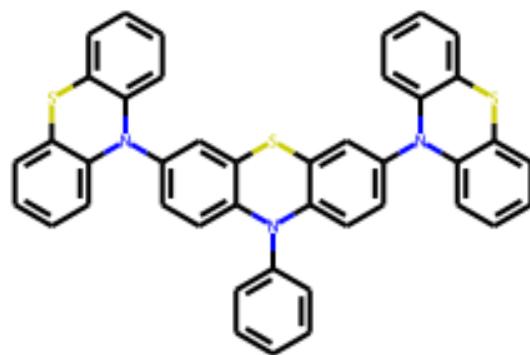


No.72

SMILES:

c1ccc(N2c3ccc(N4c5ccccc5Sc5ccccc54)cc3Sc3cc(N4c5ccccc5Sc5ccccc54)ccc32)cc1

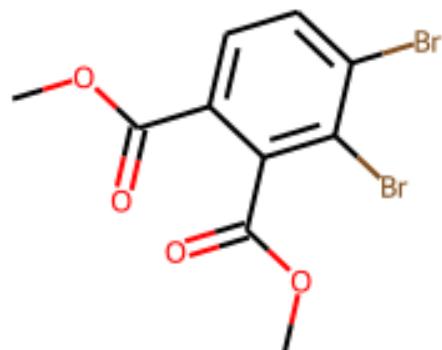
prob: 0.81



No.73

SMILES: COC(=O)c1ccc(Br)c(Br)c1C(=O)OC

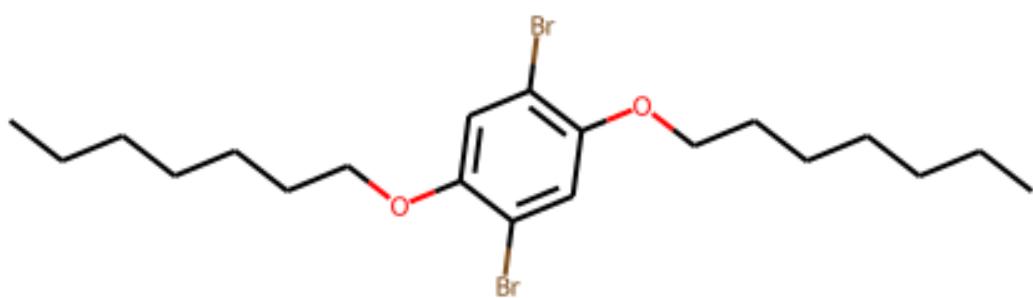
prob: 0.81



No.74

SMILES: CCCCCCBr1cc(OCCCCCC)cc1Br

prob: 0.81



No.75

SMILES: COC(=O)c1c(Br)c(C(=O)OC)c(Br)c(C(=O)OC)c1Br

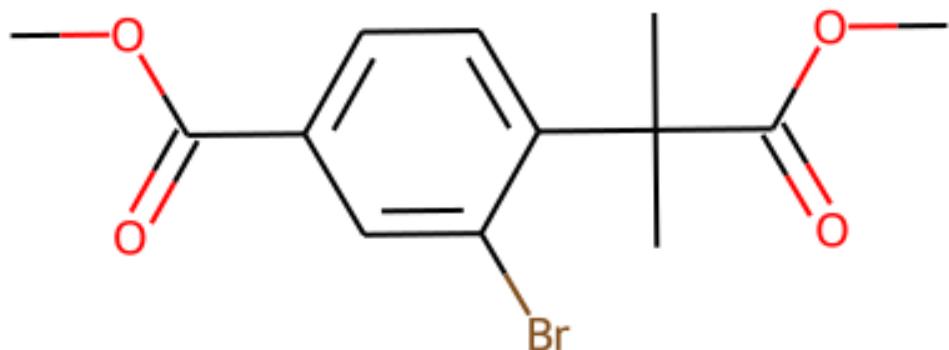
prob: 0.81



No.76

SMILES: COC(=O)c1ccc(C(C)(C)C(=O)OC)c(Br)c1

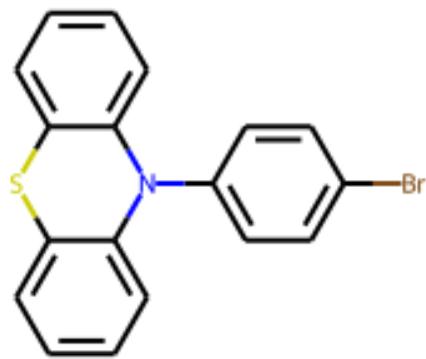
prob: 0.81



No.77

SMILES: Brcc1ccc(N2c3cccc3Sc3cccc32)cc1

prob: 0.8

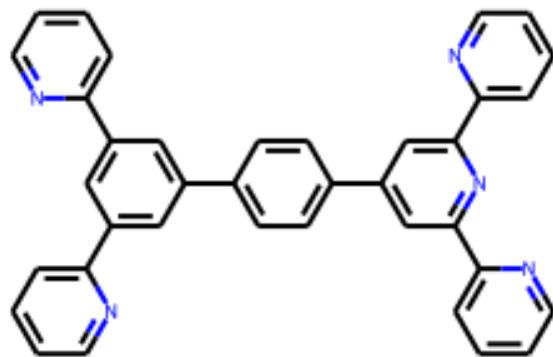


No.78

SMILES:

c1ccc(-c2cc(-c3ccc(-c4cc(-c5ccccc5)nc(-c5ccccc5)c4)cc3)cc(-c3ccccc3)c2)nc1

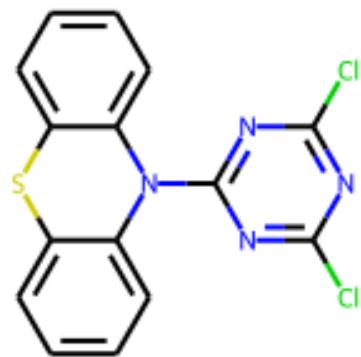
prob: 0.8



No.79

SMILES: Clc1nc(Cl)nc(N2c3cccc3Sc3cccc32)n1

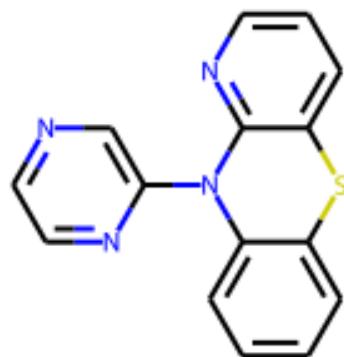
prob: 0.8



No.80

SMILES: c1ccc2c(c1)Sc1cccn1N2c1cnccn1

prob: 0.8

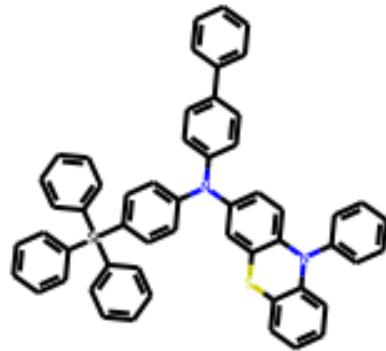


No.81

SMILES: c1ccc(-c2ccc(N(c3ccc([Si](C)c4cccc4)(c4cccc4)c4cccc4)cc3)c3ccc4c(c3)Sc3

ccccc3N4c3cccc3)cc2)cc1

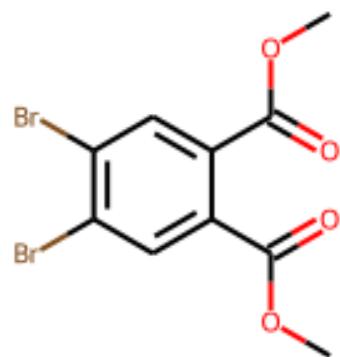
prob: 0.8



No.82

SMILES: COC(=O)c1cc(Br)c(Br)cc1C(=O)OC

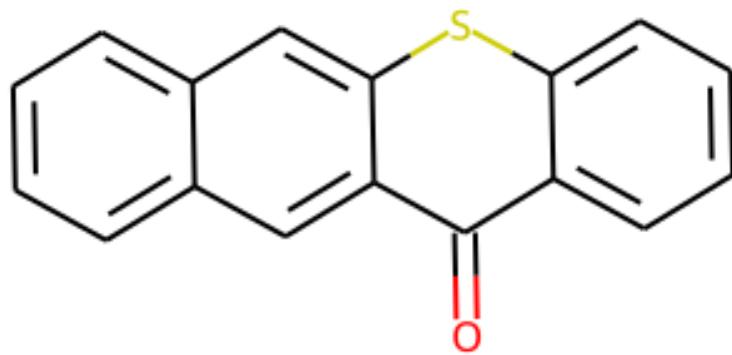
prob: 0.8



No.83

SMILES: O=c1c2cccc2sc2cc3cccc3cc12

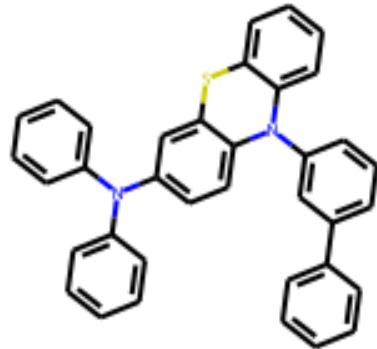
prob: 0.8



No.84

SMILES: c1ccc(-c2cccc(N3c4ccccc4Sc4cc(N(c5ccccc5)c5ccccc5)ccc43)c2)cc1

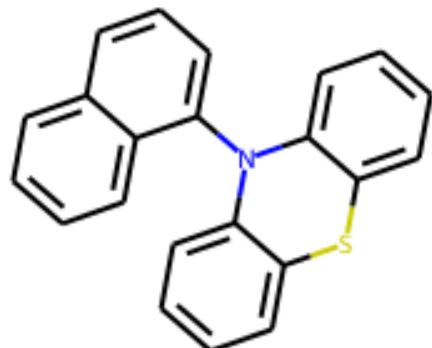
prob: 0.8



No.85

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cccc2ccccc12

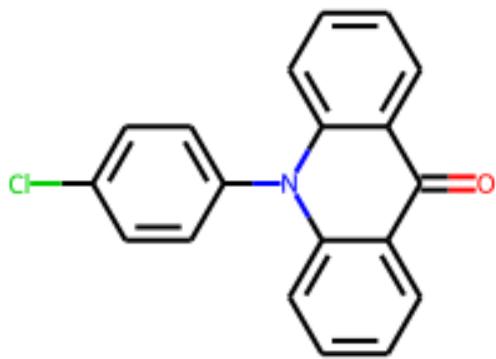
prob: 0.8



No.86

SMILES: O=c1c2ccccc2n(-c2ccc(Cl)cc2)c2ccccc12

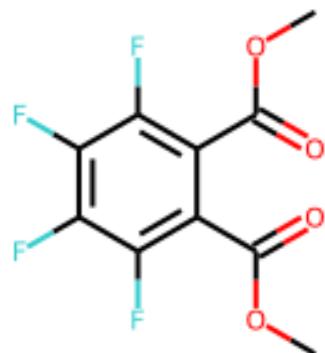
prob: 0.8



No.87

SMILES: COC(=O)c1c(F)cc(F)c(F)c(F)c1C(=O)OC

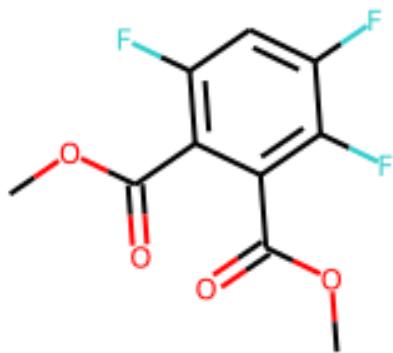
prob: 0.8



No.88

SMILES: COC(=O)c1c(F)cc(F)c(F)c1C(=O)OC

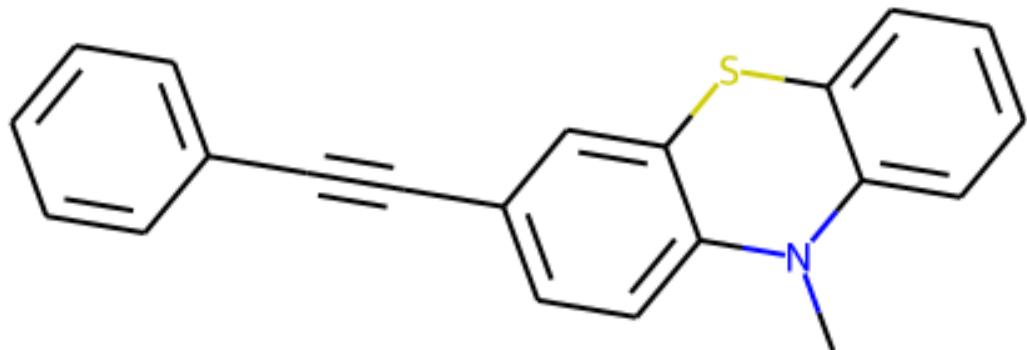
prob: 0.8



No.89

SMILES: CN1c2ccccc2Sc2cc(C#Cc3ccccc3)ccc21

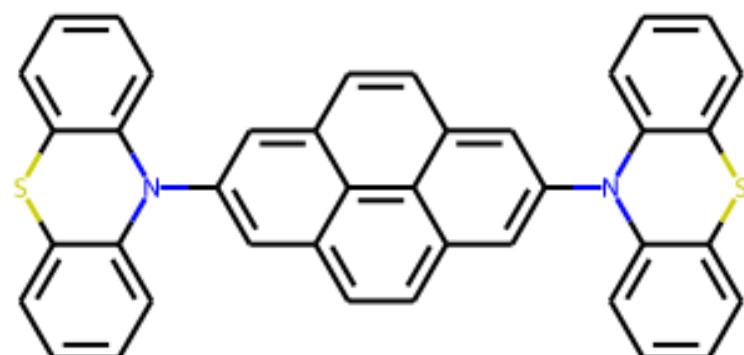
prob: 0.8



No.90

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cc2ccc3cc(N4c5ccccc5Sc5ccccc54)cc4ccc(c1)c2c34

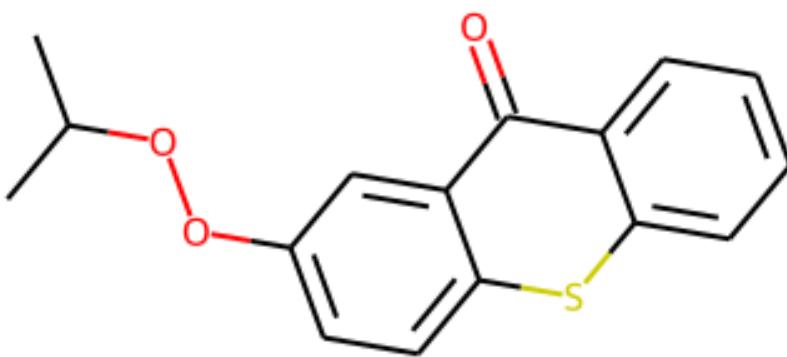
prob: 0.8



No.91

SMILES: CC(C)Oc1ccc2sc3ccccc3c(=O)c2c1

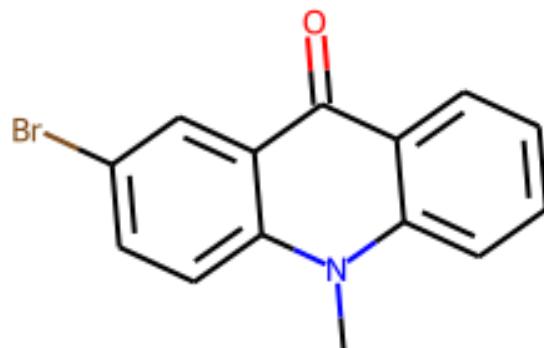
prob: 0.8



No.92

SMILES: Cn1c2ccccc2c(=O)c2cc(Br)ccc21

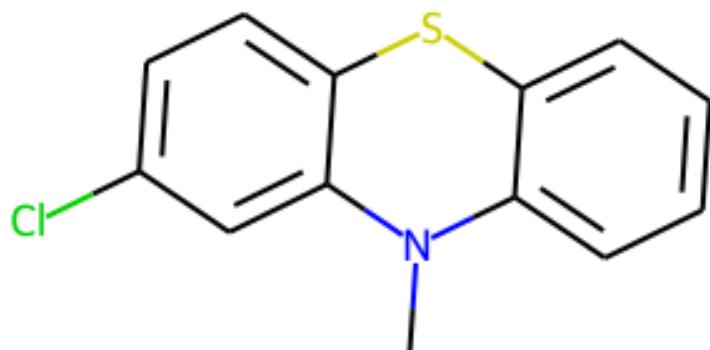
prob: 0.8



No.93

SMILES: CN1c2ccccc2Sc2ccc(Cl)cc21

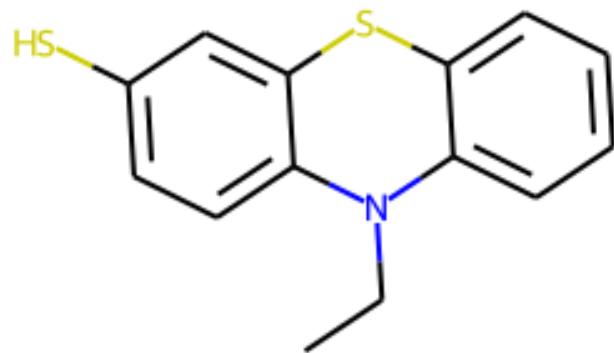
prob: 0.8



No.94

SMILES: CCN1c2ccccc2Sc2cc(S)ccc21

prob: 0.8



No.95

SMILES: c1ccc(-c2cc(N3c4ccccc4Sc4ccccc43)cc(-c3ccccc3)n2)cc1

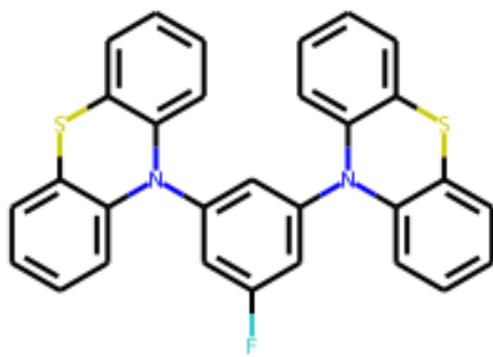
prob: 0.8



No.96

SMILES: Fc1cc(N2c3ccccc3Sc3ccccc32)cc(N2c3ccccc3Sc3ccccc32)c1

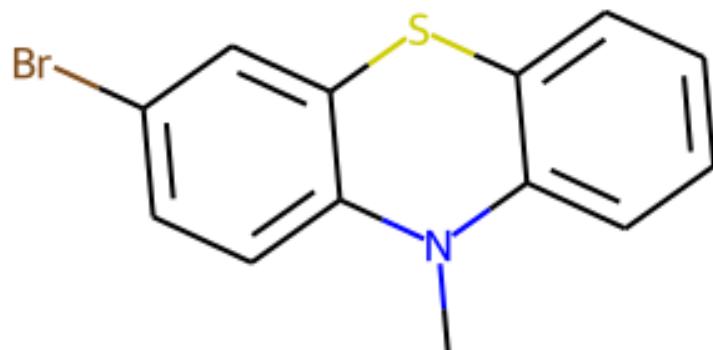
prob: 0.8



No.97

SMILES: CN1c2ccccc2Sc2cc(Br)ccc21

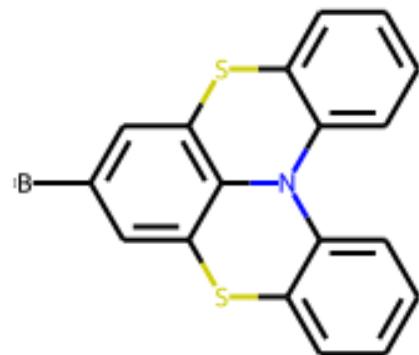
prob: 0.8



No.98

SMILES: [B]c1cc2c3c(c1)Sc1ccccc1N3c1ccccc1S2

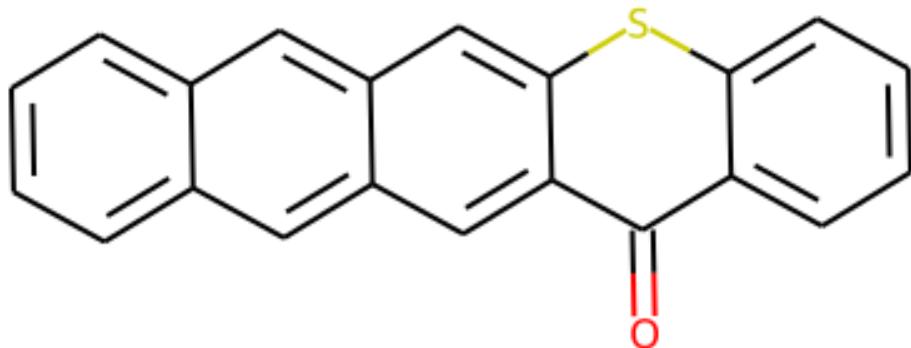
prob: 0.8



No.99

SMILES: O=c1c2ccccc2sc2cc3cc4ccccc4cc3cc12

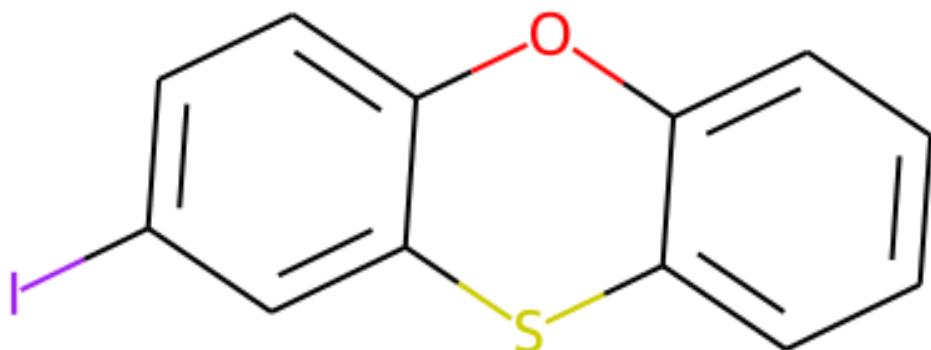
prob: 0.8



No.100

SMILES: Ic1ccc2c(c1)Sc1ccccc102

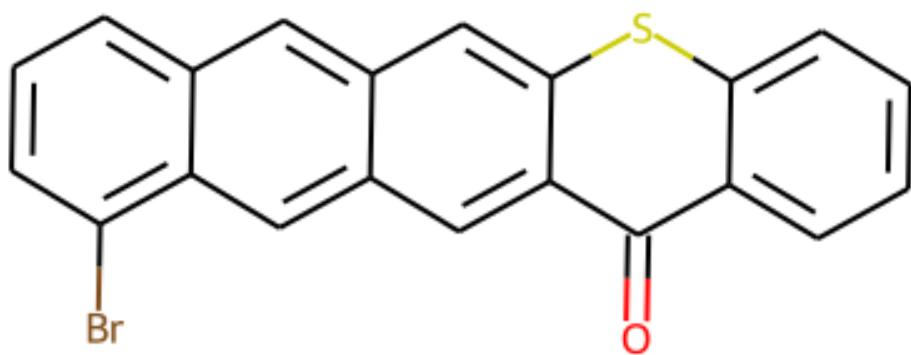
prob: 0.8



No.101

SMILES: O=c1c2ccccc2sc2cc3cc4cccc(Br)c4cc3cc12

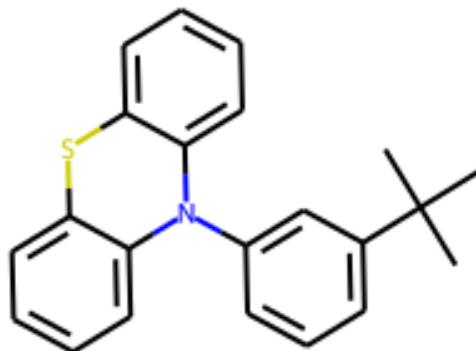
prob: 0.8



No.102

SMILES: CC(C)(C)c1ccccc(N2c3cccc3Sc3cccc32)c1

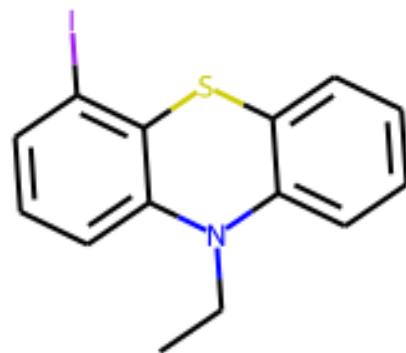
prob: 0.8



No.103

SMILES: CCN1c2ccccc2Sc2c(I)cccc21

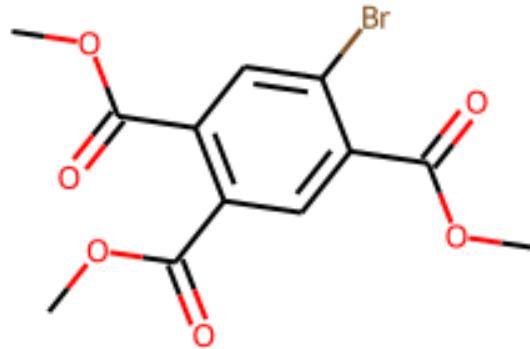
prob: 0.8



No.104

SMILES: COC(=O)c1cc(C(=O)OC)c(C(=O)OC)cc1Br

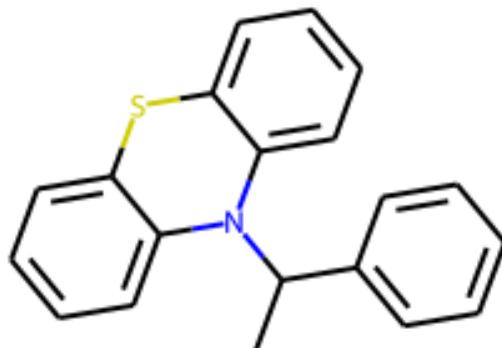
prob: 0.8



No.105

SMILES: CC(c1ccccc1)N1c2ccccc2Sc2ccccc21

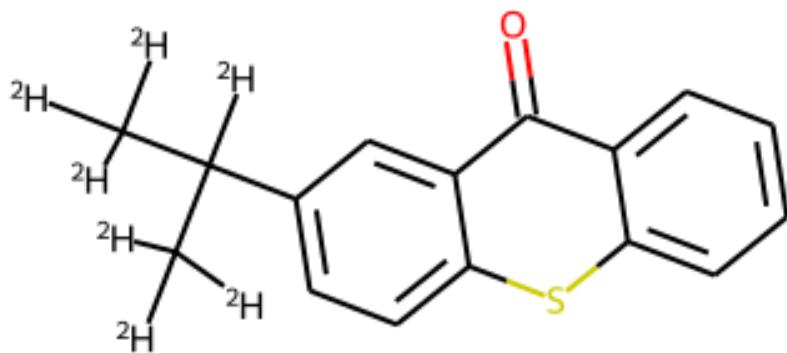
prob: 0.8



No.106

SMILES: [2H]C([2H])([2H])C([2H])(c1ccc2sc3ccccc3c(=O)c2c1)C([2H])([2H])[2H]

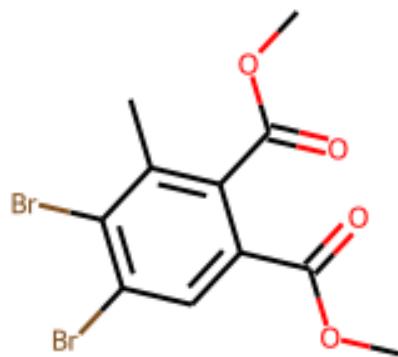
prob: 0.8



No.107

SMILES: COC(=O)c1cc(Br)c(Br)c(C)c1C(=O)OC

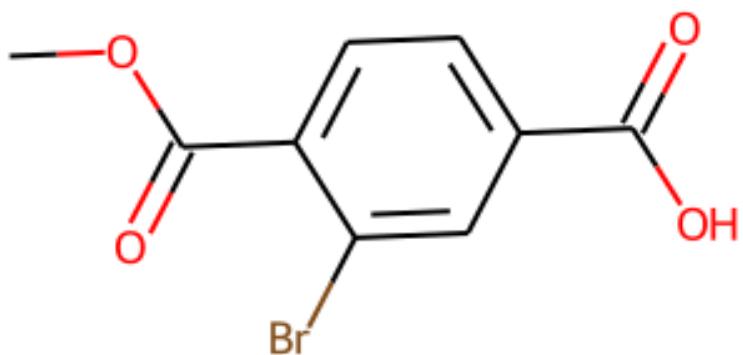
prob: 0.8



No.108

SMILES: COC(=O)c1ccc(C(=O)O)cc1Br

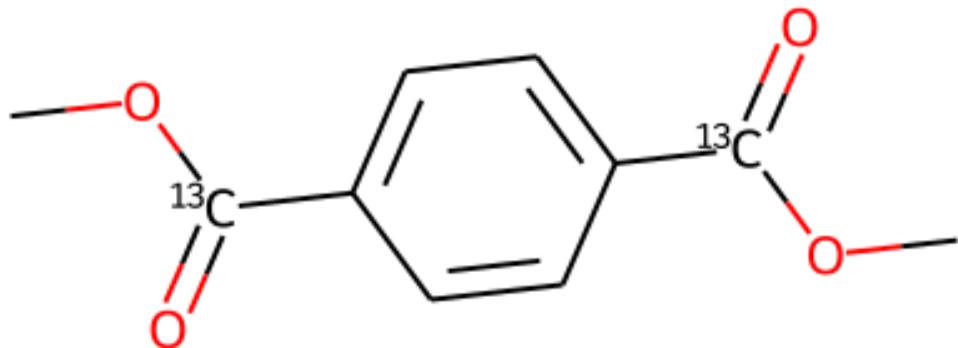
prob: 0.79



No.109

SMILES: CO[13C](=O)c1ccc([13C](=O)OC)cc1

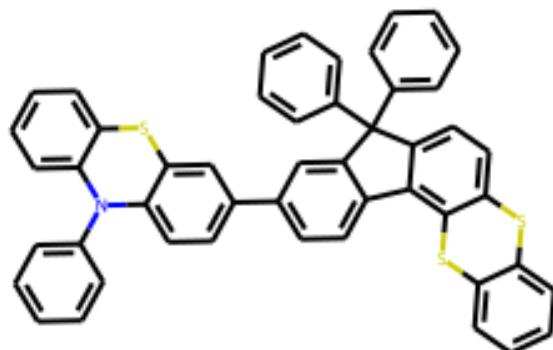
prob: 0.79



No.110

SMILES: c1ccc(N2c3cccc3Sc3cc(-c4ccc5c(c4)C(c4cccc4)(c4cccc4)c4ccc6c(c4-5)Sc4cccc4S6)ccc32)cc1

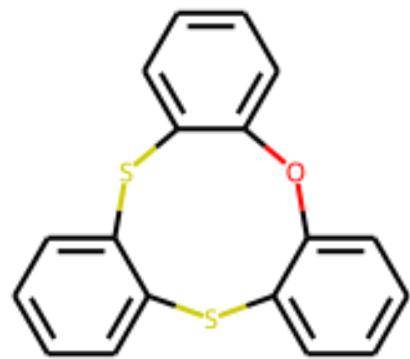
prob: 0.79



No.111

SMILES: c1ccc2c(c1)Oc1ccccc1Sc1ccccc1S2

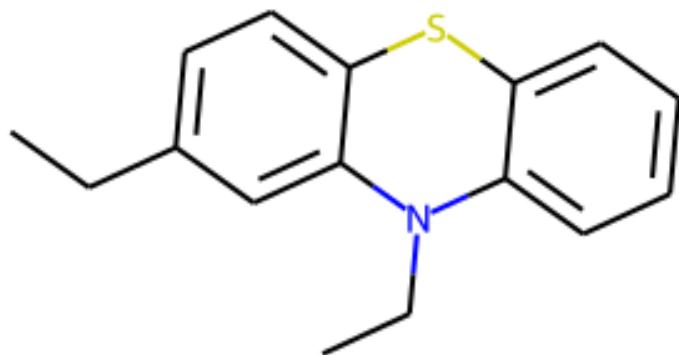
prob: 0.79



No.112

SMILES: CCc1ccc2c(c1)N(CC)c1ccccc1S2

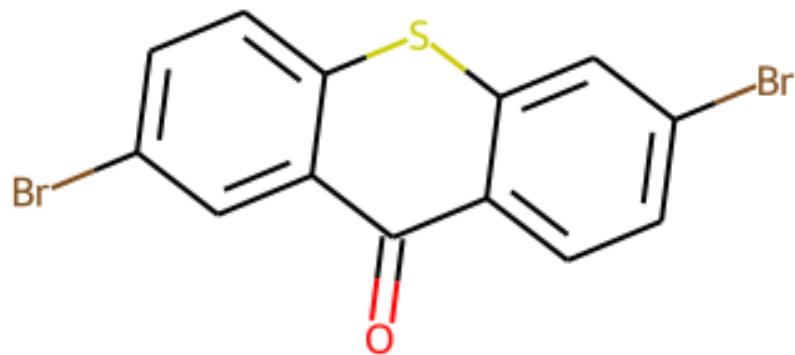
prob: 0.79



No.113

SMILES: O=c1c2ccc(Br)cc2sc2ccc(Br)cc12

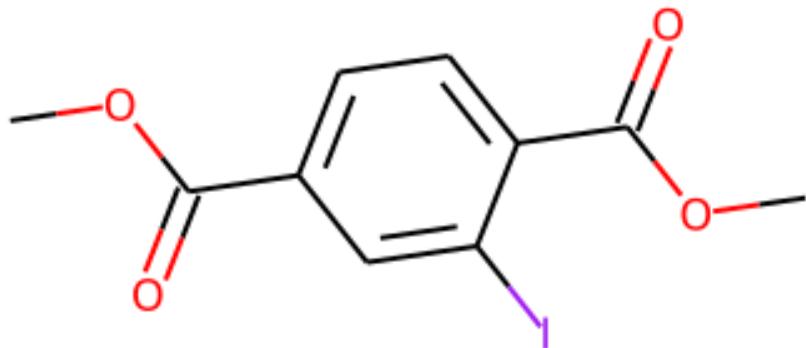
prob: 0.79



No.114

SMILES: COC(=O)c1ccc(C(=O)OC)c(I)c1

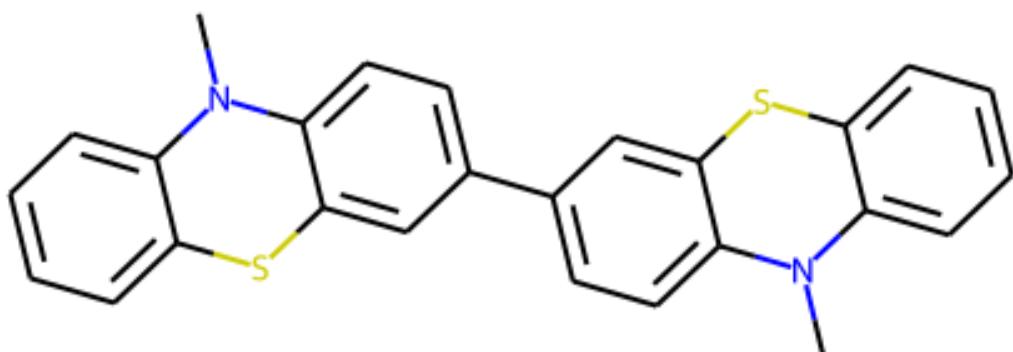
prob: 0.79



No.115

SMILES: CN1c2cccc2Sc2cc(-c3ccc4c(c3)Sc3cccc3N4C)ccc21

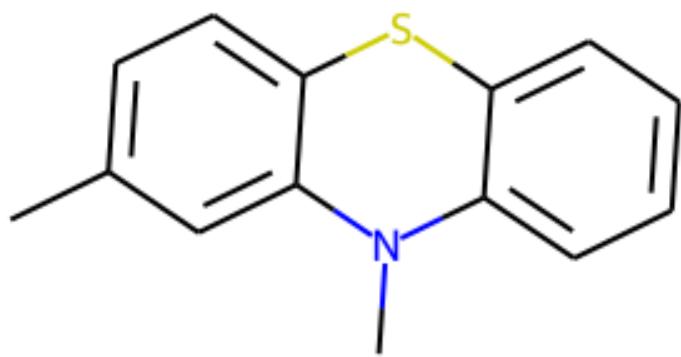
prob: 0.79



No.116

SMILES: Cc1ccc2c(c1)N(C)c1ccccc1S2

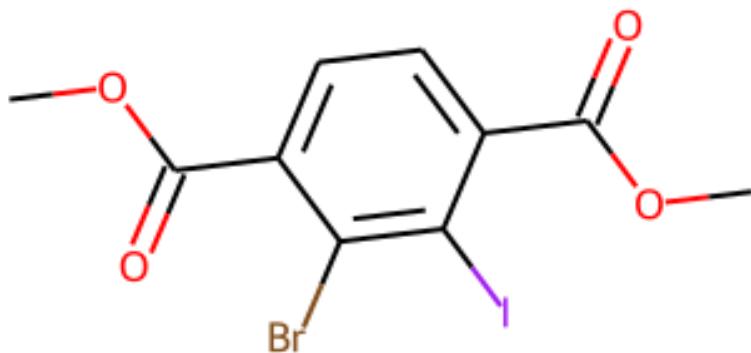
prob: 0.79



No.117

SMILES: COC(=O)c1ccc(C(=O)OC)c(I)c1Br

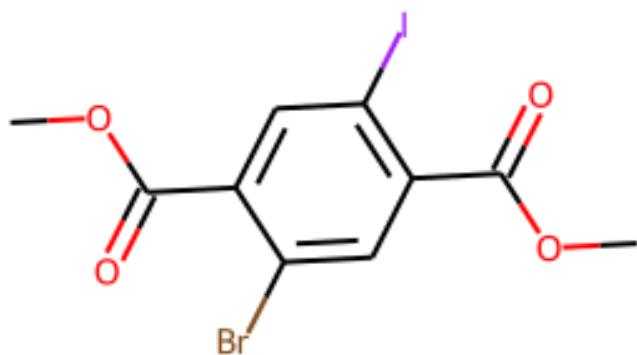
prob: 0.79



No.118

SMILES: COC(=O)c1cc(I)c(C(=O)OC)cc1Br

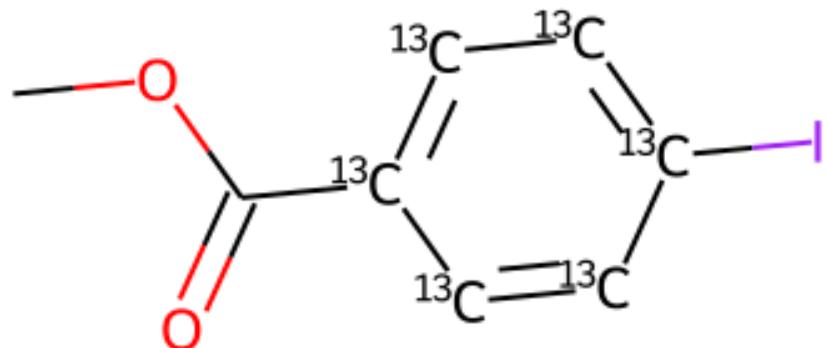
prob: 0.79



No.119

SMILES: COC(=O) [13c]1[13cH] [13cH] [13c] (I) [13cH] [13cH] 1

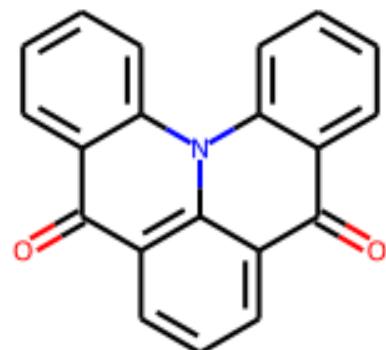
prob: 0.79



No.120

SMILES: O=c1c2ccccc2n2c3ccccc3c(=O)c3cccc1c32

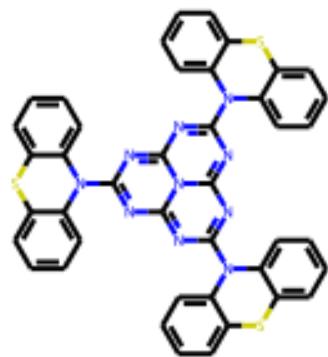
prob: 0.79



No.121

SMILES: c1ccc2c(c1)Sc1ccccc1N2C1=NC2=NC(N3c4ccccc4Sc4ccccc43)=NC3=NC(N4c5ccccc5S
c5ccccc54)=NC(=N1)N23

prob: 0.79



No.122

SMILES:

c1ccc2c(c1)Sc1ccccc1N2c1cc(N2c3ccccc3Sc3ccccc32)cc(N2c3ccccc3Sc3ccccc32)c1

prob: 0.79

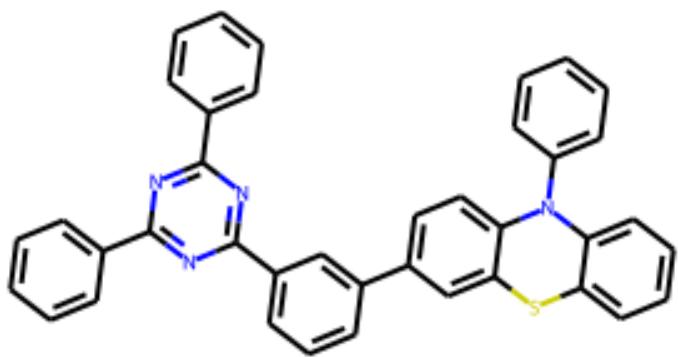


No.123

SMILES:

c1ccc(-c2nc(-c3ccccc3)nc(-c3cccc(-c4ccc5c(c4)Sc4ccccc4N5c4ccccc4)c3)n2)cc1

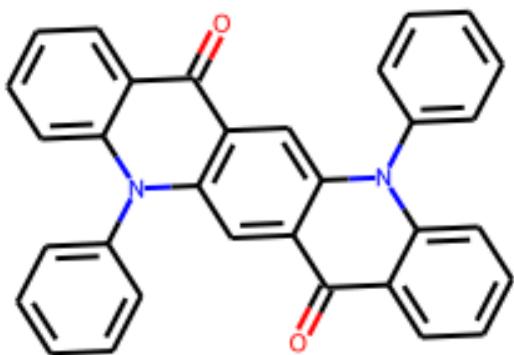
prob: 0.79



No.124

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2cc3c(=O)c4ccccc4n(-c4ccccc4)c3cc12

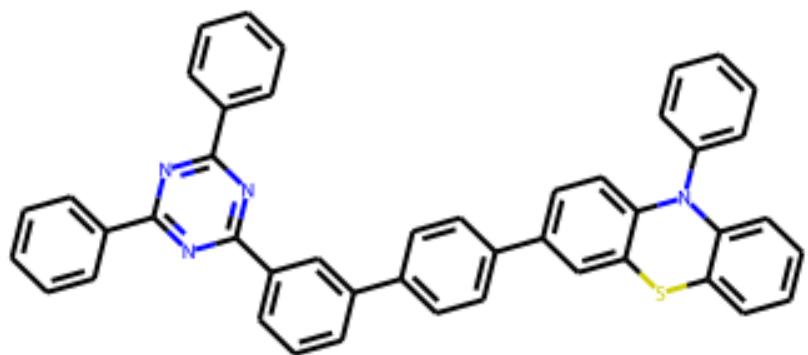
prob: 0.79



No.125

SMILES: c1ccc(-c2nc(-c3ccccc3)nc(-c3cccc(-c4ccc(-c5ccc6c(c5)Sc5ccccc5N6c5ccccc5)cc4)c3)n2)cc1

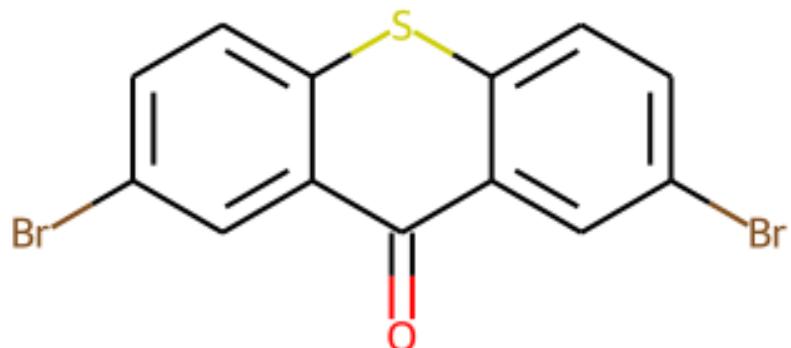
prob: 0.79



No.126

SMILES: O=c1c2cc(Br)ccc2sc2ccc(Br)cc12

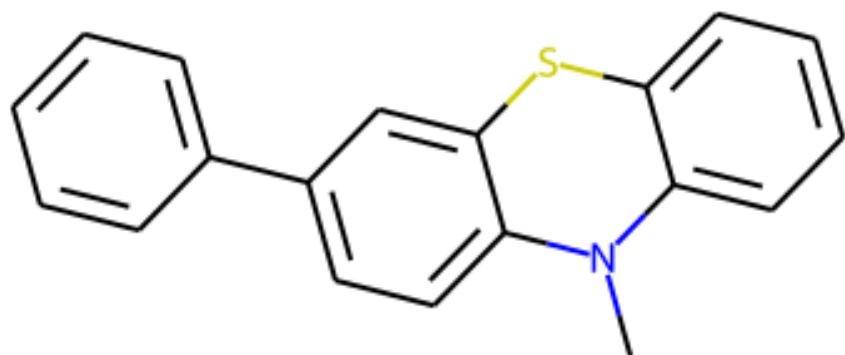
prob: 0.79



No.127

SMILES: CN1c2cccc2Sc2cc(-c3ccccc3)ccc21

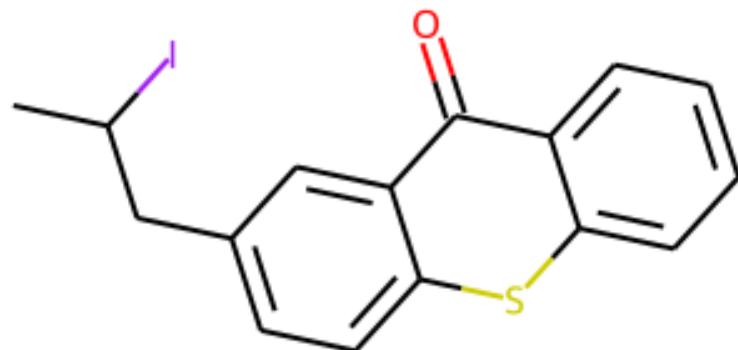
prob: 0.79



No.128

SMILES: CC(I)Cc1ccc2sc3ccccc3c(=O)c2c1

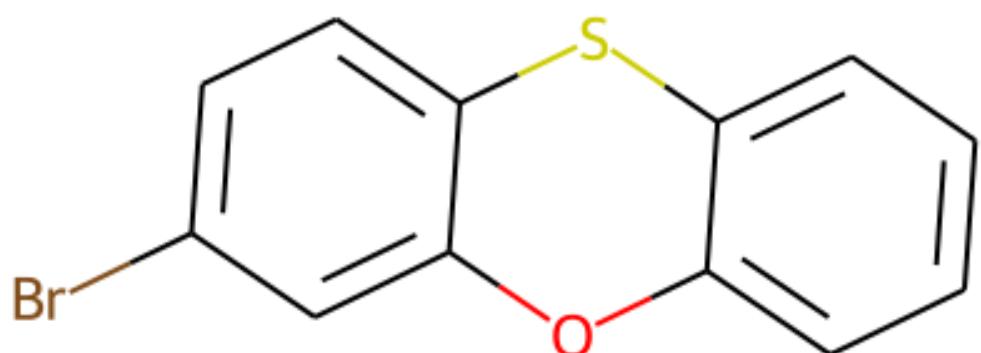
prob: 0.79



No.129

SMILES: Brc1ccc2c(c1)Oc1ccccc1S2

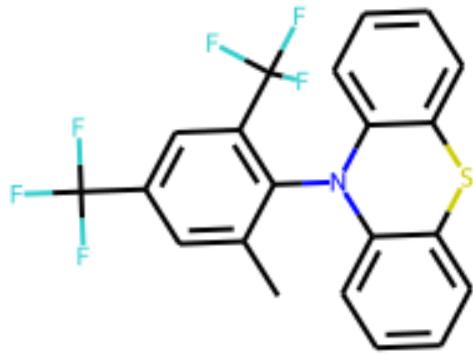
prob: 0.79



No.130

SMILES: Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1N1c2ccccc2Sc2ccccc21

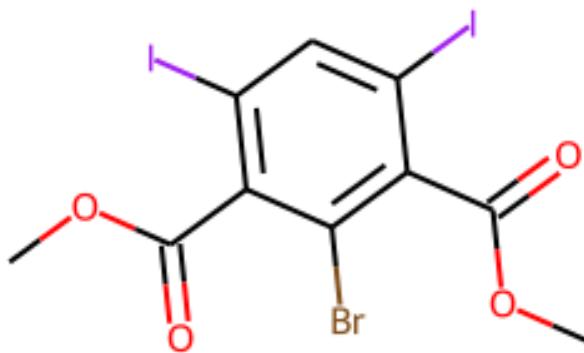
prob: 0.79



No.131

SMILES: COC(=O)c1c(I)cc(I)c(C(=O)OC)c1Br

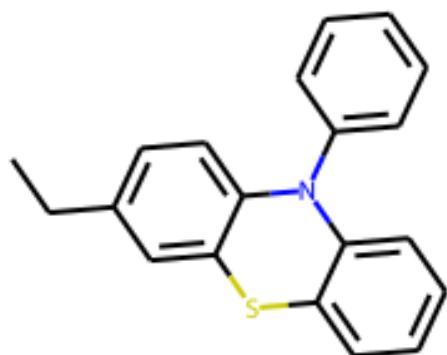
prob: 0.79



No.132

SMILES: CCc1ccc2c(c1)Sc1ccccc1N2c1ccccc1

prob: 0.79



No.133

SMILES: Cc1ccc2c(c1)Sc1ccccc1N2C

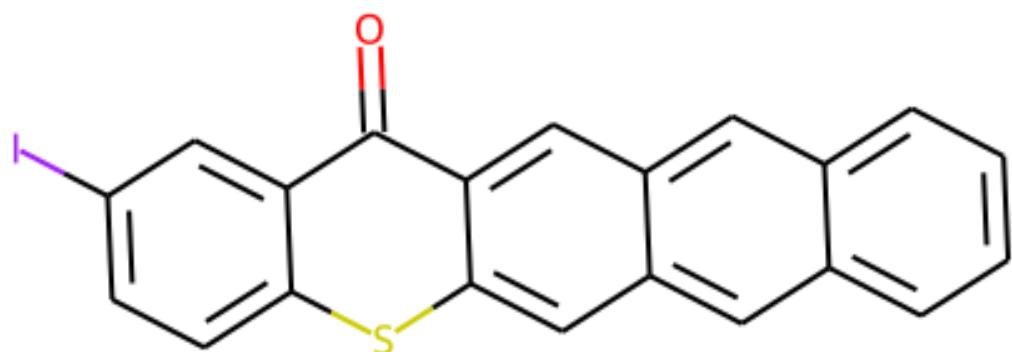
prob: 0.79



No.134

SMILES: O=c1c2cc(I)ccc2sc2cc3cc4cccc4cc3cc12

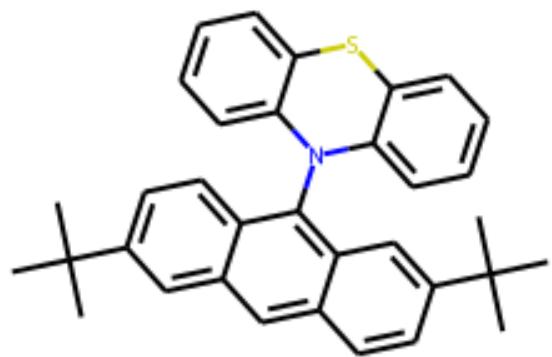
prob: 0.79



No.135

SMILES: CC(C)(C)c1ccc2c(N3c4cccc4Sc4cccc43)c3cc(C(C)(C)C)ccc3cc2c1

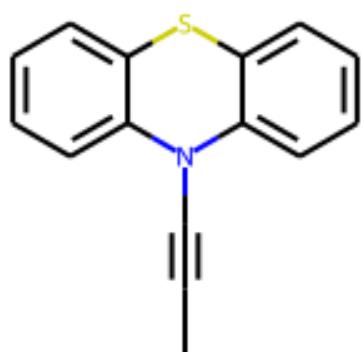
prob: 0.79



No.136

SMILES: CC#CN1c2ccccc2Sc2ccccc21

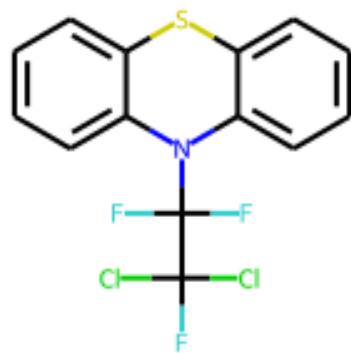
prob: 0.79



No.137

SMILES: FC(C1)(C1)C(F)(F)N1c2ccccc2Sc2ccccc21

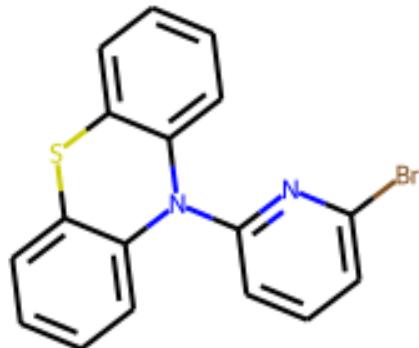
prob: 0.79



No.138

SMILES: Brc1ccccc(N2c3ccccc3Sc3ccccc32)n1

prob: 0.79

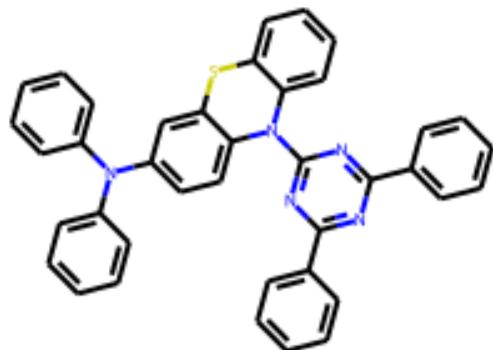


No.139

SMILES:

c1ccc(-c2nc(-c3ccccc3)nc(N3c4cccc4Sc4cc(N(c5cccc5)c5cccc5)ccc43)n2)cc1

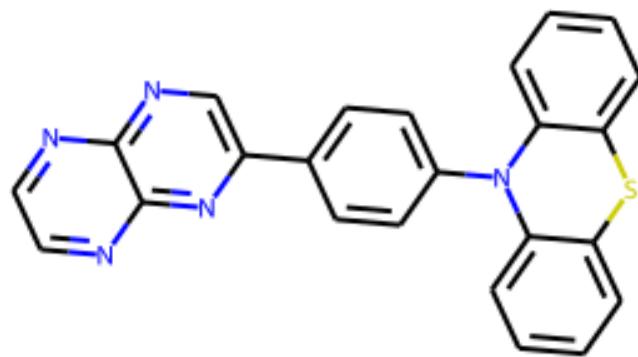
prob: 0.79



No.140

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2cnc3nccnc3n2)cc1

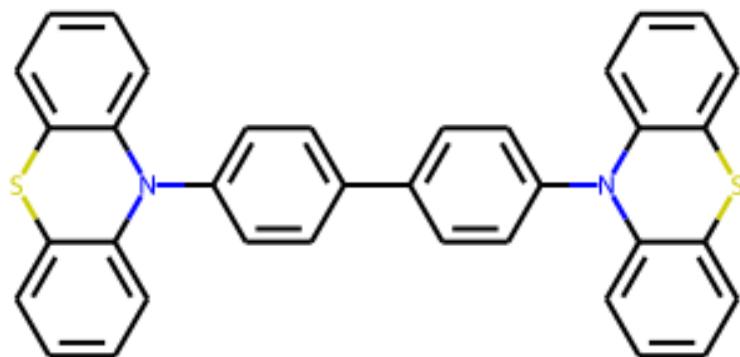
prob: 0.78



No.141

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2ccc(N3c4ccccc4Sc4ccccc43)cc2)cc1

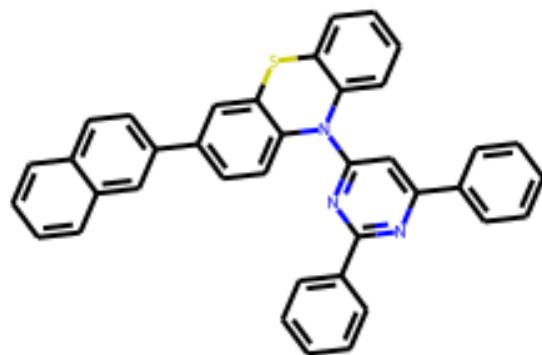
prob: 0.78



No.142

SMILES: c1ccc(-c2cc(N3c4ccccc4Sc4cc(-c5ccc6ccccc6c5)ccc43)nc(-c3ccccc3)n2)cc1

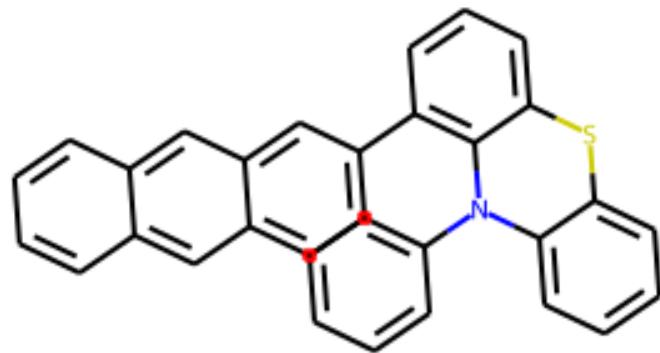
prob: 0.78



No.143

SMILES: c1ccc(N2c3cccc3Sc3cccc(-c4ccc5cc6cccc6cc5c4)c32)cc1

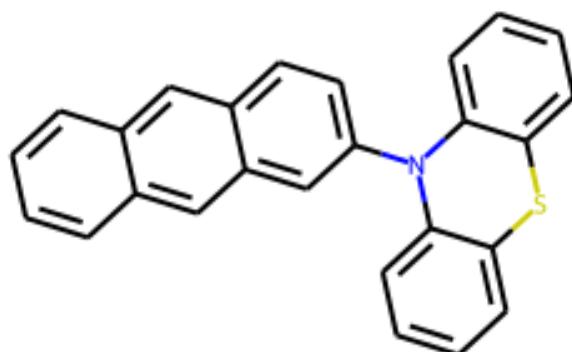
prob: 0.78



No.144

SMILES: c1ccc2c(c1)Sc1cccc1N2c1ccc2cc3cccc3cc2c1

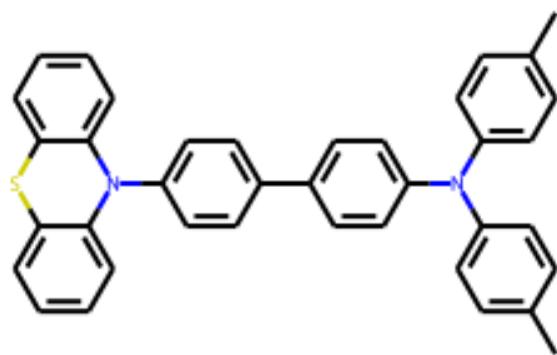
prob: 0.78



No.145

SMILES: Cc1ccc(N(c2ccc(C)cc2)c2ccc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)cc2)cc1

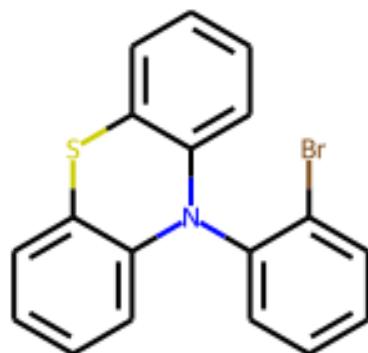
prob: 0.78



No.146

SMILES: Brcccc1N1c2ccccc2Sc2ccccc21

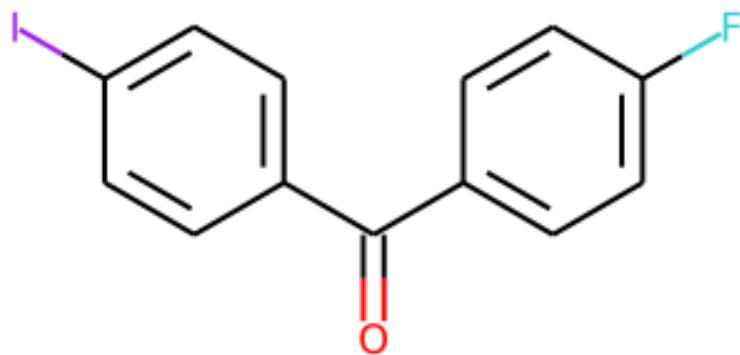
prob: 0.78



No.147

SMILES: O=C(c1ccc(F)cc1)c1ccc(I)cc1

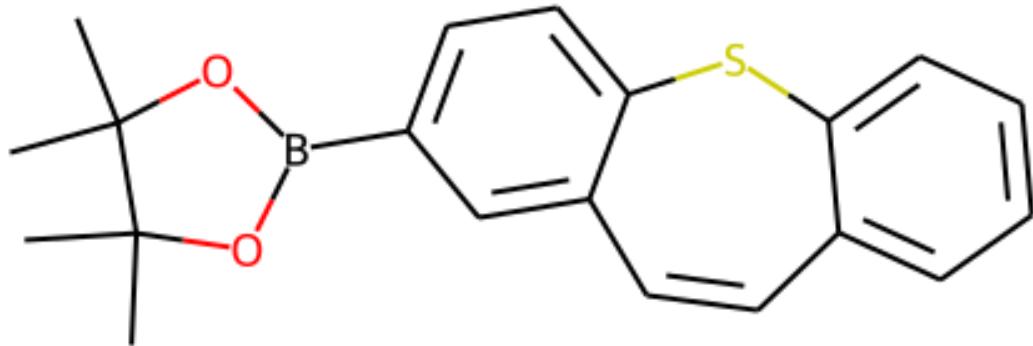
prob: 0.78



No.148

SMILES: CC1(C)OB(c2ccc3c(c2)C=Cc2ccccc2S3)OC1(C)C

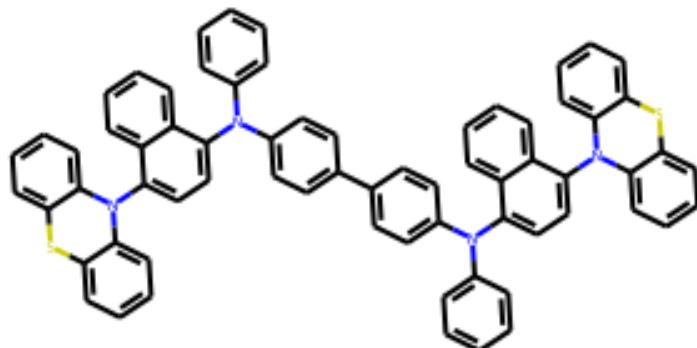
prob: 0.78



No.149

SMILES: c1ccc(N(c2ccc(-c3ccc(N(c4cccc4)c4ccc(N5c6ccccc6Sc6ccccc65)c5ccccc45)cc3)cc2)c2ccc(N3c4cccc4Sc4cccc43)c3ccccc23)cc1

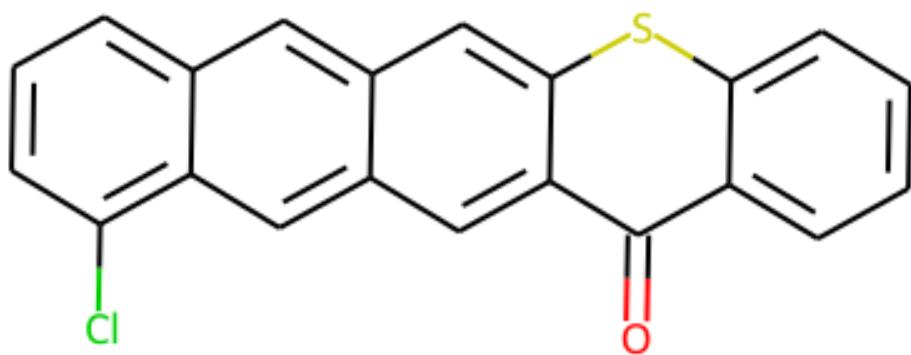
prob: 0.78



No.150

SMILES: O=c1c2ccccc2sc2cc3cc4cccc(Cl)c4cc3cc12

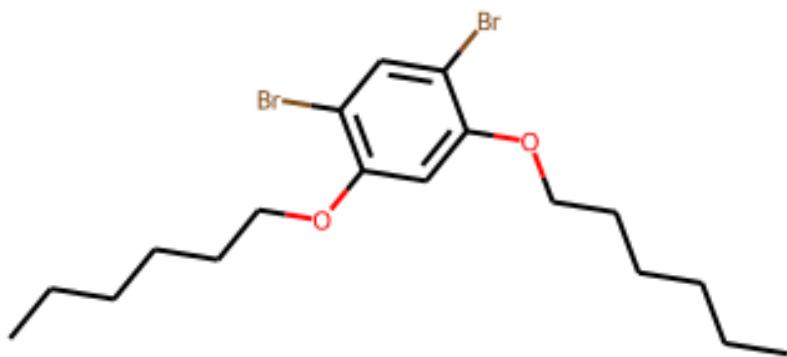
prob: 0.78



No.151

SMILES: CCCCCCC0c1cc(OCCCCCC)c(Br)cc1Br

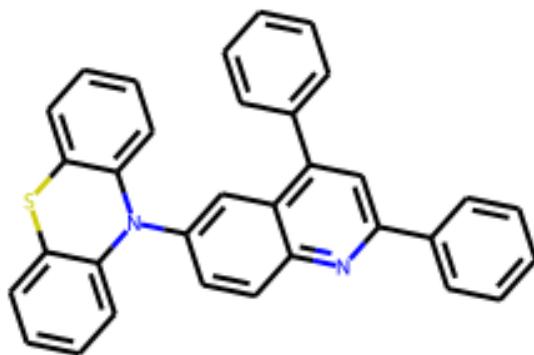
prob: 0.78



No.152

SMILES: c1ccc(-c2cc(-c3cccc3)c3cc(N4c5ccccc5Sc5ccccc54)ccc3n2)cc1

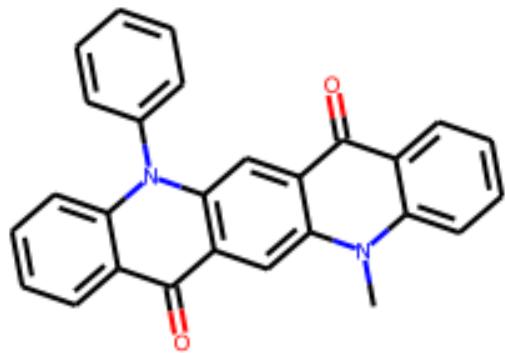
prob: 0.78



No.153

SMILES: Cn1c2ccccc2c(=O)c2cc3c(cc21)c(=O)c1ccccc1n3-c1ccccc1

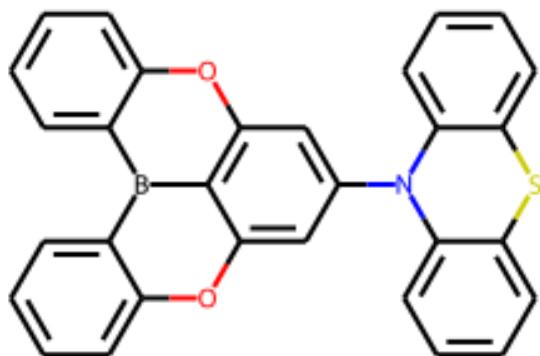
prob: 0.78



No.154

SMILES: c1ccc2c(c1)Oc1cc(N3c4ccccc4Sc4ccccc43)cc3c1B2c1ccccc103

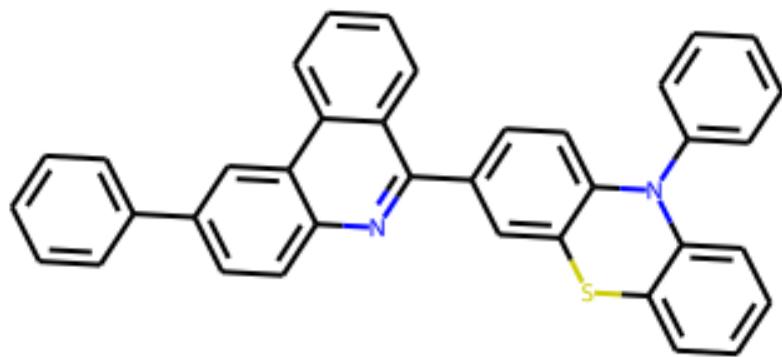
prob: 0.78



No.155

SMILES: c1ccc(-c2ccc3nc(-c4ccc5c(c4)Sc4ccccc4N5c4ccccc4)c4ccccc4c3c2)cc1

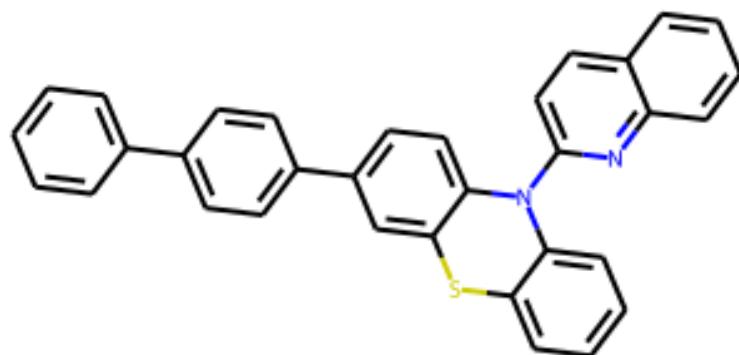
prob: 0.78



No.156

SMILES: c1ccc(-c2ccc(-c3ccc4c(c3)Sc3cccc3N4c3ccc4ccccc4n3)cc2)cc1

prob: 0.78

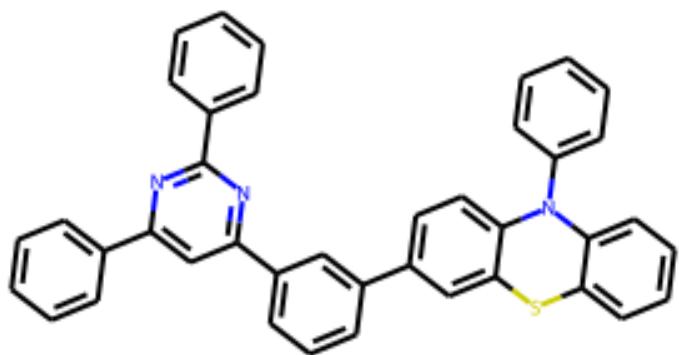


No.157

SMILES:

c1ccc(-c2cc(-c3cccc(-c4ccc5c(c4)Sc4cccc4N5c4ccccc4)c3)nc(-c3cccc3)n2)cc1

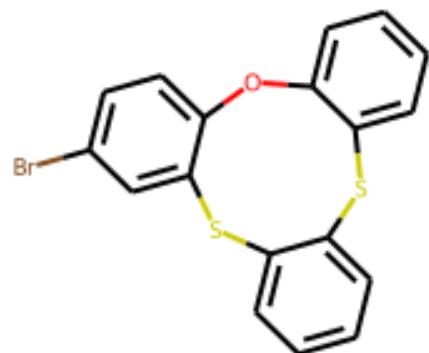
prob: 0.78



No.158

SMILES: Brcc1ccc2c(c1)Sc1ccccc1Sc1ccccc1O2

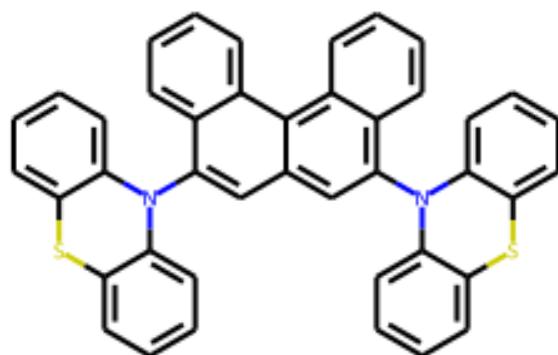
prob: 0.78



No.159

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cc2cc(N3c4ccccc4Sc4ccccc43)c3ccccc3c2c2ccccc12

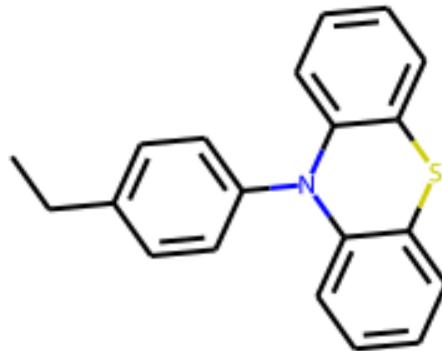
prob: 0.78



No.160

SMILES: CCc1ccc(N2c3cccc3Sc3cccc32)cc1

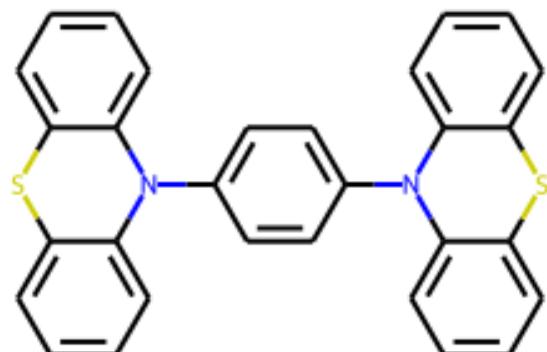
prob: 0.78



No.161

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(N2c3cccc3Sc3cccc32)cc1

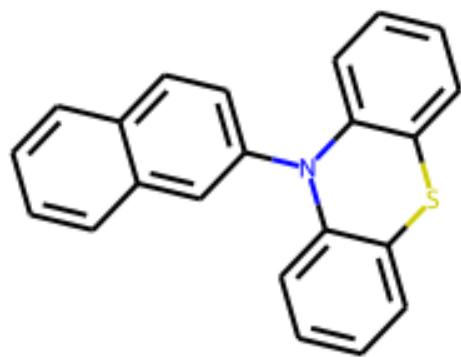
prob: 0.78



No.162

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2ccccc2c1

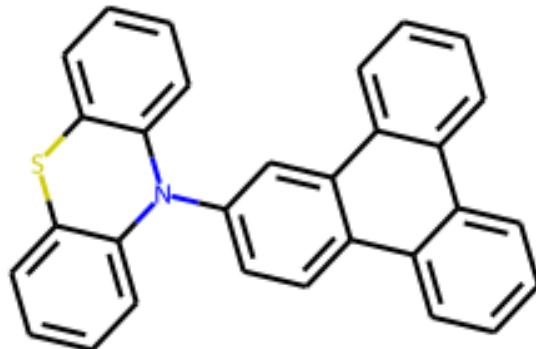
prob: 0.78



No. 163

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2c3ccccc3c3ccccc3c2c1

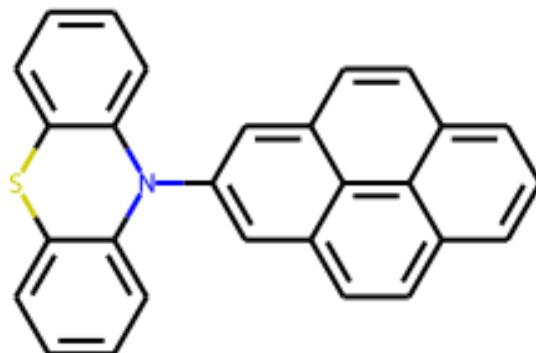
prob: 0.78



No. 164

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cc2ccc3cccc4ccc(c1)c2c34

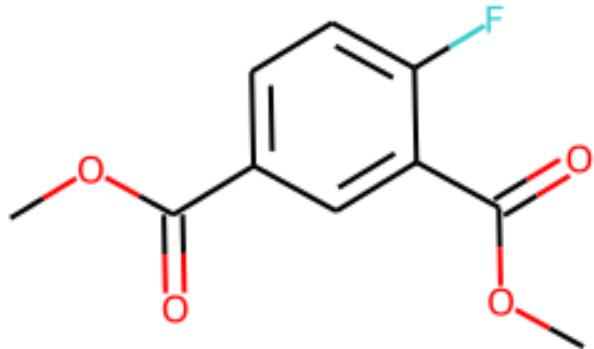
prob: 0.78



No.165

SMILES: COC(=O)c1ccc(F)c(C(=O)OC)c1

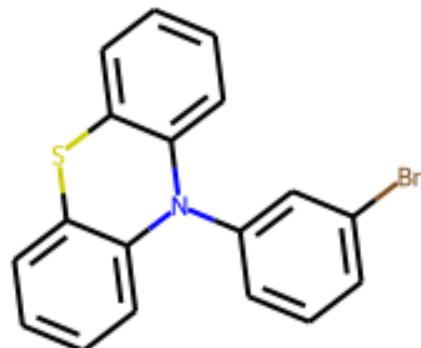
prob: 0.78



No.166

SMILES: Brc1ccccc(N2c3ccccc3Sc3ccccc32)c1

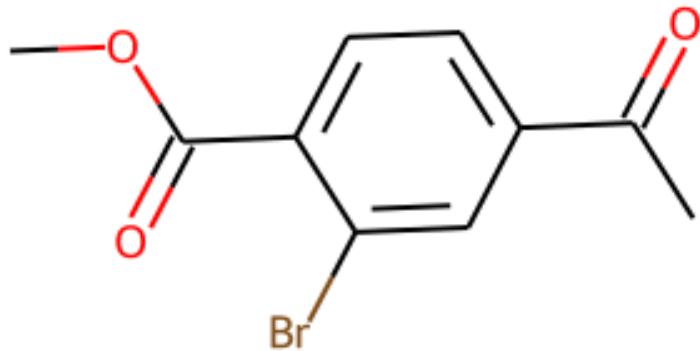
prob: 0.78



No.167

SMILES: COC(=O)c1ccc(C(C)=O)cc1Br

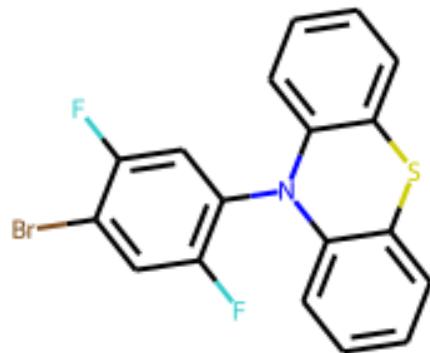
prob: 0.78



No.168

SMILES: Fc1cc(N2c3ccccc3Sc3ccccc32)c(F)cc1Br

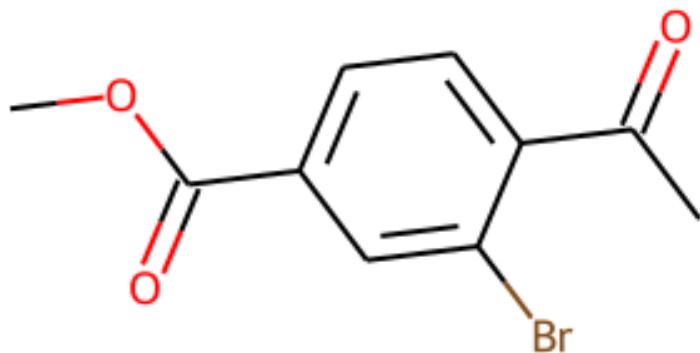
prob: 0.78



No.169

SMILES: COC(=O)c1ccc(C(C)=O)c(Br)c1

prob: 0.78

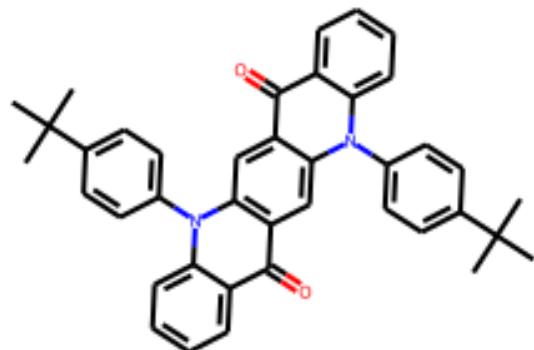


No.170

SMILES:

CC(C)(C)c1ccc(-n2c3cccc3c(=O)c3cc4c(cc32)c(=O)c2ccccc2n4-c2ccc(C(C)(C)C)cc2)cc1

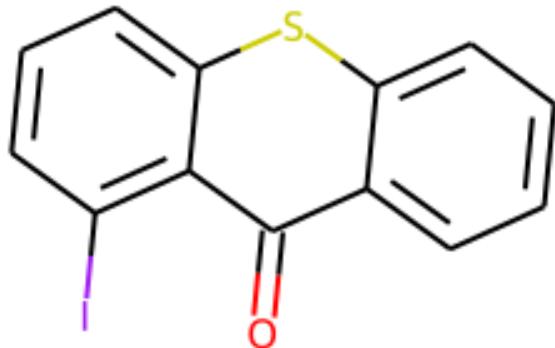
prob: 0.78



No.171

SMILES: O=c1c2ccccc2sc2cccc(I)c12

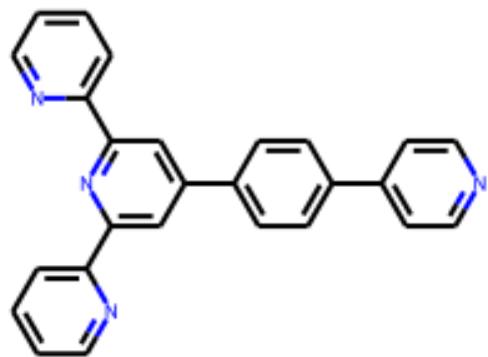
prob: 0.78



No.172

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccncc4)cc3)cc(-c3cccn3)n2)nc1

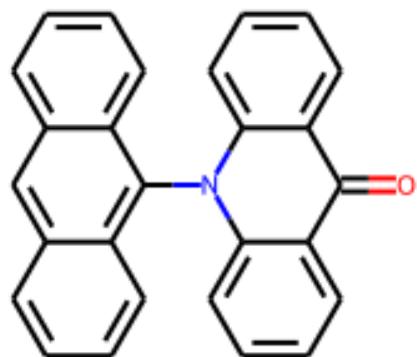
prob: 0.78



No.173

SMILES: O=c1c2ccccc2n(-c2c3ccccc3cc3ccccc23)c2ccccc12

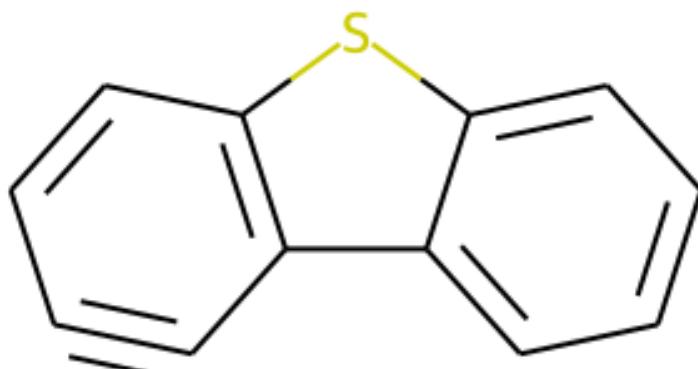
prob: 0.78



No.174

SMILES: c1ccc2sc3ccccc3c2c#1

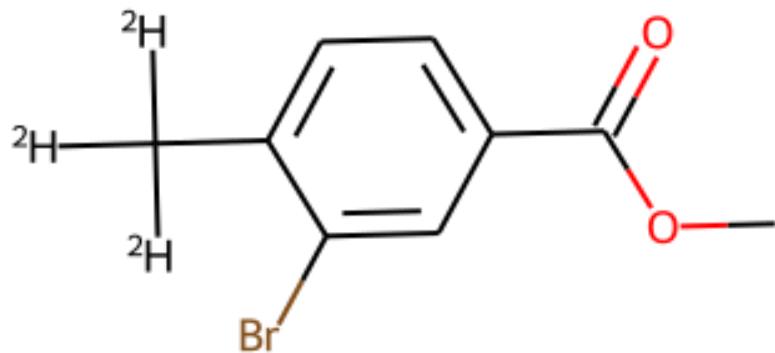
prob: 0.78



No.175

SMILES: [2H]C([2H])([2H])c1ccc(C(=O)OC)cc1Br

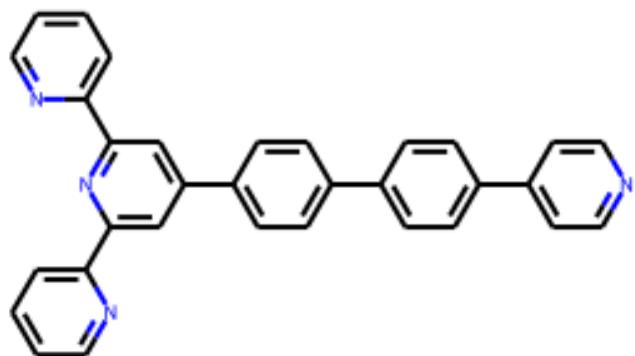
prob: 0.78



No.176

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccc(-c5ccncc5)cc4)cc3)cc(-c3cccn3)n2)nc1

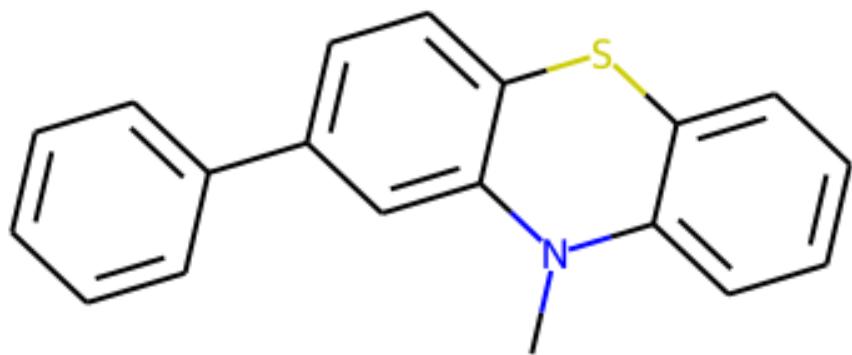
prob: 0.78



No.177

SMILES: CN1c2cccc2Sc2ccc(-c3ccccc3)cc21

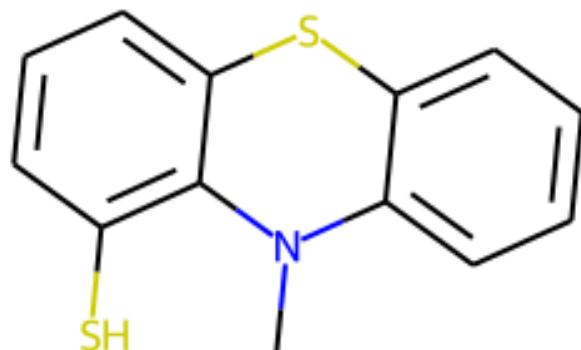
prob: 0.78



No.178

SMILES: CN1c2ccccc2Sc2cccc(S)c21

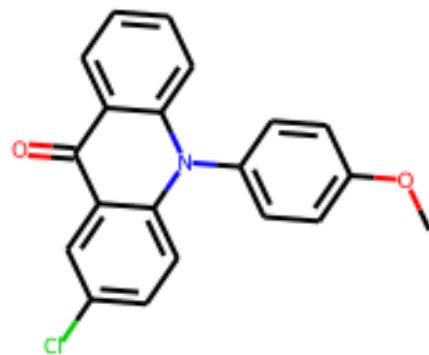
prob: 0.78



No.179

SMILES: C0c1ccc(-n2c3ccccc3c(=O)c3cc(Cl)ccc32)cc1

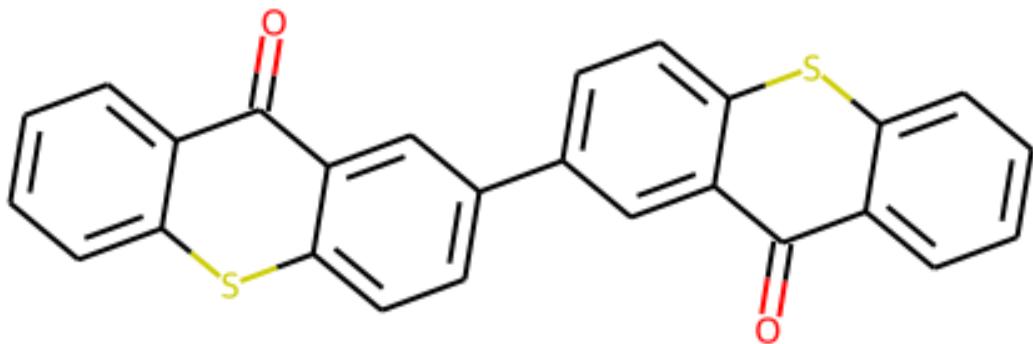
prob: 0.78



No.180

SMILES: O=c1c2ccccc2sc2ccc(-c3ccc4sc5ccccc5c(=O)c4c3)cc12

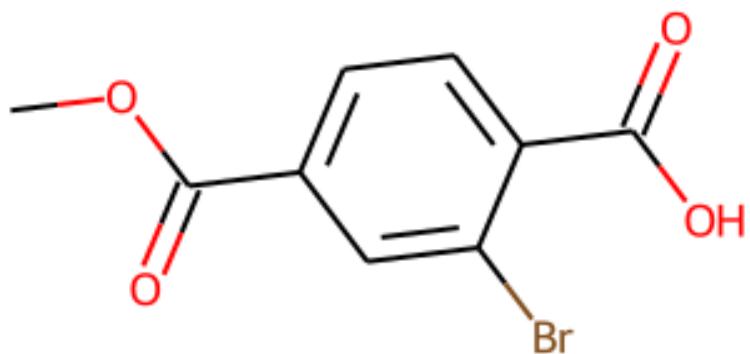
prob: 0.78



No.181

SMILES: COC(=O)c1ccc(C(=O)O)c(Br)c1

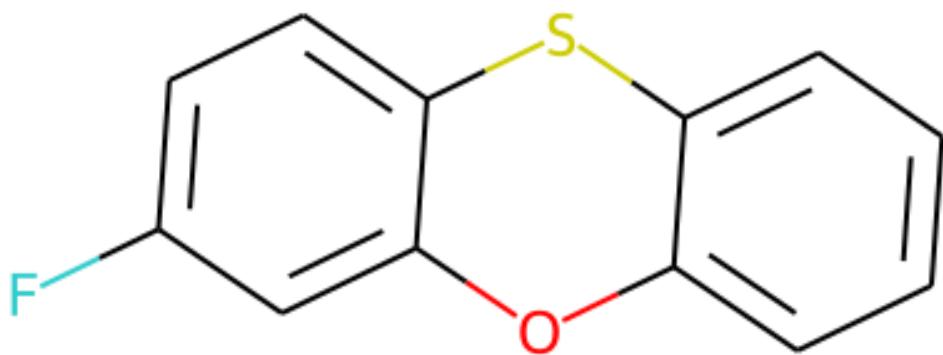
prob: 0.78



No.182

SMILES: Fc1ccc2c(c1)Oc1ccccc1S2

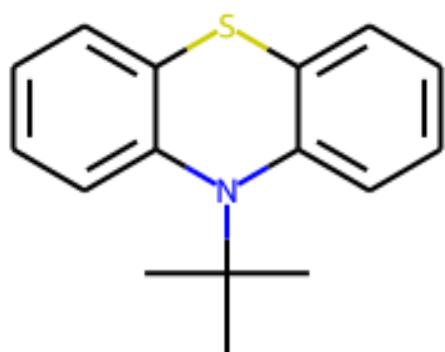
prob: 0.77



No.183

SMILES: CC(C)(C)N1c2ccccc2Sc2ccccc21

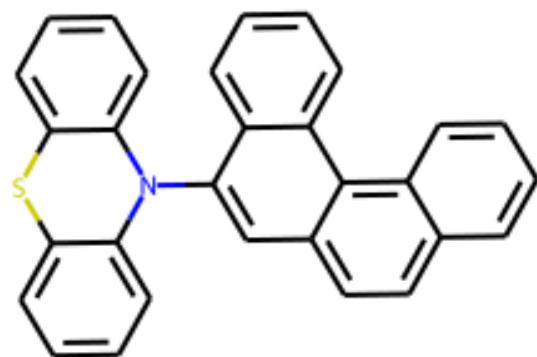
prob: 0.77



No.184

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cc2ccc3ccccc3c2c2ccccc12

prob: 0.77

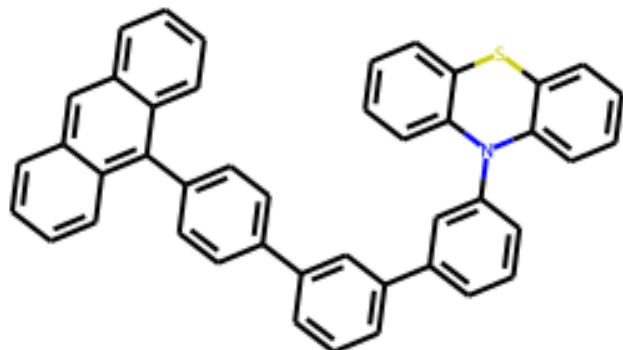


No.185

SMILES:

c1cc(-c2ccc(-c3c4cccc4cc4cccc34)cc2)cc(-c2cccc(N3c4cccc4Sc4cccc43)c2)c1

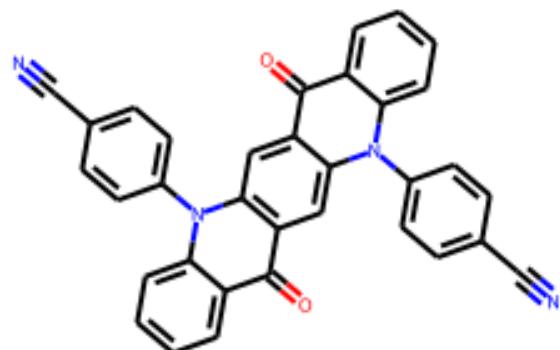
prob: 0.77



No.186

SMILES: N#Cc1ccc(-n2c3cccc3c(=O)c3cc4c(cc32)c(=O)c2cccc2n4-c2ccc(C#N)cc2)cc1

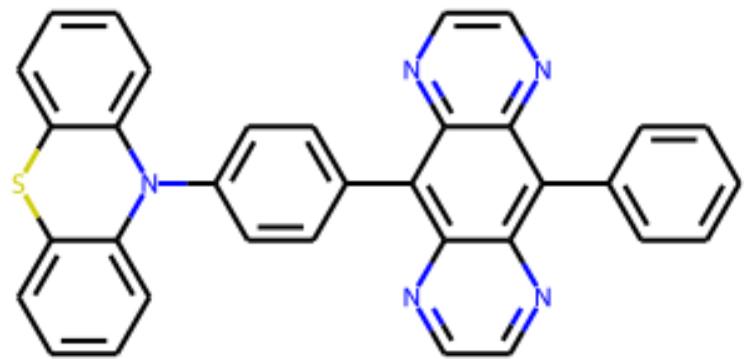
prob: 0.77



No.187

SMILES: c1ccc(-c2c3nccnc3c(-c3ccc(N4c5cccc5Sc5cccc54)cc3)c3nccnc23)cc1

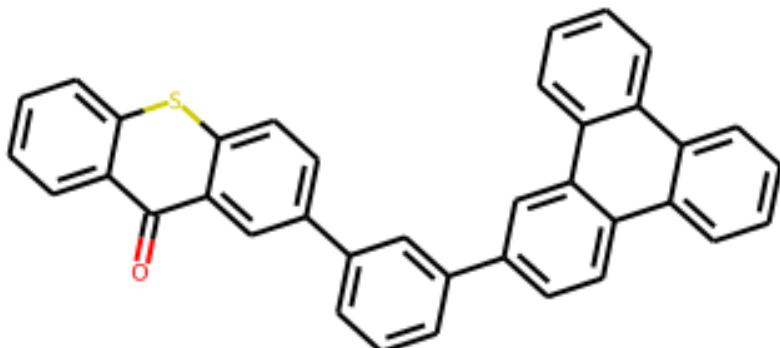
prob: 0.77



No.188

SMILES: O=c1c2ccccc2sc2ccc(-c3cccc(-c4ccc5c6ccccc6c6ccccc6c5c4)c3)cc12

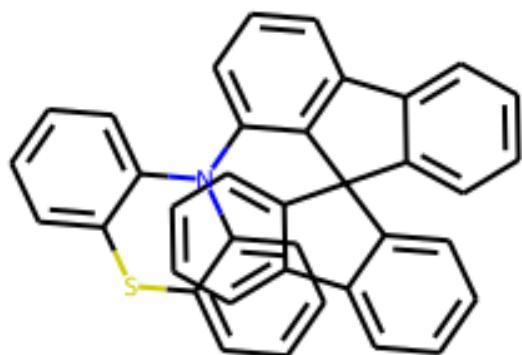
prob: 0.77



No.189

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cccc2c1C1(c3ccccc3-c3ccccc31)c1ccccc1-2

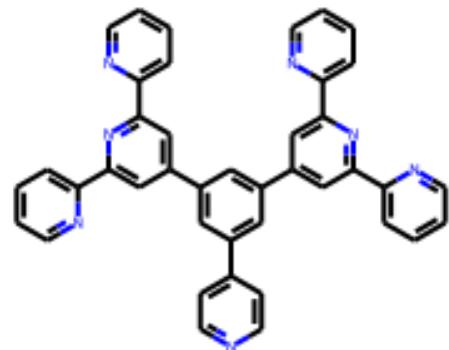
prob: 0.77



No.190

SMILES: c1ccc(-c2cc(-c3cc(-c4ccncc4)cc(-c4cc(-c5ccccn5)nc(-c5ccccn5)c4)c3)cc(-c3ccccn3)n2)nc1

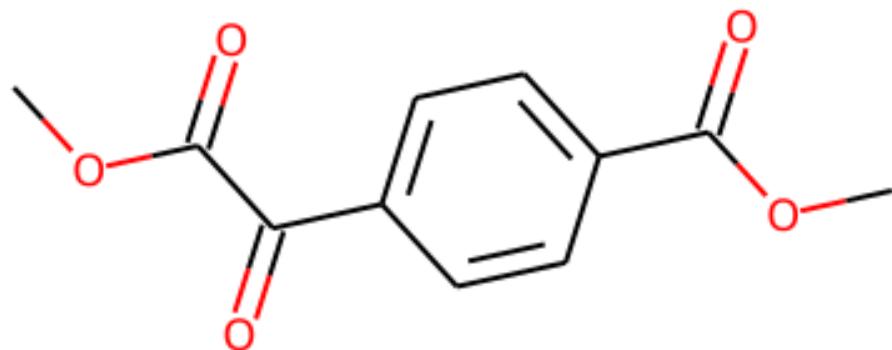
prob: 0.77



No.191

SMILES: COC(=O)C(=O)c1ccc(C(=O)OC)cc1

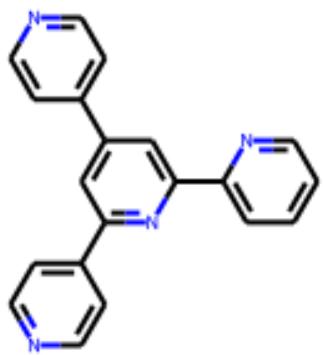
prob: 0.77



No.192

SMILES: c1ccc(-c2cc(-c3ccncc3)cc(-c3ccncc3)n2)nc1

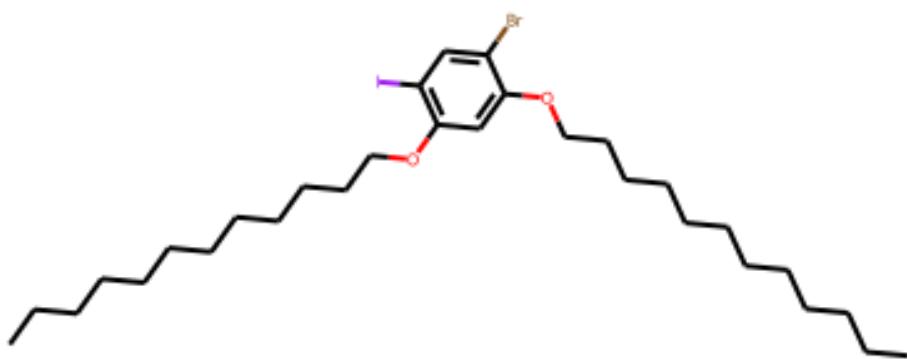
prob: 0.77



No.193

SMILES: CCCCCCCCCCCC0c1cc(OCCCCCC)cc(I)cc1Br

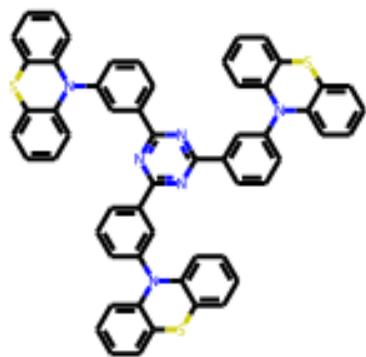
prob: 0.77



No.194

SMILES: c1cc(-c2nc(-c3cccc(N4c5ccccc5Sc5cccc54)c3)nc(-c3cccc(N4c5ccccc5Sc5cccc54)c3)n2)cc(N2c3cccc3Sc3cccc32)c1

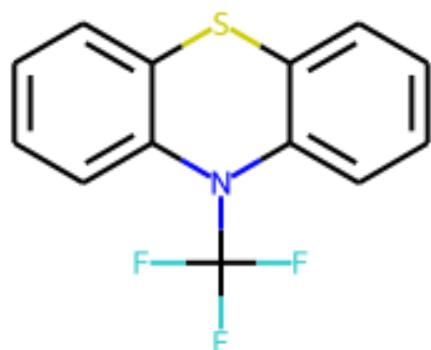
prob: 0.77



No.195

SMILES: FC(F)(F)N1c2ccccc2Sc2ccccc21

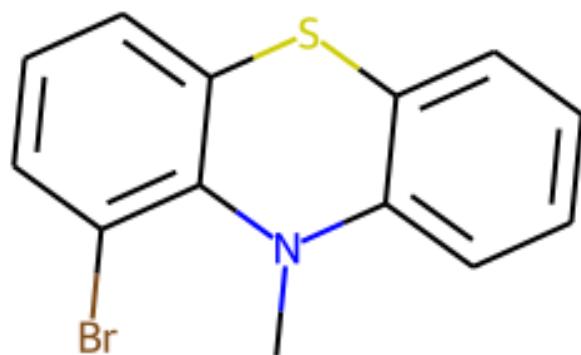
prob: 0.77



No.196

SMILES: CN1c2ccccc2Sc2cccc(Br)c21

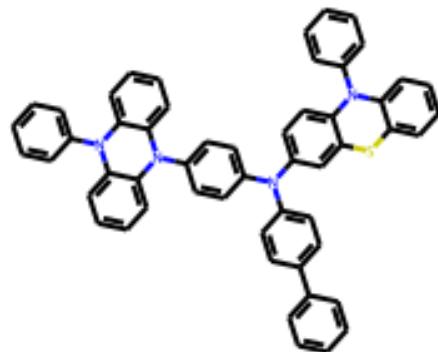
prob: 0.77



No.197

SMILES: c1ccc(-c2ccc(N(c3ccc(N4c5cccc5N(c5cccc5)c5cccc54)cc3)c3ccc4c(c3)Sc3ccc3N4c3cccc3)cc2)cc1

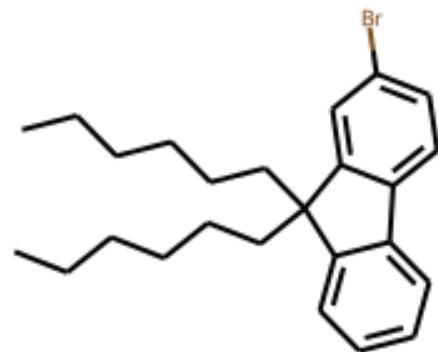
prob: 0.77



No.198

SMILES: CCCCCC1(CCCCC) c2cccc2-c2ccc(Br)cc21

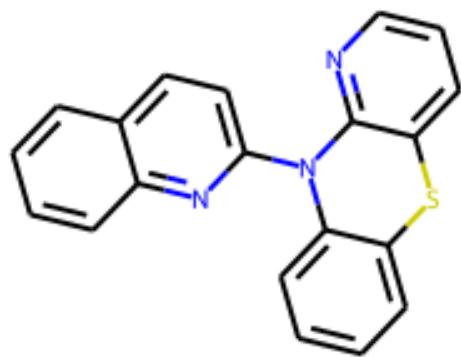
prob: 0.77



No.199

SMILES: c1ccc2c(c1)Sc1ccnc1N2c1ccc2cccc2n1

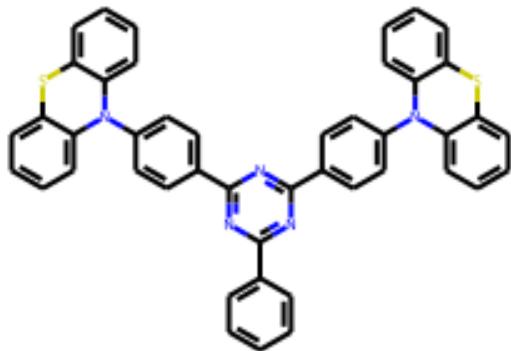
prob: 0.77



No.200

SMILES: c1ccc(-c2nc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)nc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)n2)cc1

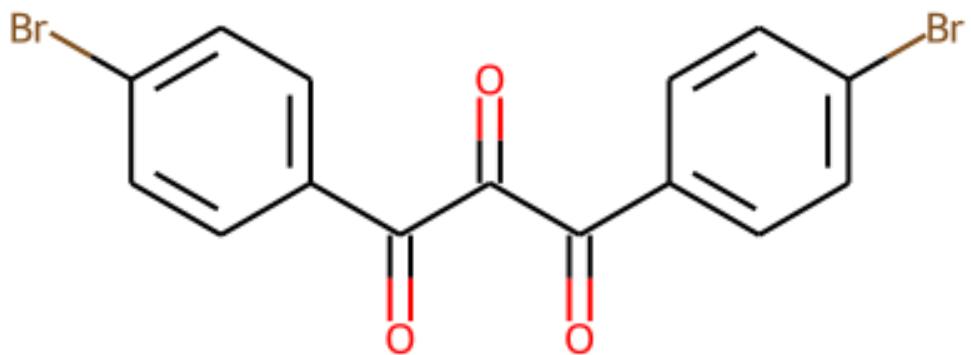
prob: 0.77



No.201

SMILES: O=C(C(=O)c1ccc(Br)cc1)C(=O)c1ccc(Br)cc1

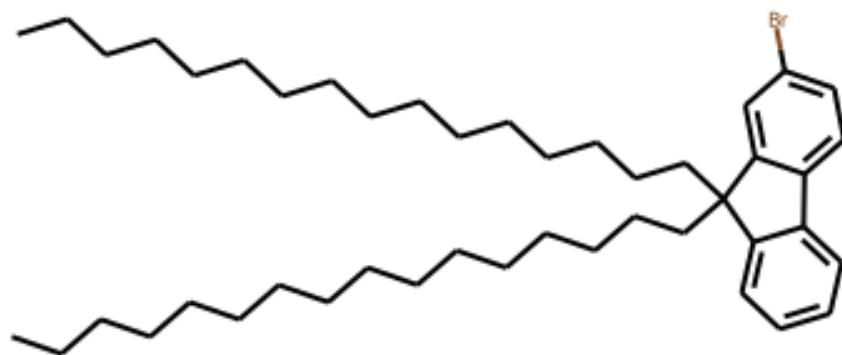
prob: 0.77



No. 202

SMILES: CCCCCCCCCCCCCCCC1(CCCCCCCCCCCCC) c2ccccc2-c2ccc(Br)cc21

prob: 0.77

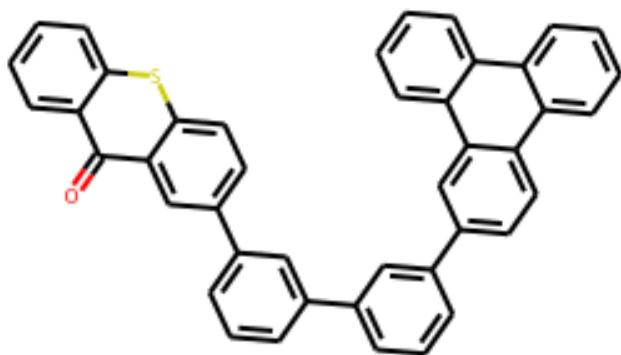


No. 203

SMILES:

0=c1c2ccccc2sc2ccc(-c3cccc(-c4cccc(-c5ccc6c7cccc7c7cccc7c6c5)c4)c3)cc12

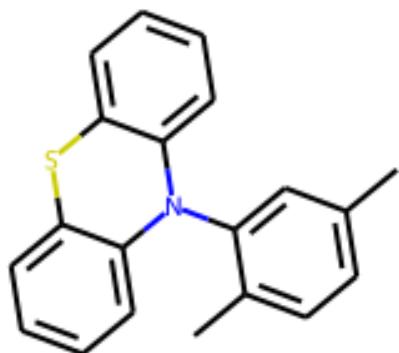
prob: 0.77



No.204

SMILES: Cc1ccc(C)c(N2c3cccc3Sc3cccc32)c1

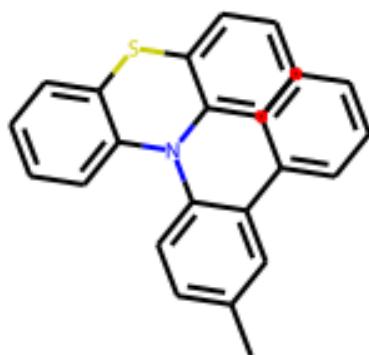
prob: 0.77



No.205

SMILES: Cc1ccc(N2c3cccc3Sc3cccc32)c(-c2cccc2)c1

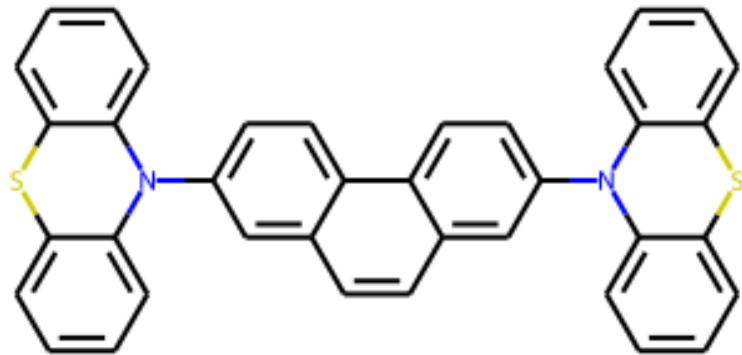
prob: 0.77



No.206

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2c(ccc3cc(N4c5ccccc5Sc5ccccc54)ccc32)c1

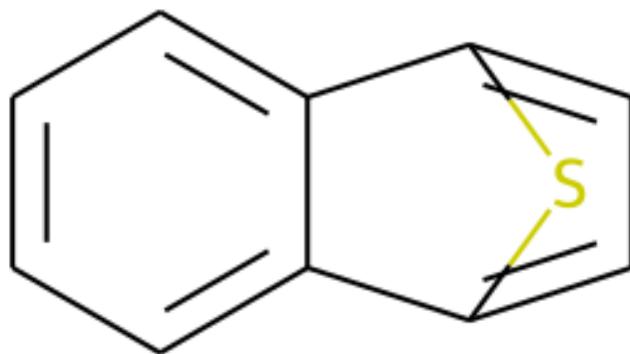
prob: 0.77



No.207

SMILES: c1ccc2c3ccc(s3)c2c1

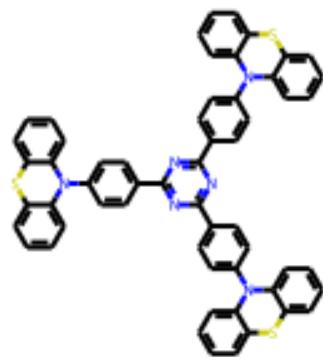
prob: 0.77



No.208

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2nc(-c3ccc(N4c5ccccc5Sc5ccccc54)cc3)nc(-c3ccc(N4c5ccccc5Sc5ccccc54)cc3)n2)cc1

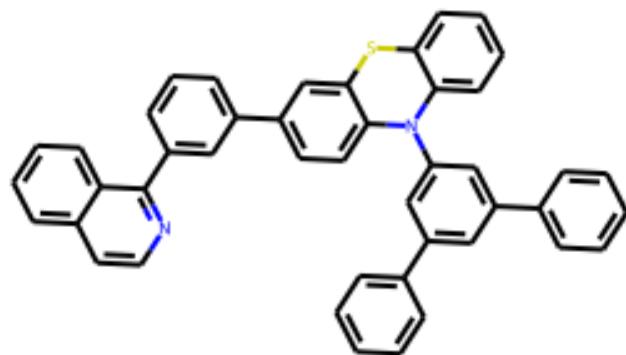
prob: 0.77



No.209

SMILES:

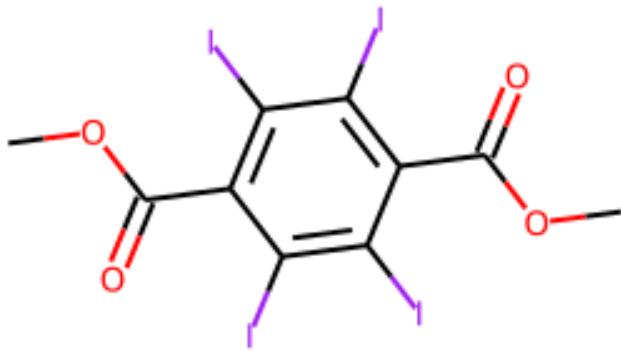
c1ccc(-c2cc(-c3cccc3)cc(N3c4ccccc4Sc4cc(-c5cccc(-c6nccc7ccccc67)c5)ccc43)c2)cc1
prob: 0.77



No.210

SMILES: COC(=O)c1c(I)c(I)c(C(=O)OC)c(I)c1I

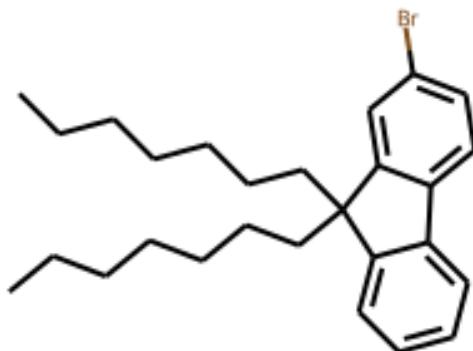
prob: 0.77



No. 211

SMILES: CCCCCCCC1(CCCCCC)c2ccccc2-c2ccc(Br)cc21

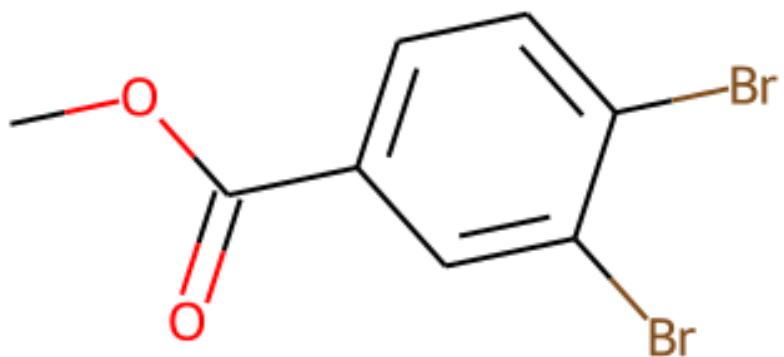
prob: 0.77



No. 212

SMILES: COC(=O)c1ccc(Br)c(Br)c1

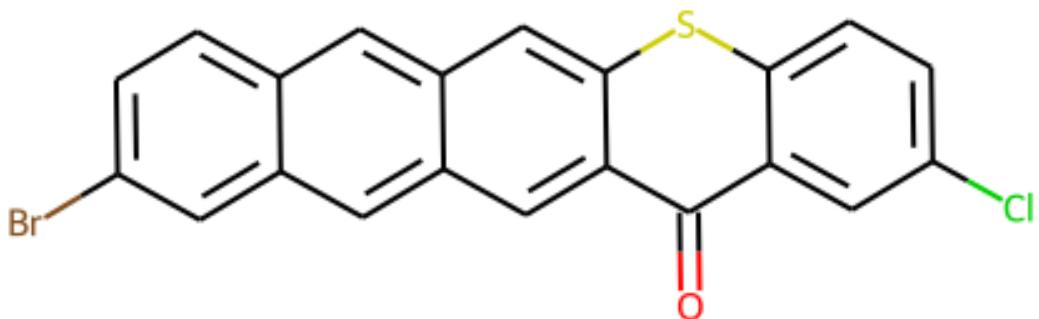
prob: 0.77



No.213

SMILES: O=c1c2cc(Cl)ccc2sc2cc3cc4ccc(Br)cc4cc3cc12

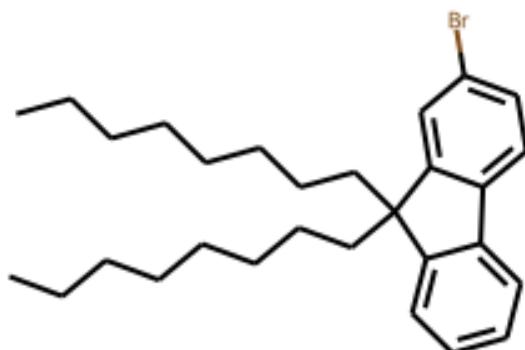
prob: 0.77



No.214

SMILES: CCCCCCCCC1(CCCCCCCC)c2cccc2-c2ccc(Br)cc21

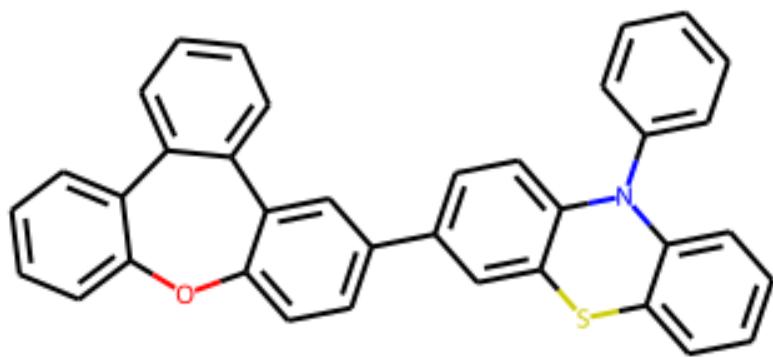
prob: 0.77



No.215

SMILES: c1ccc(N2c3cccc3Sc3cc(-c4ccc5c(c4)-c4ccccc4-c4ccccc405)ccc32)cc1

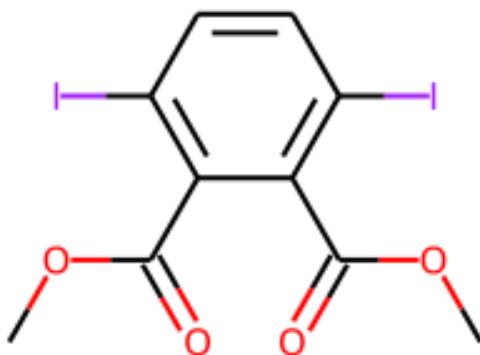
prob: 0.77



No. 216

SMILES: COC(=O)c1c(I)ccc(I)c1C(=O)OC

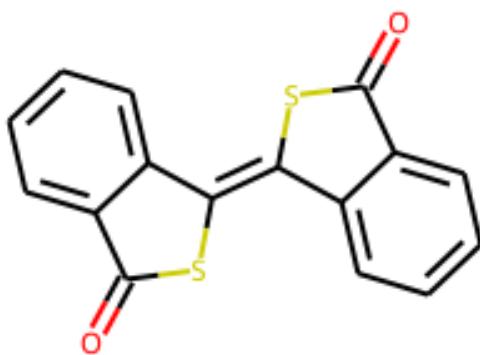
prob: 0.77



No. 217

SMILES: O=C1SC(=C2SC(=O)c3ccccc32)c2ccccc21

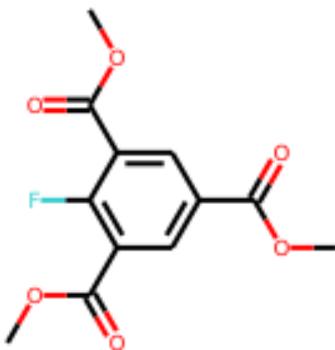
prob: 0.77



No.218

SMILES: COC(=O)c1cc(C(=O)OC)c(F)c(C(=O)OC)c1

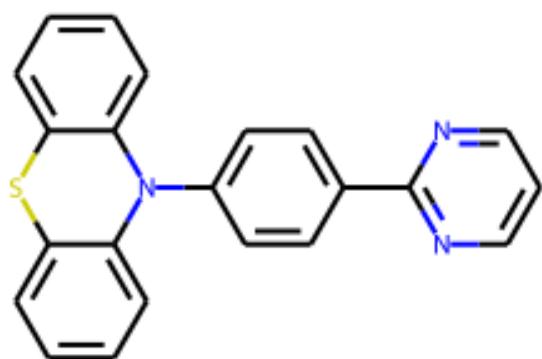
prob: 0.77



No.219

SMILES: c1cnc(-c2ccc(N3c4cccc4Sc4cccc43)cc2)nc1

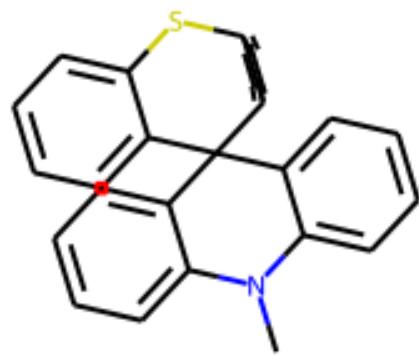
prob: 0.77



No.220

SMILES: CN1c2ccccc2C2(c3ccccc3Sc3ccccc32)c2ccccc21

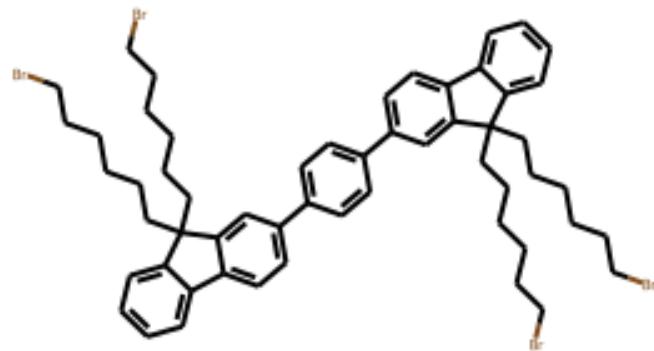
prob: 0.77



No. 221

SMILES: BrCCCCCCC1(CCCCCCBr)c2ccccc2-c2ccc(-c3ccc(-c4ccc5c(c4)C(CCCCCCBr)(CCCCCBr)c4cccc4-5)cc3)cc21

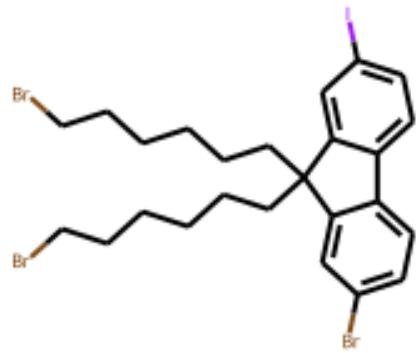
prob: 0.77



No. 222

SMILES: BrCCCCCCC1(CCCCCCBr)c2cc(Br)ccc2-c2ccc(I)cc21

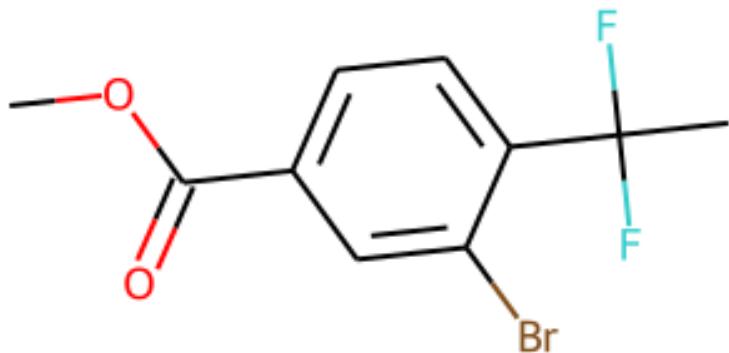
prob: 0.77



No.223

SMILES: COC(=O)c1ccc(C(C)(F)F)c(Br)c1

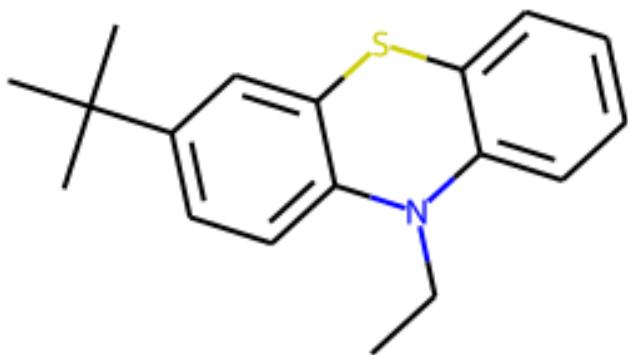
prob: 0.77



No.224

SMILES: CCN1c2ccccc2Sc2cc(C(C)(C)C)ccc21

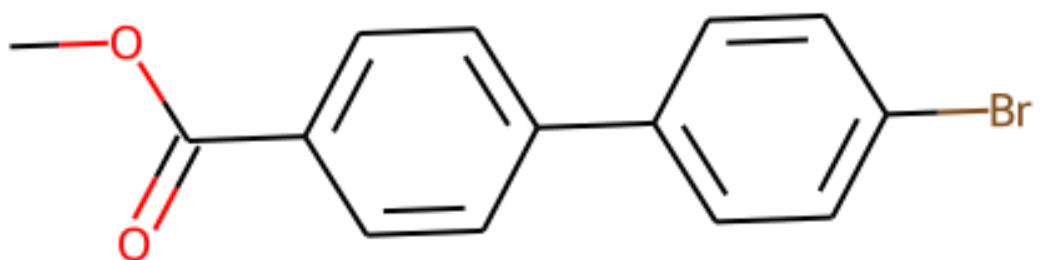
prob: 0.77



No.225

SMILES: COC(=O)c1ccc(-c2ccc(Br)cc2)cc1

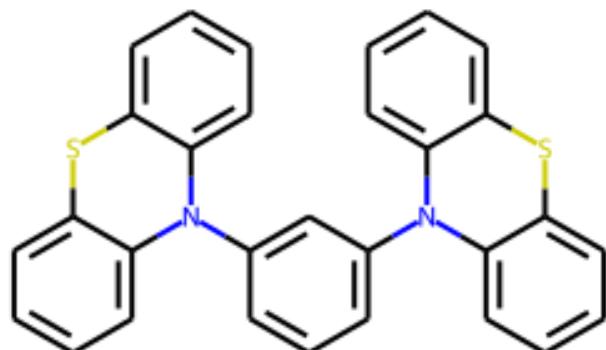
prob: 0.77



No.226

SMILES: c1cc(N2c3cccc3Sc3cccc32)cc(N2c3cccc3Sc3cccc32)c1

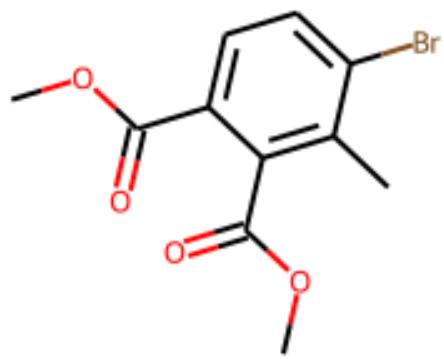
prob: 0.77



No.227

SMILES: COC(=O)c1ccc(Br)c(C)c1C(=O)OC

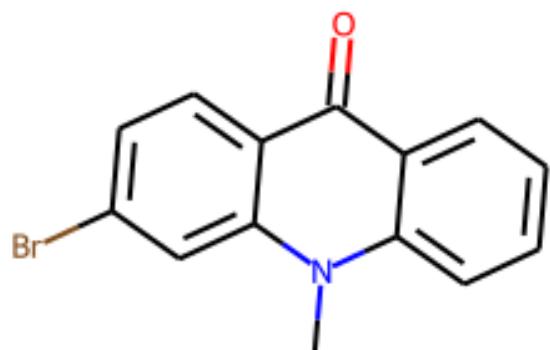
prob: 0.77



No. 228

SMILES: Cn1c2ccccc2c(=O)c2ccc(Br)cc21

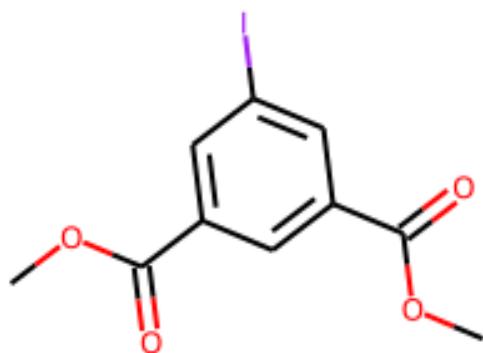
prob: 0.77



No. 229

SMILES: COC(=O)c1cc(I)cc(C(=O)OC)c1

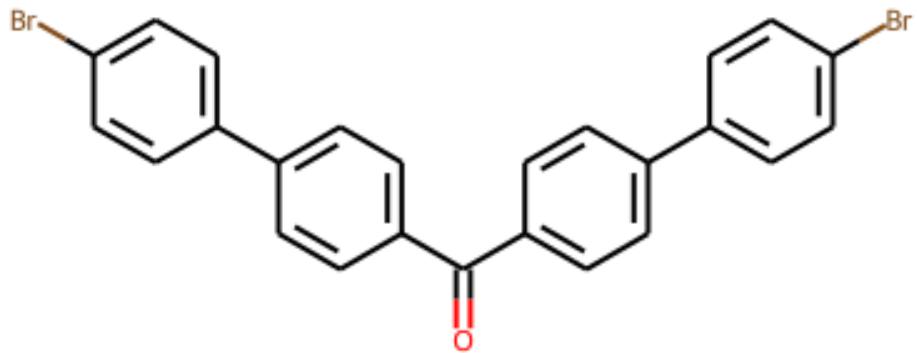
prob: 0.76



No.230

SMILES: O=C(c1ccc(-c2ccc(Br)cc2)cc1)c1ccc(-c2ccc(Br)cc2)cc1

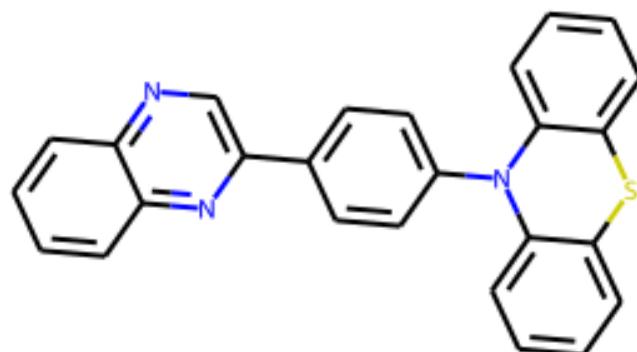
prob: 0.76



No.231

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2cnc3ccccc3n2)cc1

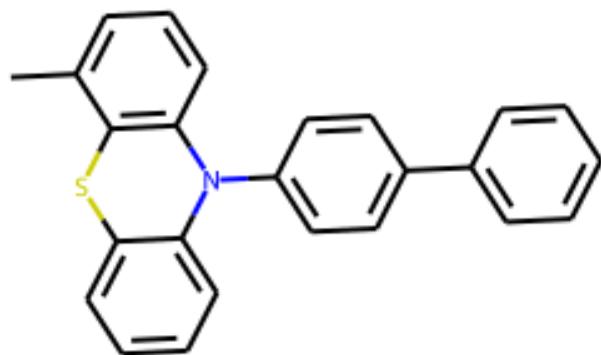
prob: 0.76



No.232

SMILES: Cc1ccccc2c1Sc1ccccc1N2c1ccc(-c2ccccc2)cc1

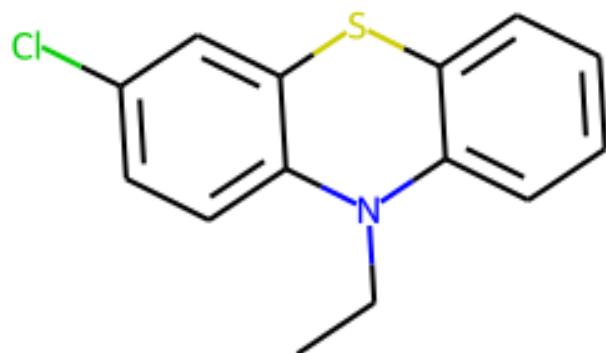
prob: 0.76



No.233

SMILES: CCN1c2ccccc2Sc2cc(Cl)ccc21

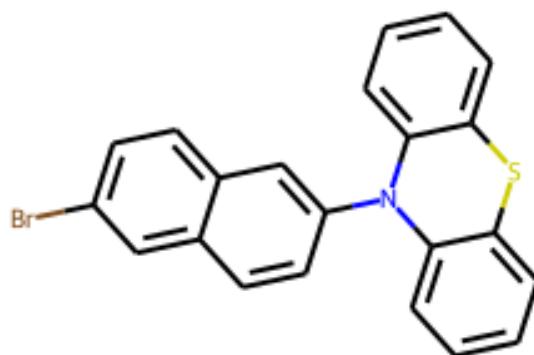
prob: 0.76



No.234

SMILES: Brc1ccc2cc(N3c4ccccc4Sc4ccccc43)ccc2c1

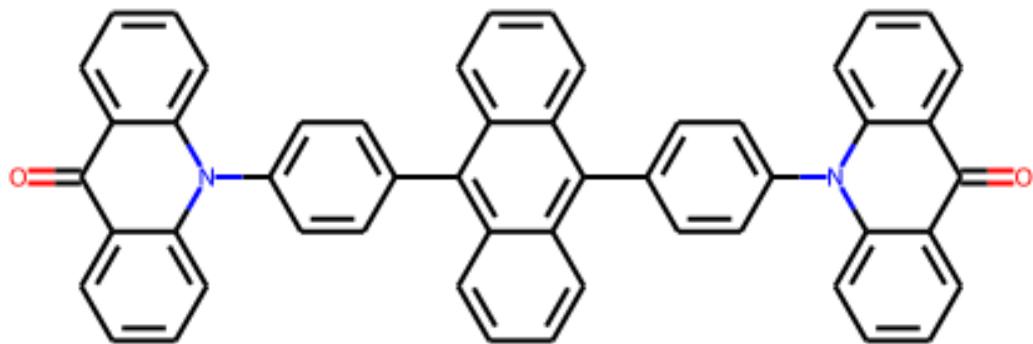
prob: 0.76



No.235

SMILES: O=c1c2ccccc2n(-c2ccc(-c3c4ccccc4c(-c4ccc(-n5c6ccccc6c(=O)c6ccccc65)cc4)c4cccc34)cc2)c2ccccc12

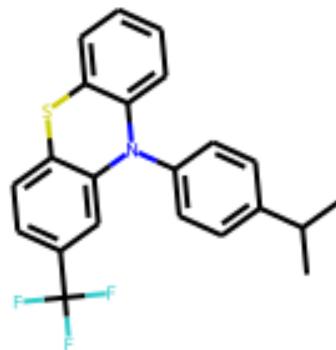
prob: 0.76



No.236

SMILES: CC(C)c1ccc(N2c3ccccc3Sc3ccc(C(F)(F)F)cc32)cc1

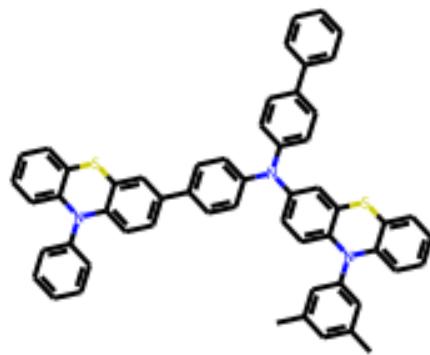
prob: 0.76



No.237

SMILES: Cc1cc(C)cc(N2c3ccccc3Sc3cc(N(c4ccc(-c5ccccc5)cc4)c4ccc(-c5ccc6c(c5)Sc5ccc5N6c5ccccc5)cc4)ccc32)c1

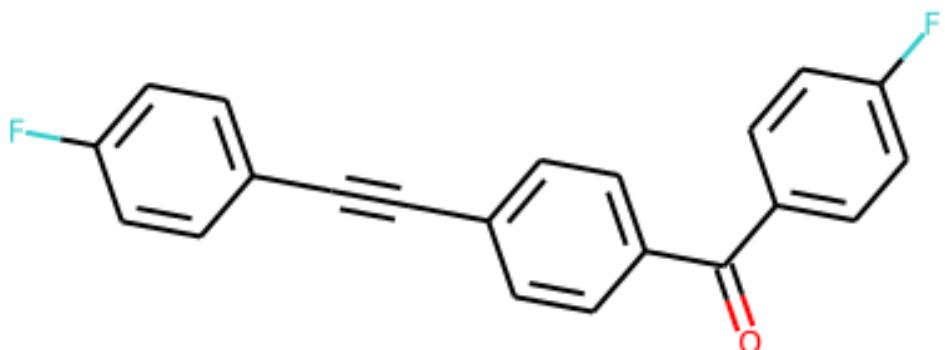
prob: 0.76



No.238

SMILES: O=C(c1ccc(F)cc1)c1ccc(C#Cc2ccc(F)cc2)cc1

prob: 0.76



No.239

SMILES: FC(F)(F)c1cc(N2c3cccc3Sc3cccc32)cc(N2c3cccc3Sc3cccc32)c1

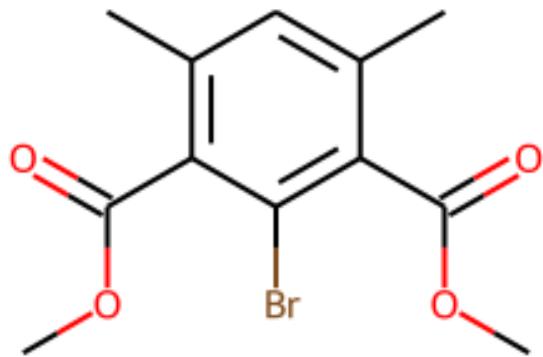
prob: 0.76



No. 240

SMILES: COC(=O)c1c(C)cc(C)c(C(=O)OC)c1Br

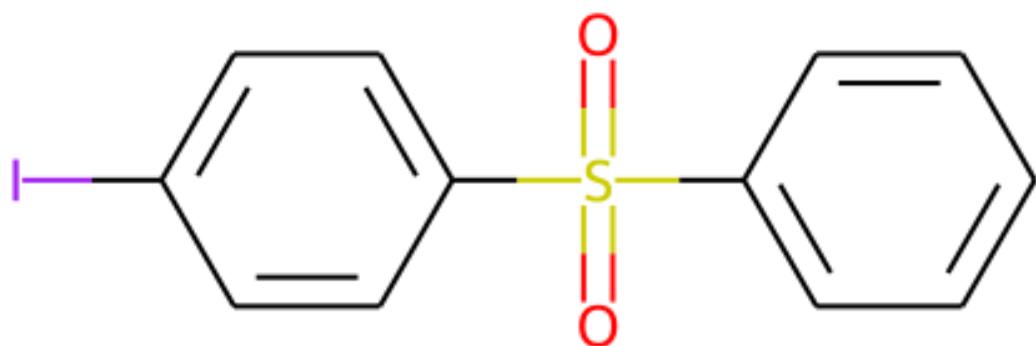
prob: 0.76



No. 241

SMILES: O=S(=O)(c1ccccc1)c1ccc(I)cc1

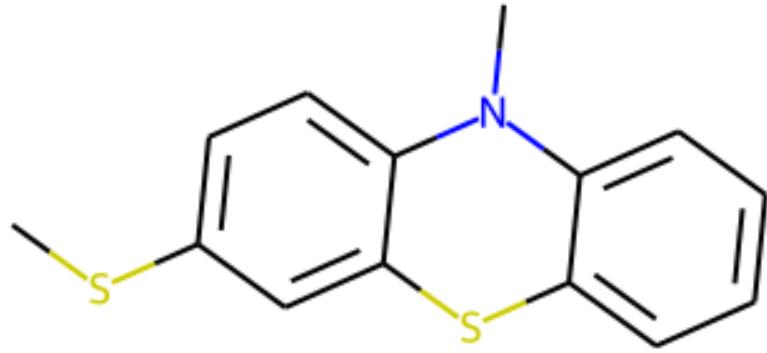
prob: 0.76



No. 242

SMILES: CSc1ccc2c(c1)Sc1ccccc1N2C

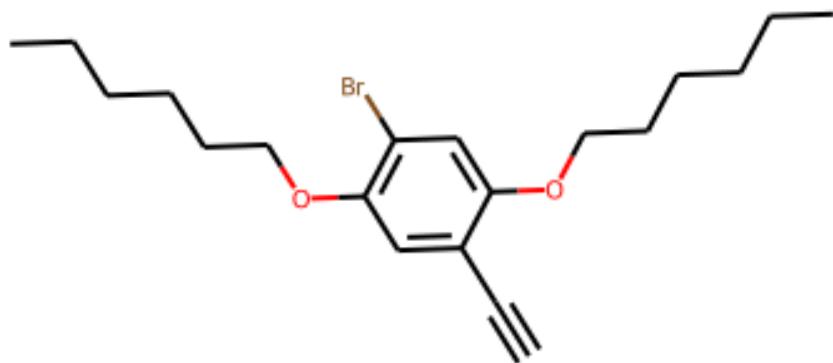
prob: 0.76



No. 243

SMILES: C#Cc1cc(OCCCCCC)c(Br)cc1OCCCCCC

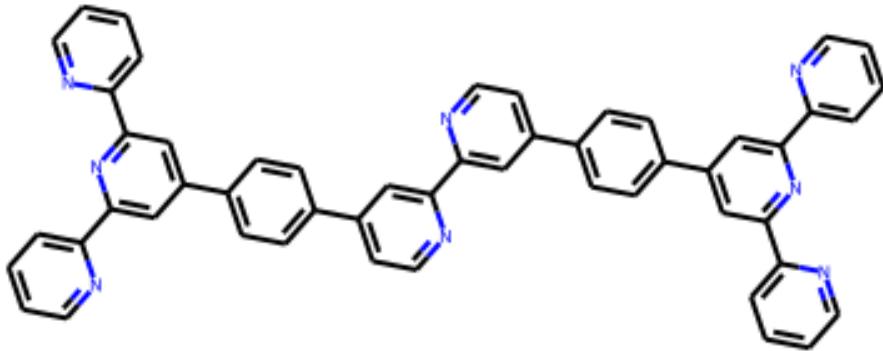
prob: 0.76



No. 244

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccnc(-c5cc(-c6ccc(-c7cc(-c8cccn8)nc(-c8cccn8)c7)cc6)ccn5)c4)cc3)cc(-c3cccn3)n2)nc1

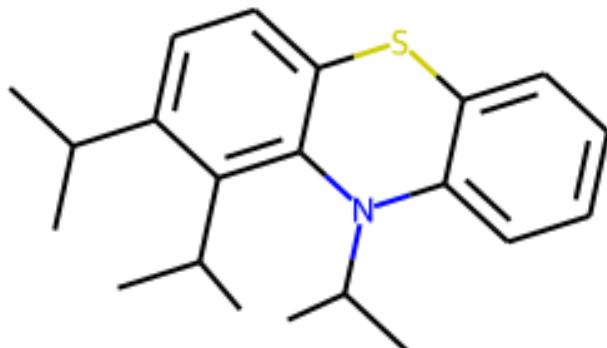
prob: 0.76



No. 245

SMILES: CC(C)c1ccc2c(c1C(C)C)N(C(C)C)c1ccccc1S2

prob: 0.76



No. 246

SMILES: Cc1cc(C)c(P(c2c(C)cc(C)cc2C)c2c(C)cc(N3c4ccccc4Sc4ccccc43)cc2C)c(C)c1

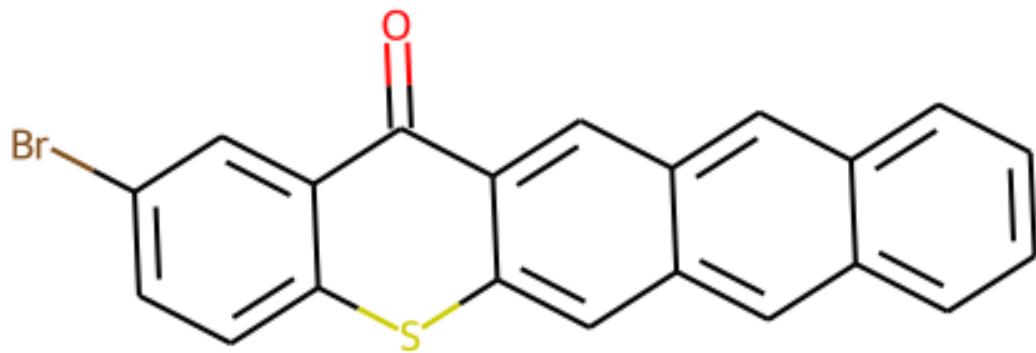
prob: 0.76



No. 247

SMILES: O=c1c2cc(Br)ccc2sc2cc3cc4cccc4cc3cc12

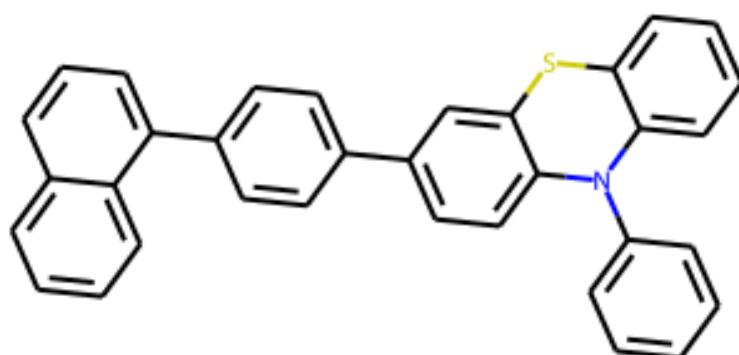
prob: 0.76



No. 248

SMILES: c1ccc(N2c3cccc3Sc3cc(-c4ccc(-c5cccc6cccc56)cc4)ccc32)cc1

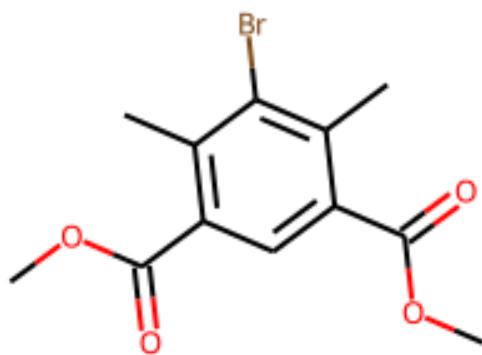
prob: 0.76



No. 249

SMILES: COC(=O)c1cc(C(=O)OC)c(C)c(Br)c1C

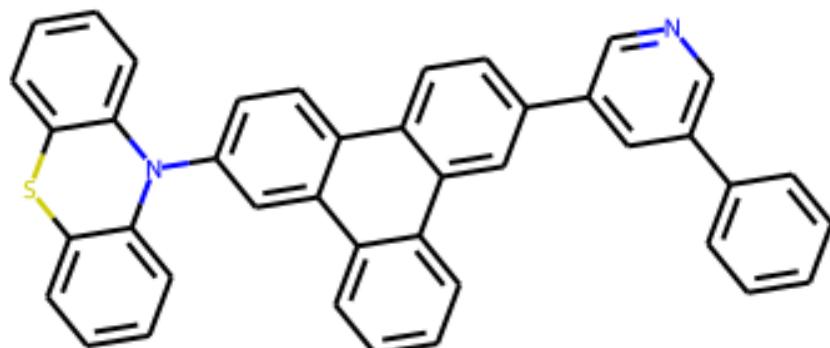
prob: 0.76



No. 250

SMILES: c1ccc(-c2cncc(-c3ccc4c5ccc(N6c7cccc7Sc7ccccc76)cc5c5ccccc5c4c3)c2)cc1

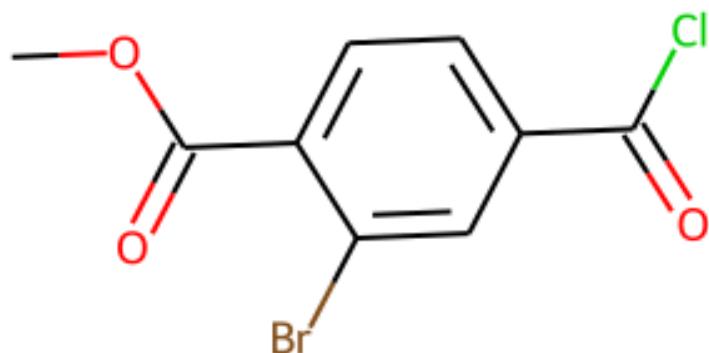
prob: 0.76



No. 251

SMILES: COC(=O)c1ccc(C(=O)Cl)cc1Br

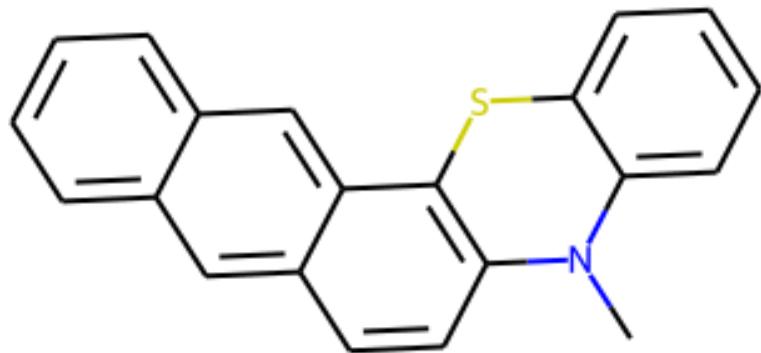
prob: 0.76



No. 252

SMILES: CN1c2ccccc2Sc2c1ccc1cc3ccccc3cc21

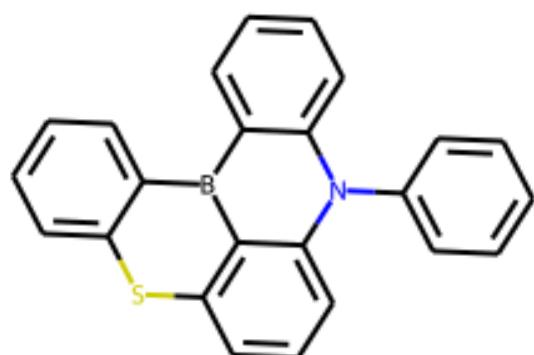
prob: 0.76



No. 253

SMILES: c1ccc(N2c3ccccc3B3c4ccccc4Sc4ccccc2c43)cc1

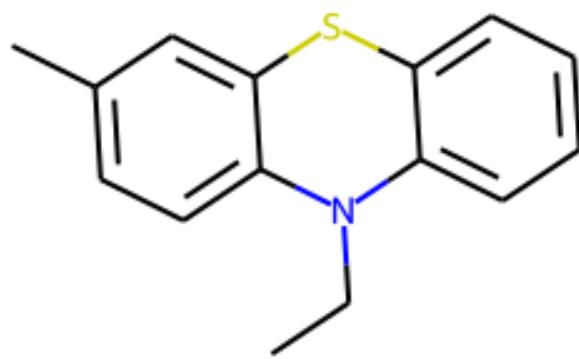
prob: 0.76



No. 254

SMILES: CCN1c2ccccc2Sc2cc(C)ccc21

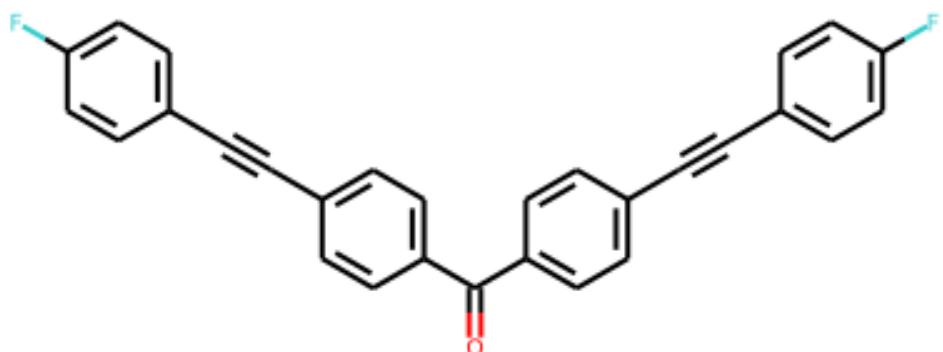
prob: 0.76



No. 255

SMILES: O=C(c1ccc(C#Cc2ccc(F)cc2)cc1)c1ccc(C#Cc2ccc(F)cc2)cc1

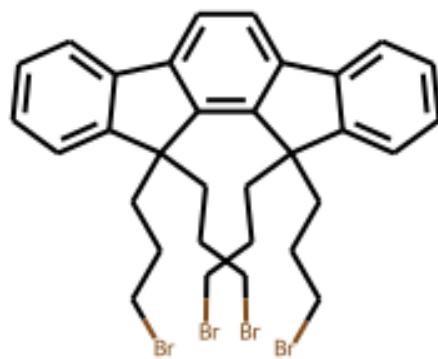
prob: 0.76



No. 256

SMILES: BrCCCC1(CCBr)cc2ccccc2-c2ccc3c(c21)C(CCBr)(CCBr)c1ccccc1-3

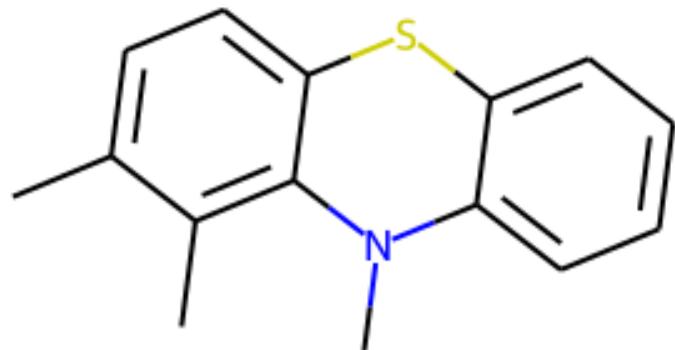
prob: 0.76



No. 257

SMILES: Cc1ccc2c(c1C)N(C)c1ccccc1S2

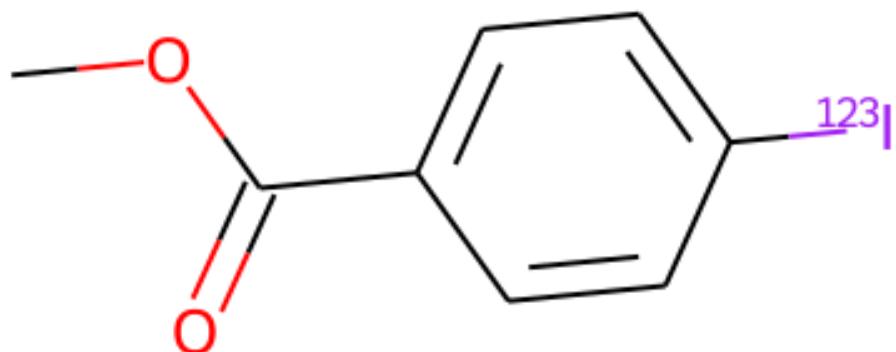
prob: 0.76



No. 258

SMILES: COC(=O)c1ccc([123I])cc1

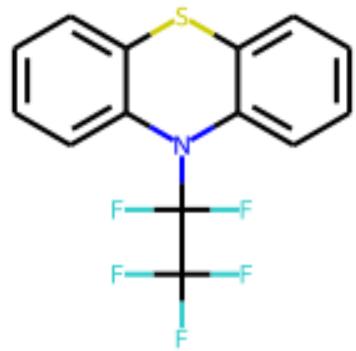
prob: 0.76



No. 259

SMILES: FC(F)(F)C(F)(F)N1c2ccccc2Sc2ccccc21

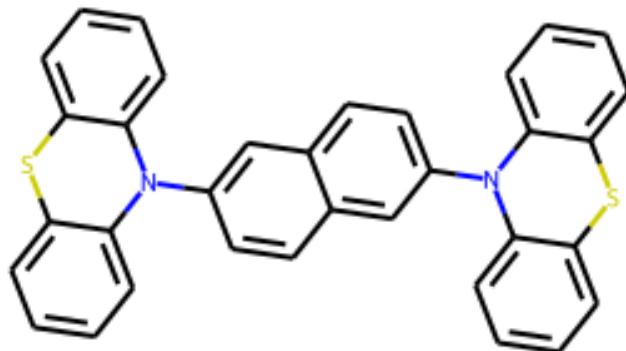
prob: 0.76



No. 260

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2cc(N3c4ccccc4Sc4ccccc43)ccc2c1

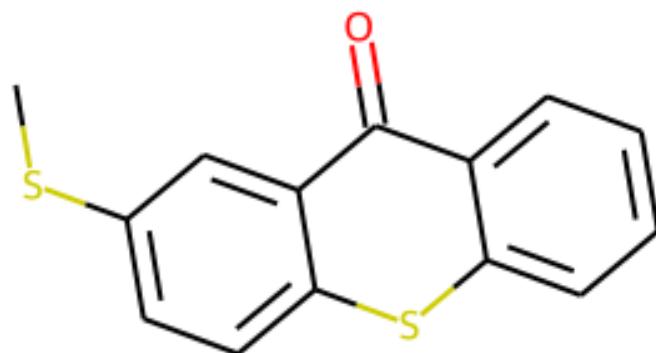
prob: 0.76



No. 261

SMILES: CSc1ccc2sc3ccccc3c(=O)c2c1

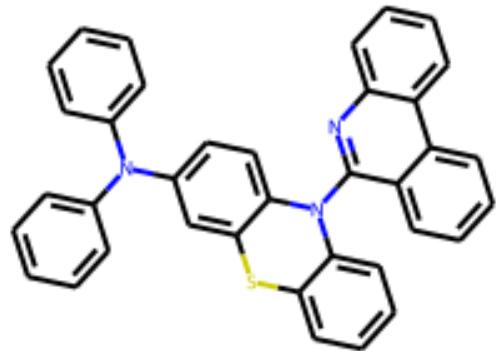
prob: 0.76



No.262

SMILES: c1ccc(N(c2ccccc2)c2ccc3c(c2)Sc2ccccc2N3c2nc3ccccc3c3ccccc23)cc1

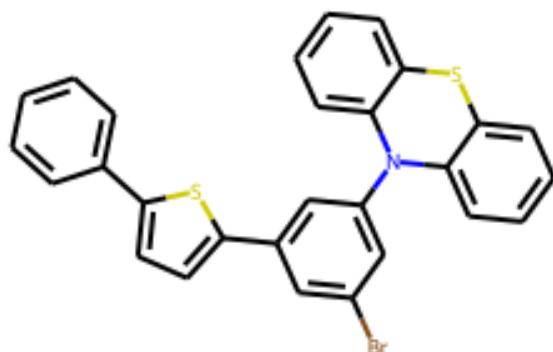
prob: 0.76



No.263

SMILES: Brc1cc(-c2ccc(-c3ccccc3)s2)cc(N2c3ccccc3Sc3ccccc2)cc1

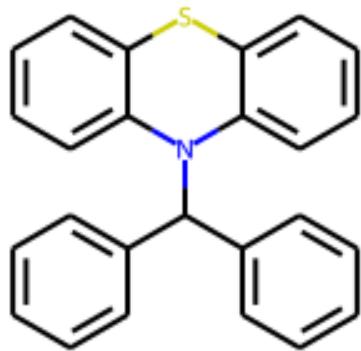
prob: 0.76



No.264

SMILES: c1ccc(C(c2ccccc2)N2c3ccccc3Sc3ccccc2)cc1

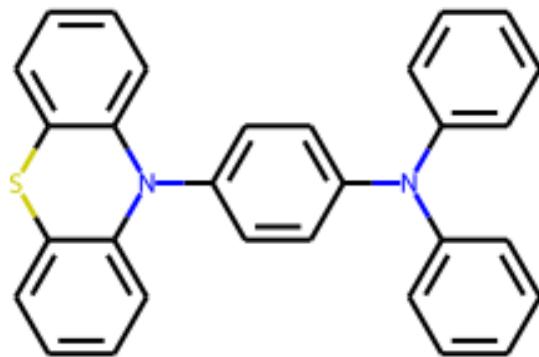
prob: 0.76



No. 265

SMILES: c1ccc(N(c2ccccc2)c2ccc(N3c4ccccc4Sc4ccccc43)cc2)cc1

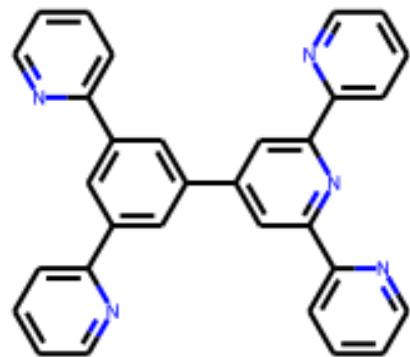
prob: 0.76



No. 266

SMILES: c1ccc(-c2cc(-c3cc(-c4cccn4)nc(-c4cccn4)c3)cc(-c3cccn3)c2)nc1

prob: 0.76

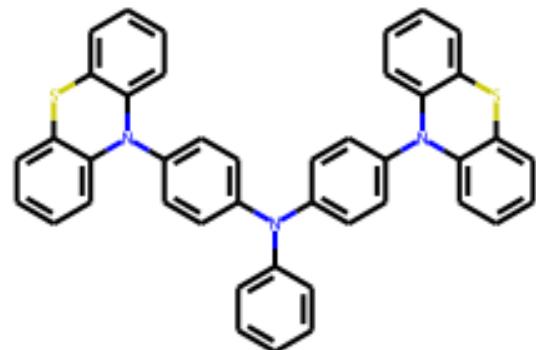


No.267

SMILES:

c1ccc(N(c2ccc(N3c4cccc4Sc4cccc43)cc2)c2ccc(N3c4cccc4Sc4cccc43)cc2)cc1

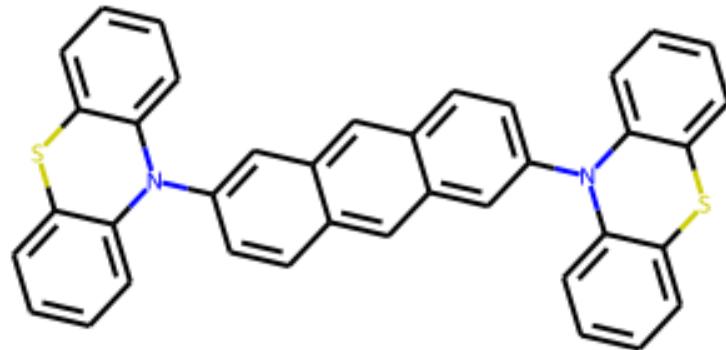
prob: 0.76



No.268

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2cc3cc(N4c5ccccc5Sc5ccccc54)ccc3cc2c1

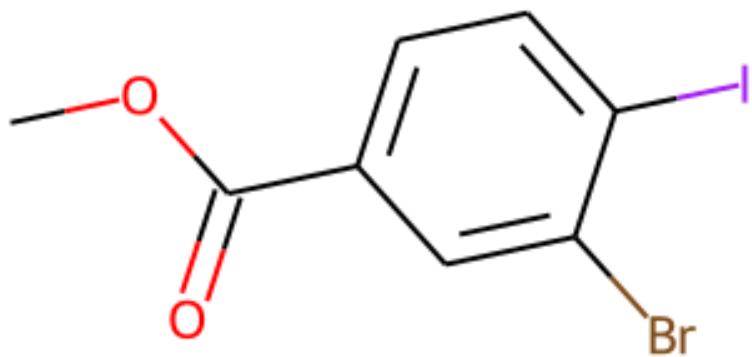
prob: 0.76



No.269

SMILES: COC(=O)c1ccc(I)c(Br)c1

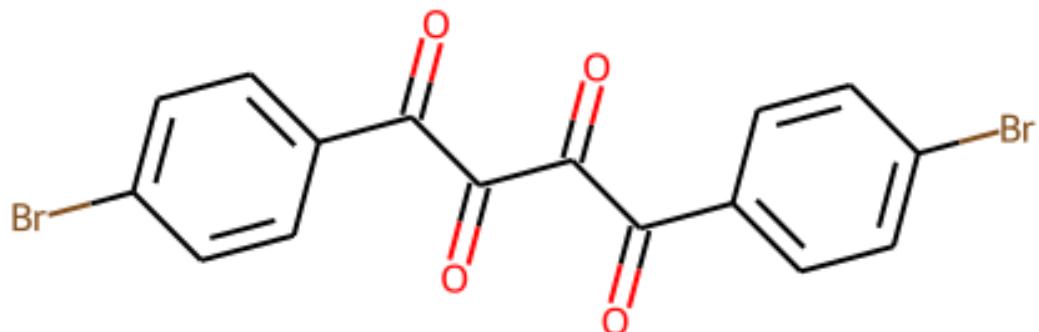
prob: 0.76



No. 270

SMILES: O=C(C(=O)C1ccc(Br)cc1)C(=O)c1ccc(Br)cc1

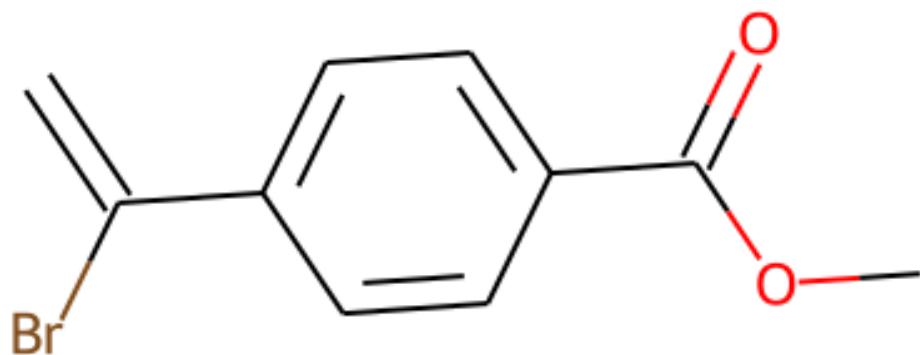
prob: 0.76



No. 271

SMILES: C=C(Br)c1ccc(C(=O)OC)cc1

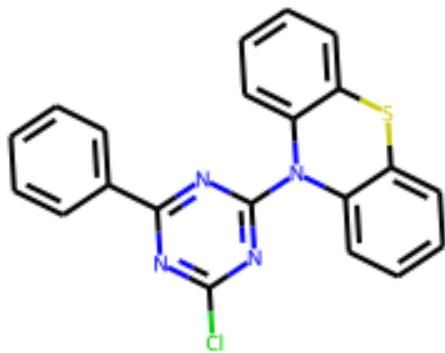
prob: 0.76



No.272

SMILES: Clc1nc(-c2ccccc2)nc(N2c3cccc3Sc3cccc32)n1

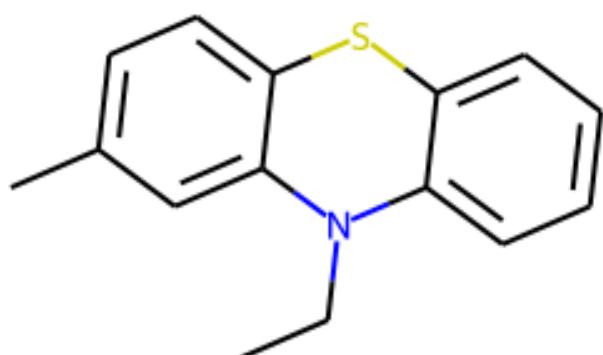
prob: 0.76



No.273

SMILES: CCN1c2ccccc2Sc2ccc(C)cc21

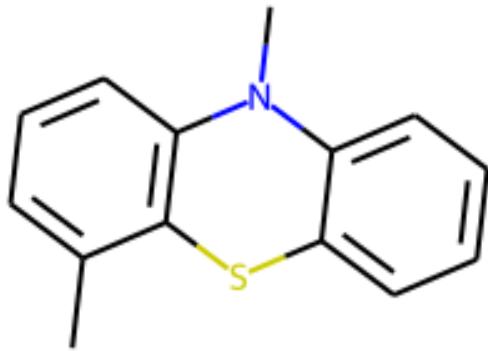
prob: 0.76



No.274

SMILES: Cc1ccccc2c1Sc1cccc1N2C

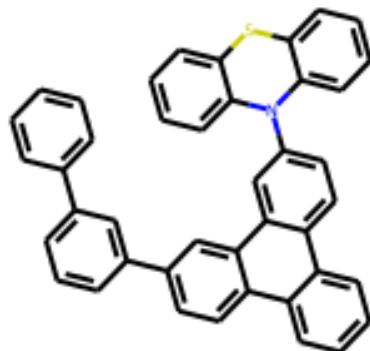
prob: 0.75



No.275

SMILES: c1ccc(-c2cccc(-c3ccc4c5cccc5c5ccc(N6c7ccccc7Sc7ccccc76)cc5c4c3)c2)cc1

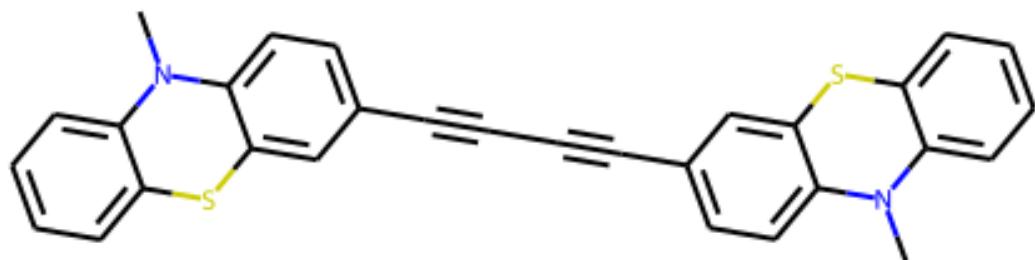
prob: 0.75



No.276

SMILES: CN1c2ccccc2Sc2cc(C#CC#Cc3ccc4c(c3)Sc3ccccc3N4C)ccc21

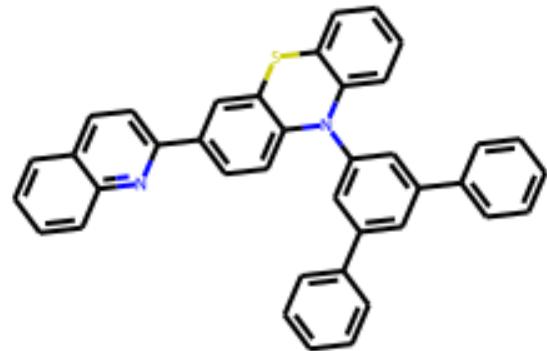
prob: 0.75



No.277

SMILES: c1ccc(-c2cc(-c3cccc3)cc(N3c4ccccc4Sc4cc(-c5ccc6ccccc6n5)ccc43)c2)cc1

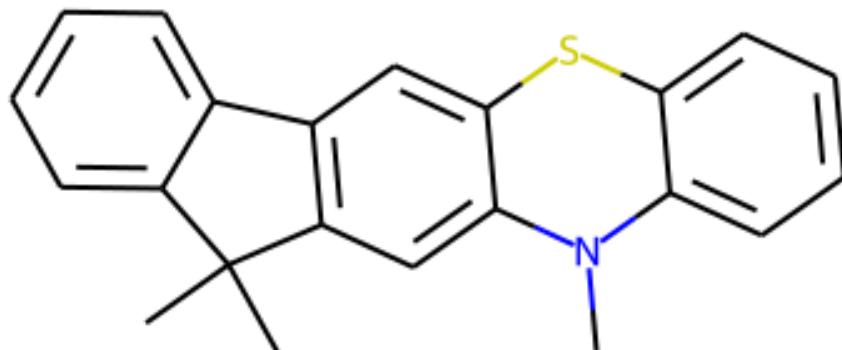
prob: 0.75



No.278

SMILES: CN1c2ccccc2Sc2cc3c(cc21)C(C)(C)c1ccccc1-3

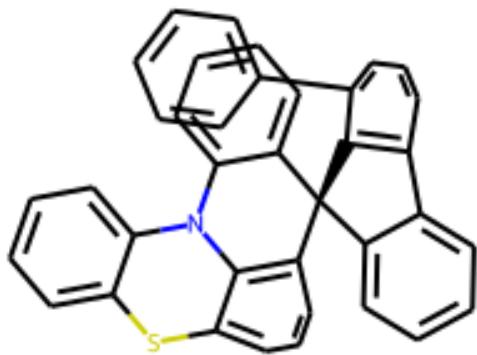
prob: 0.75



No.279

SMILES: c1ccc(-c2ccccc3c2[C@]2(c4ccccc4-3)c3ccccc3N3c4ccccc4Sc4ccccc2c43)cc1

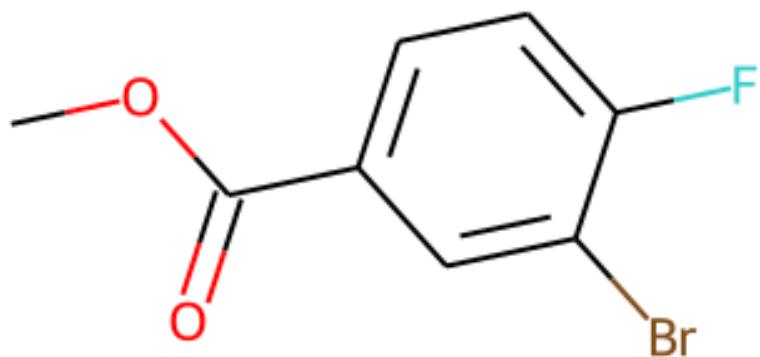
prob: 0.75



No. 280

SMILES: COC(=O)c1ccc(F)c(Br)c1

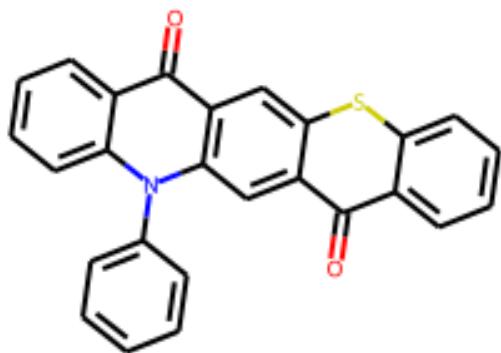
prob: 0.75



No. 281

SMILES: O=c1c2ccccc2sc2cc3c(=O)c4ccccc4n(-c4ccccc4)c3cc12

prob: 0.75

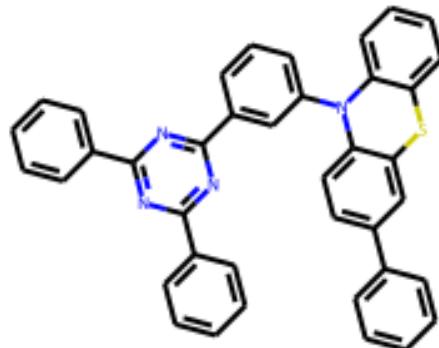


No.282

SMILES:

c1ccc(-c2ccc3c(c2)Sc2ccccc2N3c2cccc(-c3nc(-c4ccccc4)nc(-c4ccccc4)n3)c2)cc1

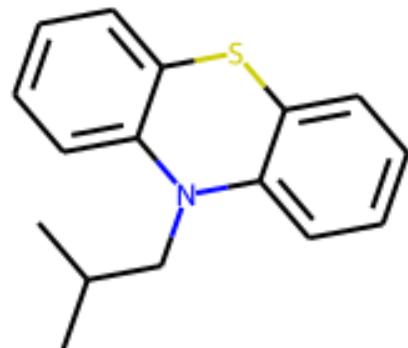
prob: 0.75



No.283

SMILES: CC(C)CN1c2ccccc2Sc2ccccc21

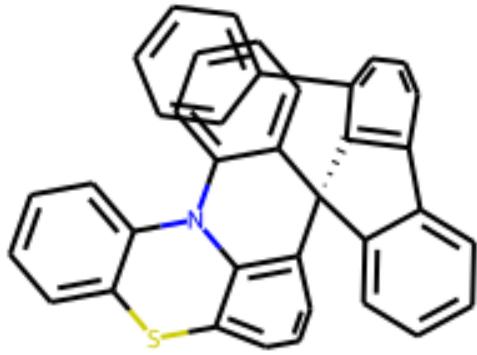
prob: 0.75



No.284

SMILES: c1ccc(-c2cccc3c2[C@H]2(c4ccccc4-3)c3ccccc3N3c4ccccc4Sc4cccc2c43)cc1

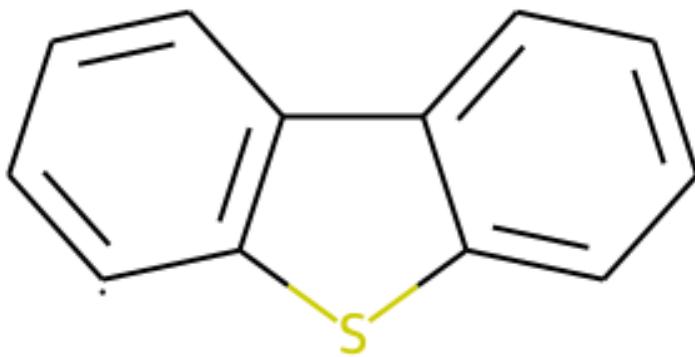
prob: 0.75



No. 285

SMILES: [c]1cccc2c1sc1ccccc12

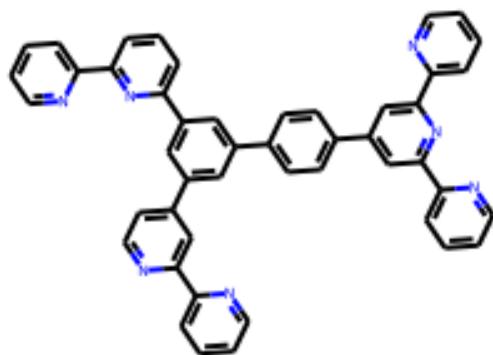
prob: 0.75



No. 286

SMILES: c1ccc(-c2cc(-c3cc(-c4ccc(-c5cc(-c6cccn6)nc(-c6cccn6)c5)cc4)cc(-c4cccc(-c5cccn5)n4)c3)ccn2)nc1

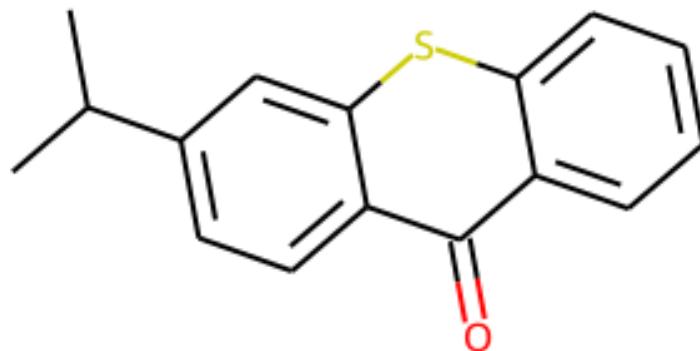
prob: 0.75



No. 287

SMILES: CC(C)c1ccc2c(=O)c3ccccc3sc2c1

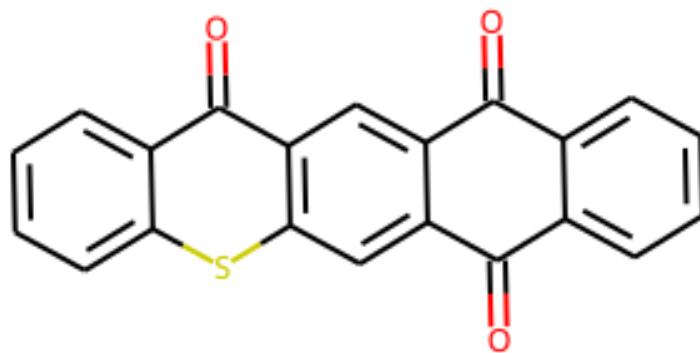
prob: 0.75



No. 288

SMILES: O=C1c2ccccc2C(=O)c2cc3c(=O)c4ccccc4sc3cc21

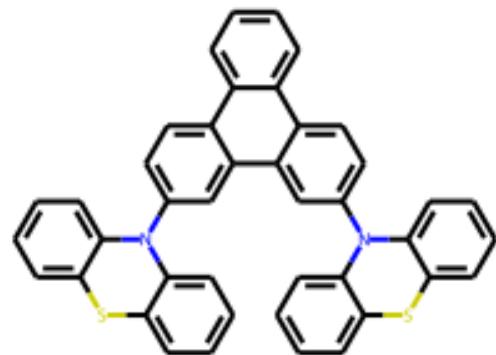
prob: 0.75



No.289

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2c3ccccc3c3ccc(N4c5ccccc5Sc5ccccc54)cc3c2c1

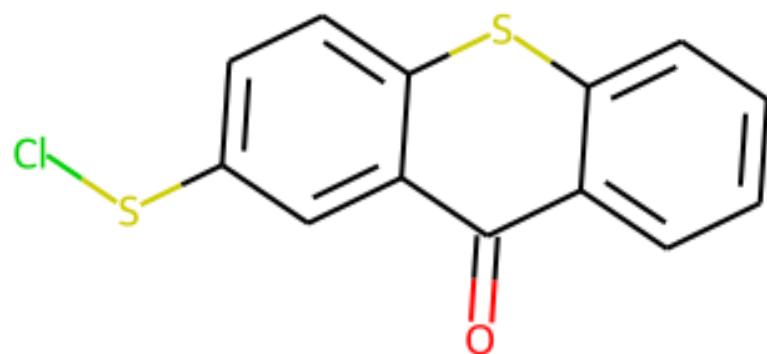
prob: 0.75



No.290

SMILES: O=c1c2ccccc2sc2ccc(SCl)cc12

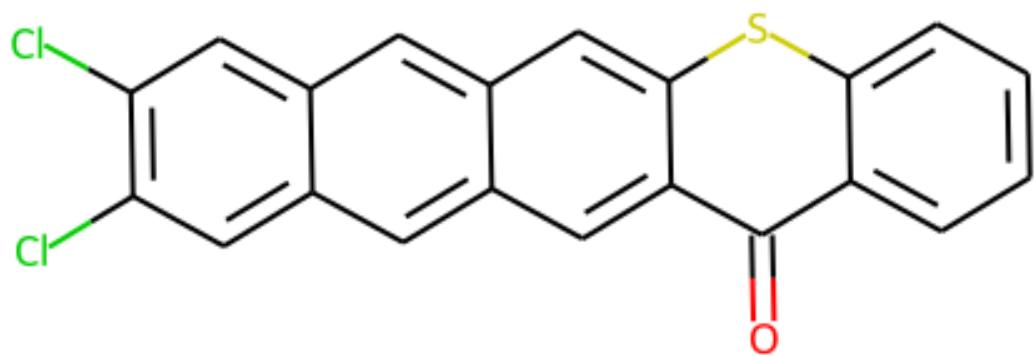
prob: 0.75



No.291

SMILES: O=c1c2ccccc2sc2cc3cc4cc(Cl)c(Cl)cc4cc3cc12

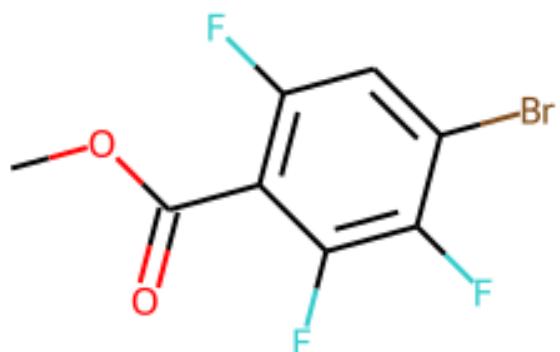
prob: 0.75



No.292

SMILES: COC(=O)c1c(F)cc(Br)c(F)c1F

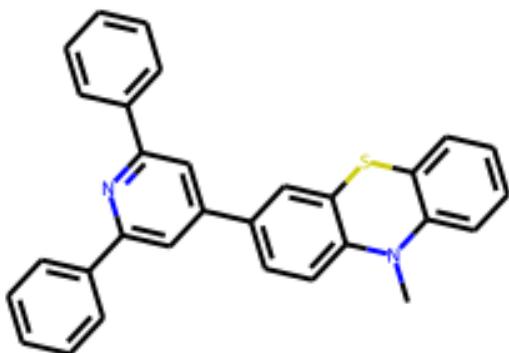
prob: 0.75



No.293

SMILES: CN1c2cccc2Sc2cc(-c3cc(-c4ccccc4)nc(-c4ccccc4)c3)ccc21

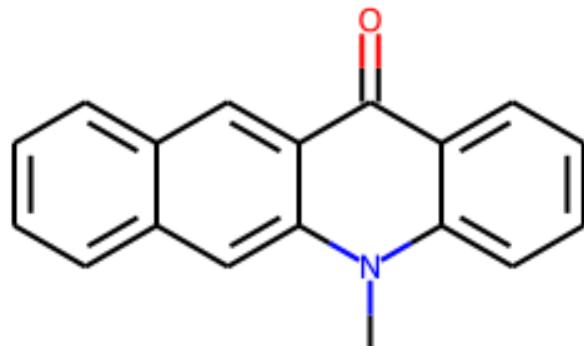
prob: 0.75



No.294

SMILES: Cn1c2ccccc2c(=O)c2cc3ccccc3cc21

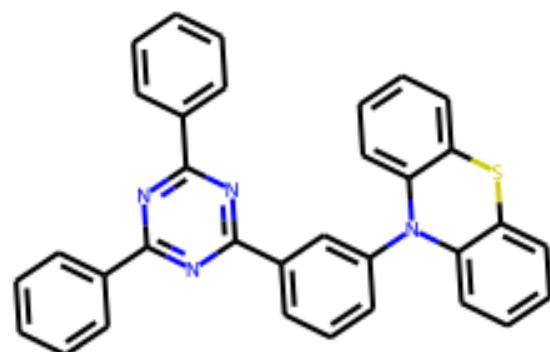
prob: 0.75



No.295

SMILES: c1ccc(-c2nc(-c3ccccc3)nc(-c3cccc(N4c5ccccc5Sc5ccccc54)c3)n2)cc1

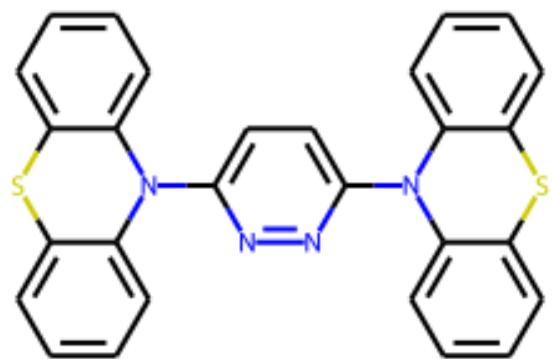
prob: 0.75



No.296

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(N2c3ccccc3Sc3ccccc32)nn1

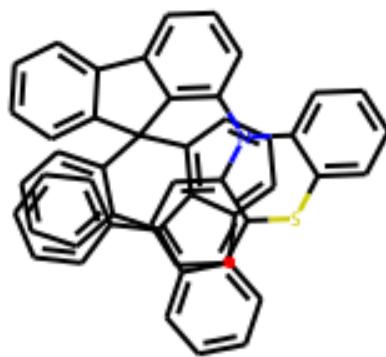
prob: 0.75



No.297

SMILES: c1ccc(C23c4ccccc4-c4cccc(c42)C2(c4ccccc4-c4cccc(N5c6ccccc6Sc6ccccc65)c42)c2ccccc23)cc1

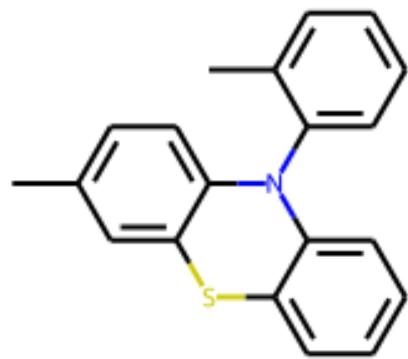
prob: 0.75



No.298

SMILES: Cc1ccc2c(c1)Sc1ccccc1N2c1ccccc1C

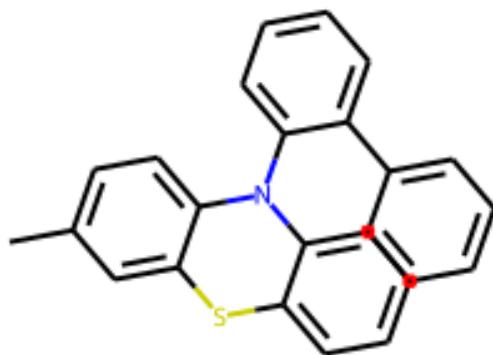
prob: 0.75



No.299

SMILES: Cc1ccc2c(c1)Sc1ccccc1N2c1ccccc1-c1ccccc1

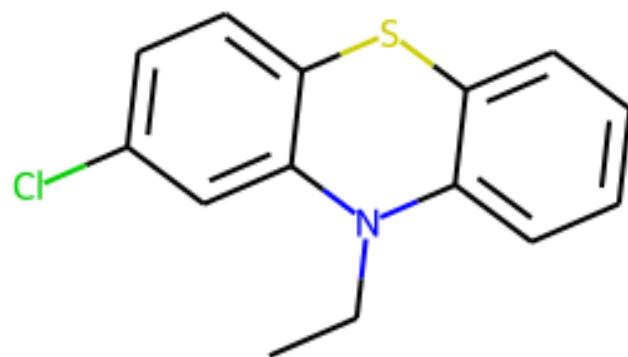
prob: 0.75



No.300

SMILES: CCN1c2ccccc2Sc2ccc(Cl)cc21

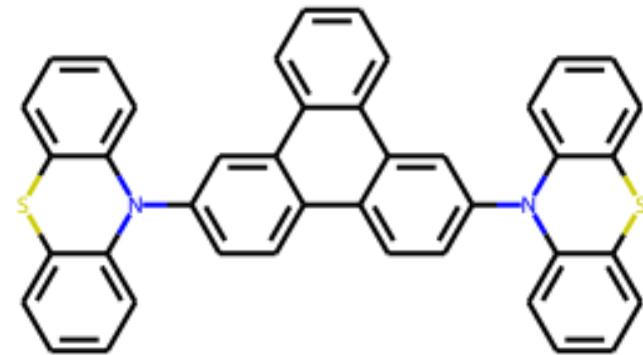
prob: 0.75



No.301

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2c3ccc(N4c5ccccc5Sc5ccccc54)cc3c3ccccc3c2c1

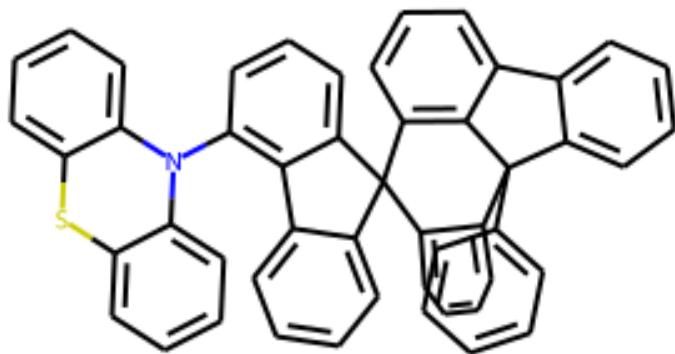
prob: 0.75



No.302

SMILES: c1ccc(C23c4ccccc4-c4cccc(c42)C2(c4ccccc4-c4c(N5c6ccccc6Sc6ccccc65)cccc42)c2ccccc23)cc1

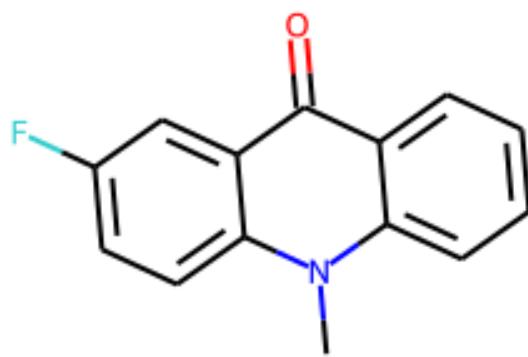
prob: 0.75



No.303

SMILES: Cn1c2ccccc2c(=O)c2cc(F)ccc21

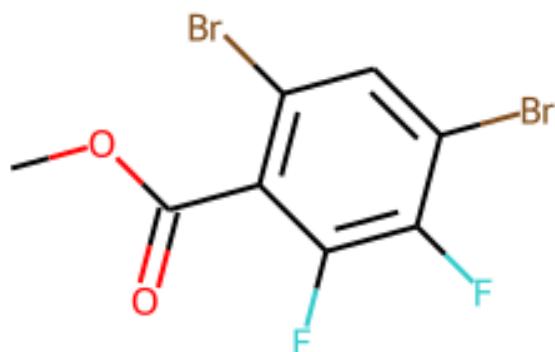
prob: 0.75



No.304

SMILES: COC(=O)c1c(Br)cc(Br)c(F)c1F

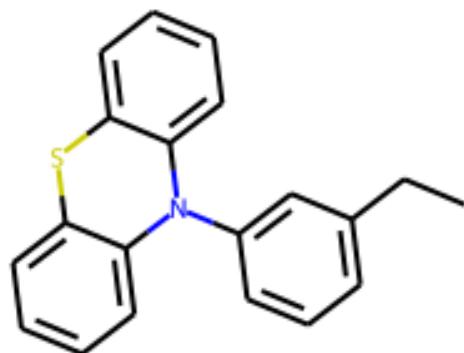
prob: 0.75



No.305

SMILES: CCc1cccc(N2c3ccccc3Sc3ccccc32)c1

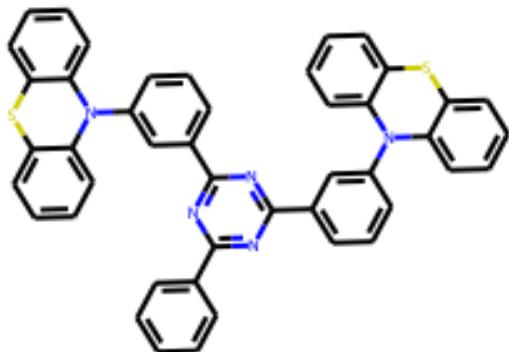
prob: 0.75



No.306

SMILES: c1ccc(-c2nc(-c3cccc(N4c5cccc5Sc5cccc54)c3)nc(-c3cccc(N4c5cccc5Sc5cccc54)c54)c3)n2)cc1

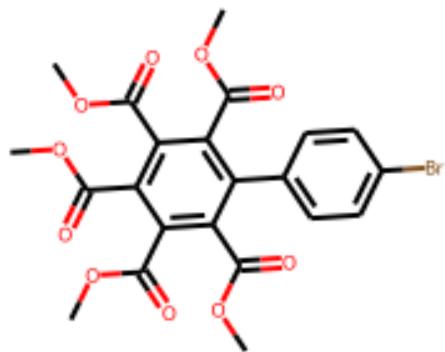
prob: 0.75



No.307

SMILES: COC(=O)c1c(C(=O)OC)c(C(=O)OC)c(-c2ccc(Br)cc2)c(C(=O)OC)c1C(=O)OC

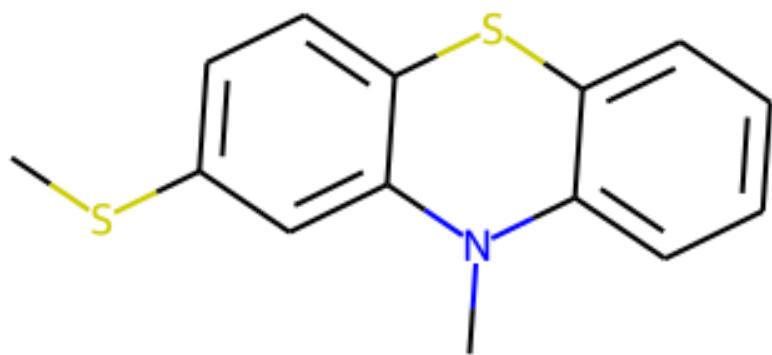
prob: 0.75



No.308

SMILES: CSc1ccc2c(c1)N(C)c1ccccc1S2

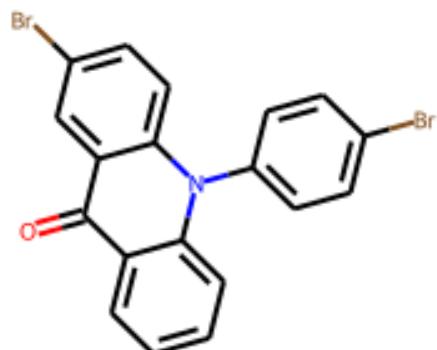
prob: 0.75



No.309

SMILES: O=c1c2ccccc2n(-c2ccc(Br)cc2)c2ccc(Br)cc12

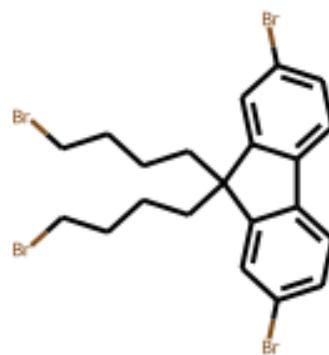
prob: 0.75



No.310

SMILES: BrCCCCC1(CCCCBBr)c2cc(Br)ccc2-c2ccc(Br)cc21

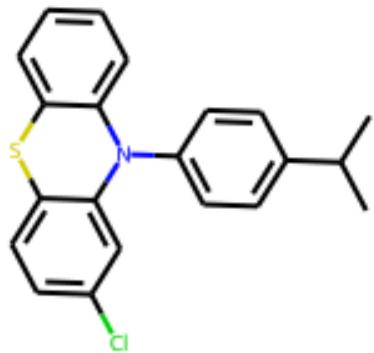
prob: 0.75



No.311

SMILES: CC(C)c1ccc(N2c3ccccc3Sc3ccc(Cl)cc32)cc1

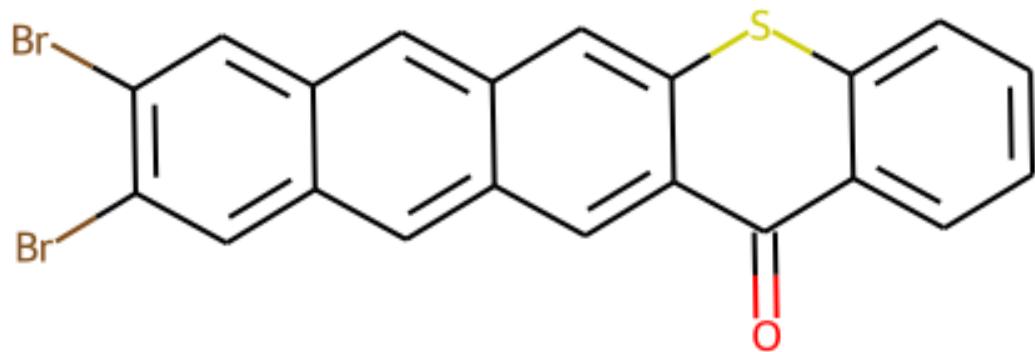
prob: 0.75



No.312

SMILES: O=c1c2cccc2sc2cc3cc4cc(Br)c(Br)cc4cc3cc12

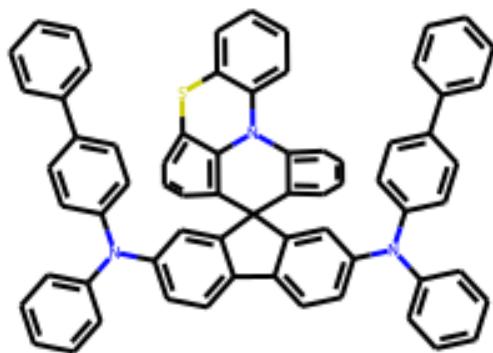
prob: 0.75



No.313

SMILES: c1ccc(-c2ccc(N(c3ccccc3)c3ccc4c(c3)C3(c5cc(N(c6ccccc6)c6ccc(-c7ccccc7)cc6)ccc5-4)c4ccccc4N4c5ccccc5Sc5cccc3c54)cc2)cc1

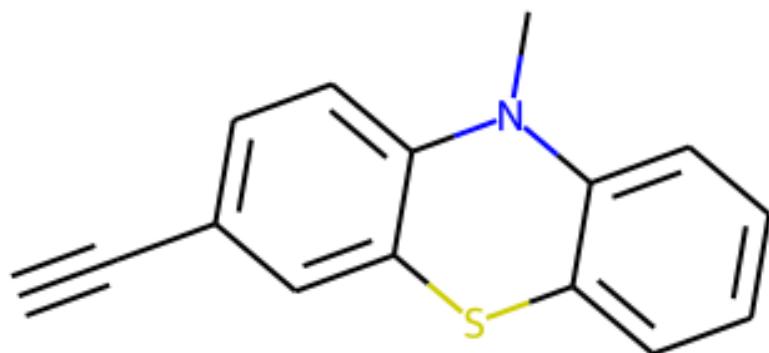
prob: 0.75



No.314

SMILES: C#Cc1ccc2c(c1)Sc1ccccc1N2C

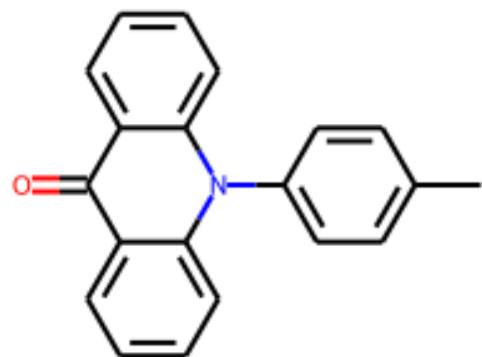
prob: 0.75



No.315

SMILES: Cc1ccc(-n2c3cccc3c(=O)c3ccccc32)cc1

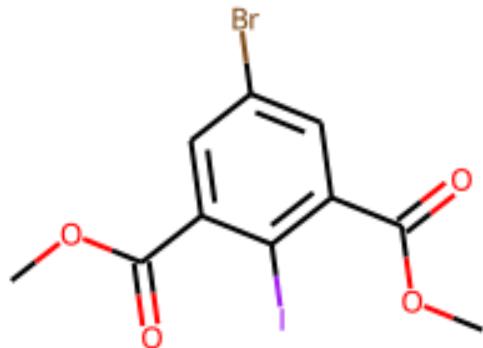
prob: 0.75



No.316

SMILES: COC(=O)c1cc(Br)cc(C(=O)OC)c1I

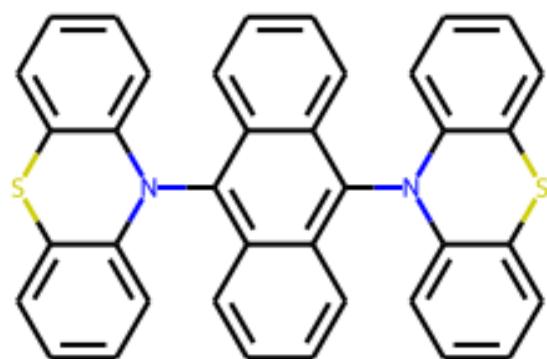
prob: 0.75



No.317

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1c2ccccc2c(N2c3ccccc3Sc3ccccc32)c2ccccc12

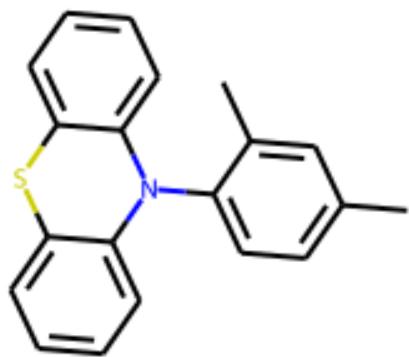
prob: 0.75



No.318

SMILES: Cc1ccc(N2c3ccccc3Sc3ccccc32)c(C)c1

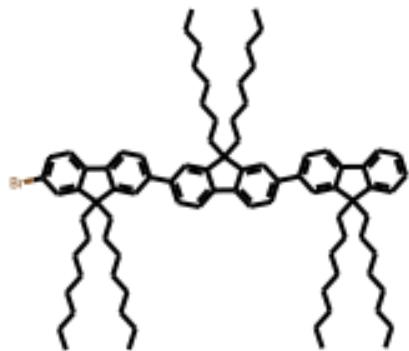
prob: 0.75



No.319

SMILES: CCCCCCCC1(CCCCCCCC)c2ccccc2-c2ccc(-c3ccc4c(c3)C(CCCCCCCC)(CCCCCCC)c3cc(-c5ccc6c(c5)C(CCCCCCCC)(CCCCCCC)c5cc(Br)ccc5-6)ccc3-4)cc21

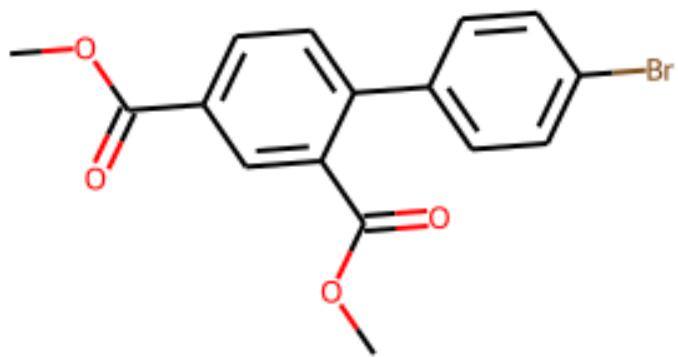
prob: 0.74



No.320

SMILES: COC(=O)c1ccc(-c2ccc(Br)cc2)c(C(=O)OC)c1

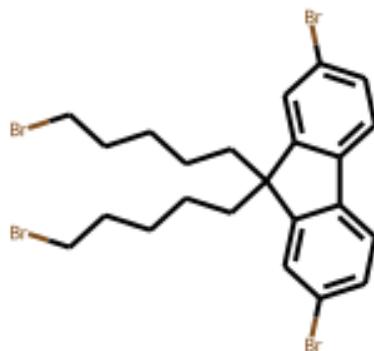
prob: 0.74



No.321

SMILES: BrCCCCC1(CCCCCBr)c2cc(Br)ccc2-c2ccc(Br)cc21

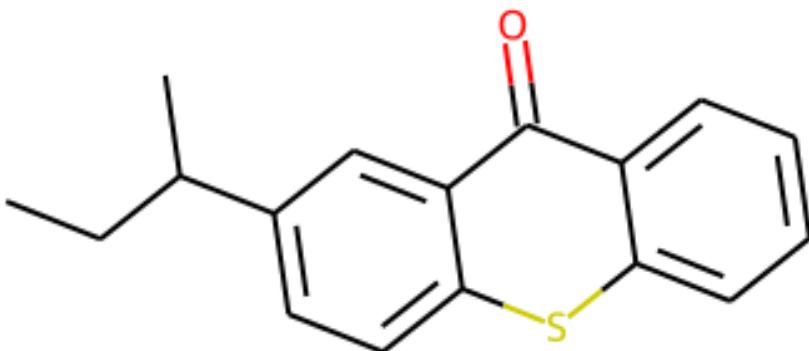
prob: 0.74



No.322

SMILES: CCC(C)c1ccc2sc3cccc3c(=O)c2c1

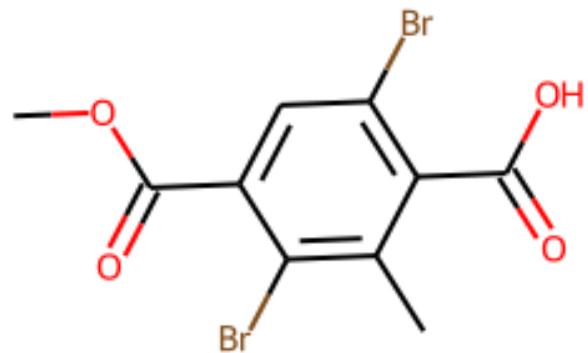
prob: 0.74



No.323

SMILES: COC(=O)c1cc(Br)c(C(=O)O)c(C)c1Br

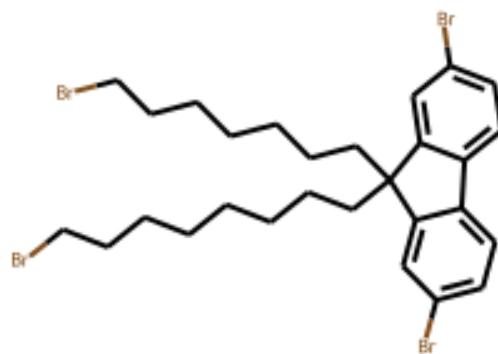
prob: 0.74



No.324

SMILES: BrCCCCCCCCC1(CCCCCCBr)c2cc(Br)ccc2-c2ccc(Br)cc21

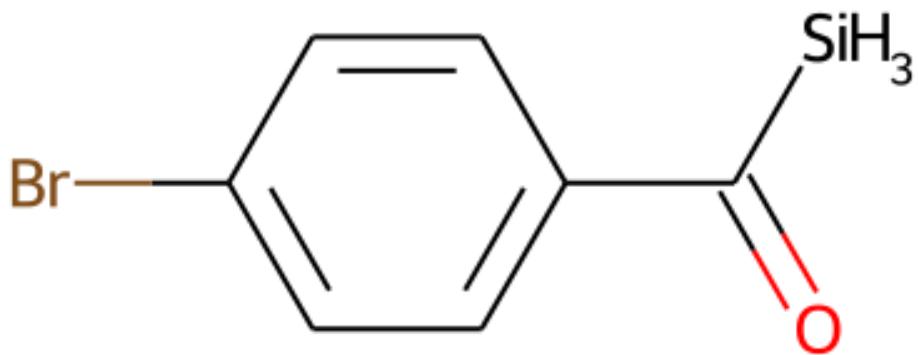
prob: 0.74



No.325

SMILES: O=C([SiH3])c1ccc(Br)cc1

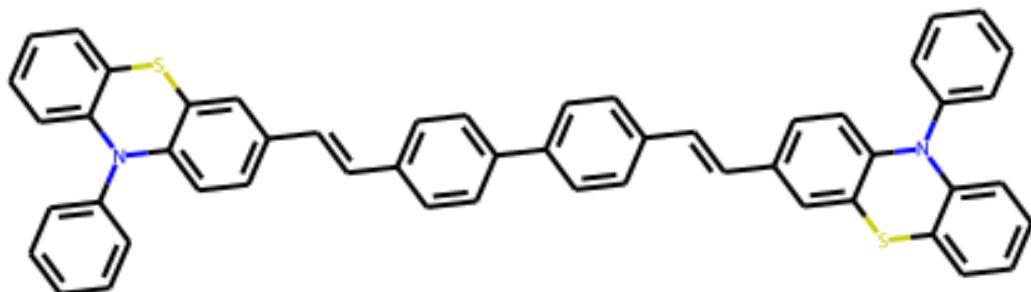
prob: 0.74



No.326

SMILES: C(=C/c1ccc2c(c1)Sc1ccccc1N2c1ccccc1)\c1ccc(-c2ccc(/C=C/c3ccc4c(c3)Sc3ccc4c3cccc3)cc2)cc1

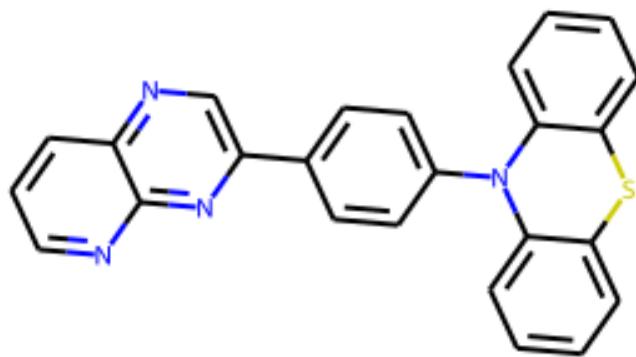
prob: 0.74



No.327

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2cnc3cccn3n2)cc1

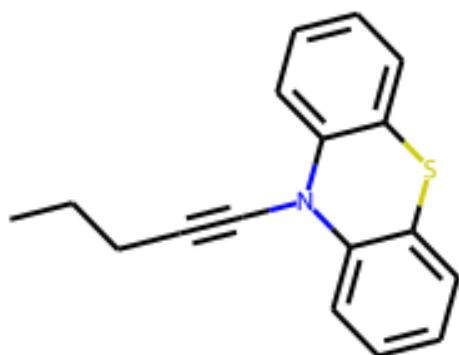
prob: 0.74



No.328

SMILES: CCCC#CN1c2ccccc2Sc2ccccc21

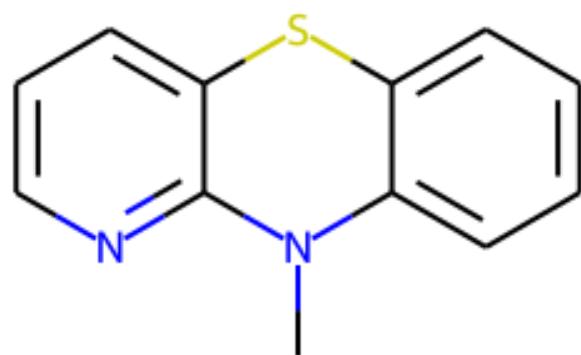
prob: 0.74



No.329

SMILES: CN1c2ccccc2Sc2cccnc21

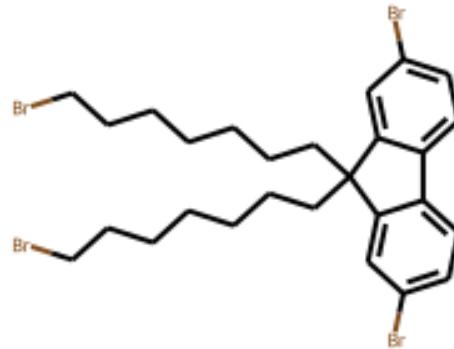
prob: 0.74



No.330

SMILES: BrCCCCCCCC1(CCCCCCBr)c2cc(Br)ccc2-c2ccc(Br)cc21

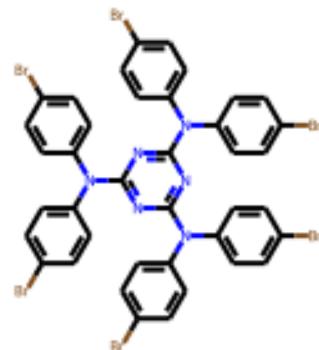
prob: 0.74



No.331

SMILES: Brc1ccc(N(c2ccc(Br)cc2)c2nc(N(c3ccc(Br)cc3)c3ccc(Br)cc3)nc(N(c3ccc(Br)cc3)c3ccc(Br)cc3)n2)cc1

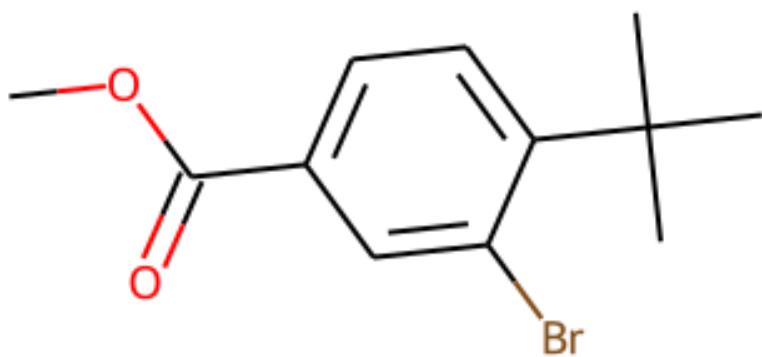
prob: 0.74



No.332

SMILES: COC(=O)c1ccc(C(C)(C)C)c(Br)c1

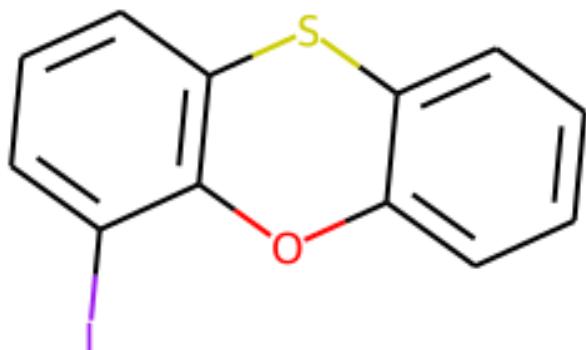
prob: 0.74



No.333

SMILES: Ic1ccccc2c10c1ccccc1S2

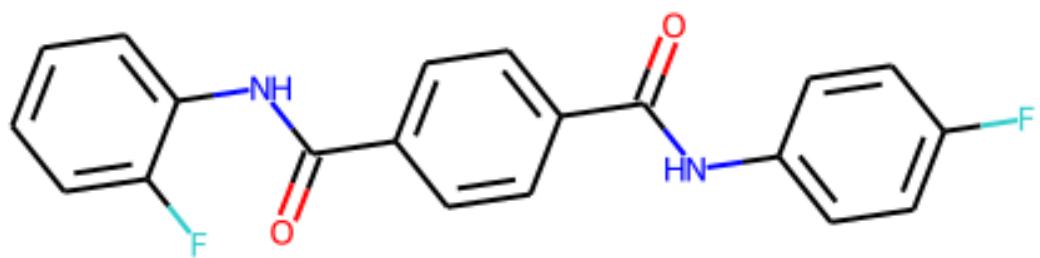
prob: 0.74



No.334

SMILES: O=C(Nc1ccc(F)cc1)c1ccc(C(=O)Nc2ccccc2F)cc1

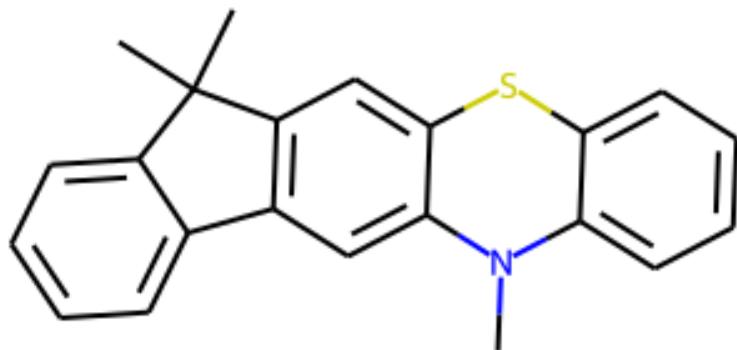
prob: 0.74



No.335

SMILES: CN1c2ccccc2Sc2cc3c(cc21)-c1ccccc1C3(C)C

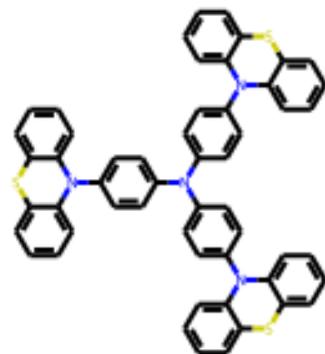
prob: 0.74



No.336

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(N(c2ccc(N3c4ccccc4Sc4ccccc43)cc2)c2ccc(N3c4cccc4Sc4ccccc43)cc2)cc1

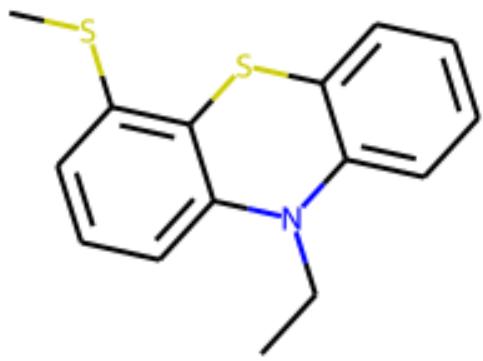
prob: 0.74



No.337

SMILES: CCN1c2ccccc2Sc2c(SC)cccc21

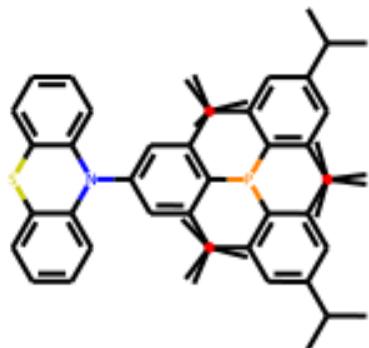
prob: 0.74



No.338

SMILES: CC(C)c1cc(C(C)C)c(P(c2c(C(C)C)cc(C(C)C)cc2C(C)C)c2c(C(C)C)cc(N3c4cccc4S)c4cccc43)cc2C(C)C)c(C(C)C)c1

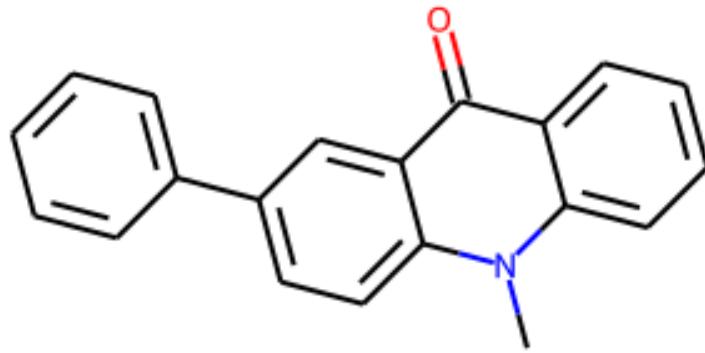
prob: 0.74



No.339

SMILES: Cn1c2ccccc2c(=O)c2cc(-c3ccccc3)ccc21

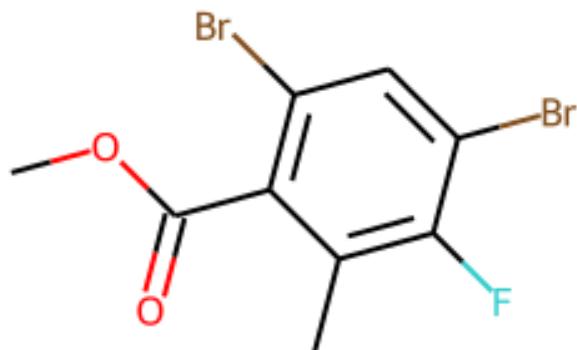
prob: 0.74



No.340

SMILES: COC(=O)c1c(Br)cc(Br)c(F)c1C

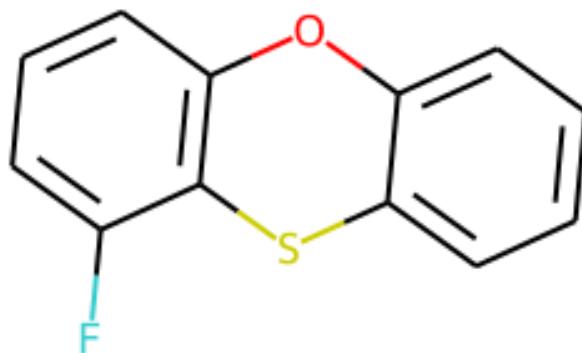
prob: 0.74



No.341

SMILES: Fc1cccc2c1Sc1ccccc102

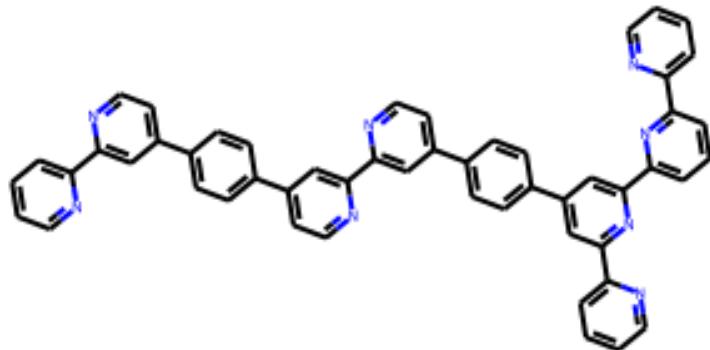
prob: 0.74



No.342

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccnc(-c5cc(-c6ccc(-c7cc(-c8ccccn8)nc(-c8cccc(-c9cccn9)n8)c7)cc6)ccn5)c4)cc3)ccn2)nc1

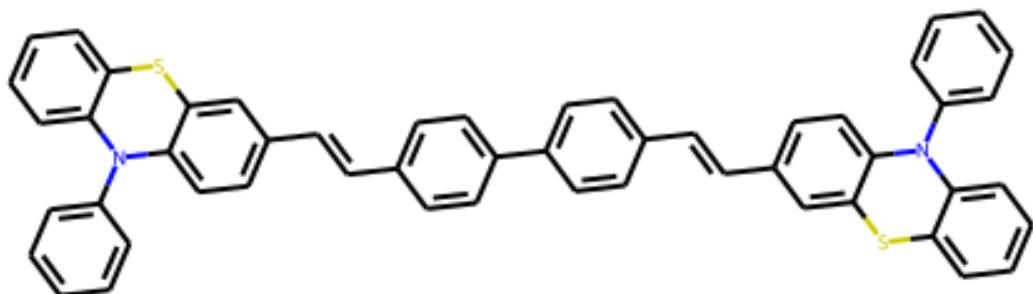
prob: 0.74



No.343

SMILES: C(=Cc1ccc2c(c1)Sc1cccc1N2c1cccc1)c1ccc(-c2ccc(C=Cc3ccc4c(c3)Sc3cccc3N4c3cccc3)cc2)cc1

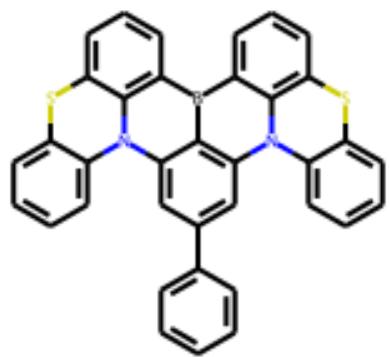
prob: 0.74



No.344

SMILES: c1ccc(-c2cc3c4c(c2)N2c5cccc5Sc5cccc(c52)B4c2cccc4c2N3c2cccc2S4)cc1

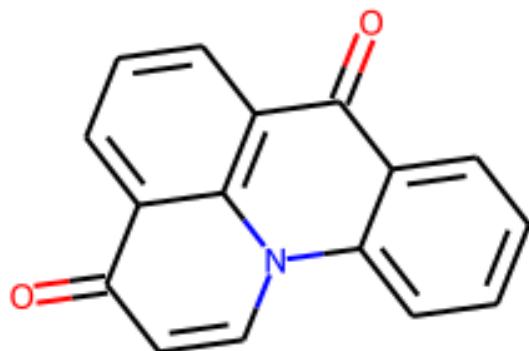
prob: 0.74



No.345

SMILES: O=c1ccn2c3cccc3c(=O)c3cccc1c32

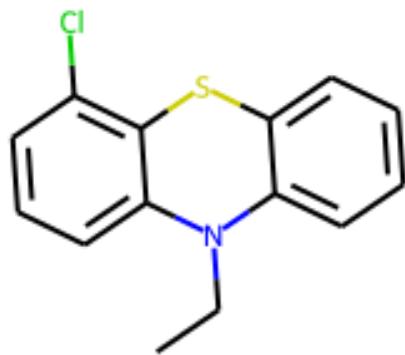
prob: 0.74



No.346

SMILES: CCN1c2ccccc2Sc2c(Cl)cccc21

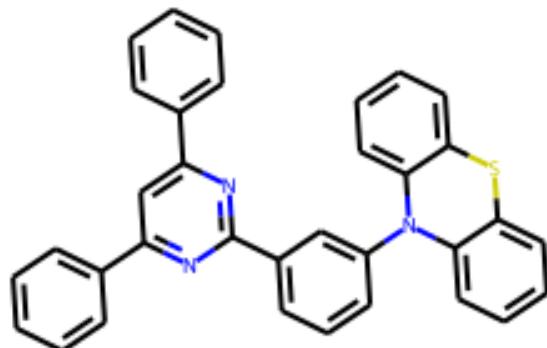
prob: 0.74



No.347

SMILES: c1ccc(-c2cc(-c3cccc3)nc(-c3cccc(N4c5cccc5Sc5cccc54)c3)n2)cc1

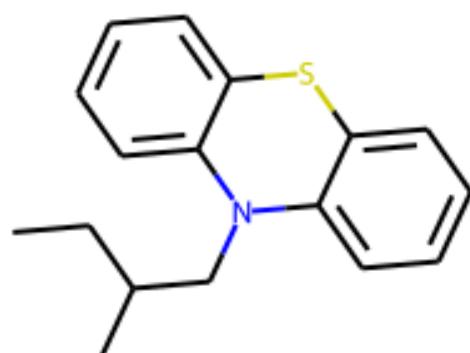
prob: 0.74



No.348

SMILES: CCC(C)CN1c2cccc2Sc2cccc21

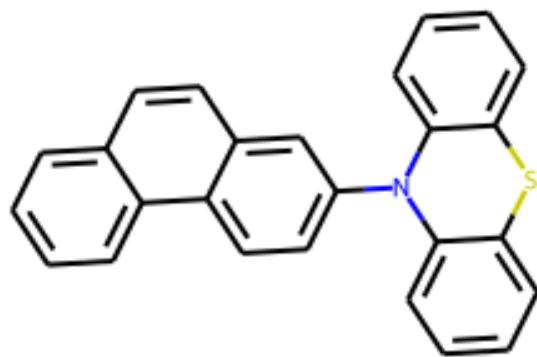
prob: 0.74



No.349

SMILES: c1ccc2c(c1)Sc1cccc1N2c1ccc2c(ccc3cccc32)c1

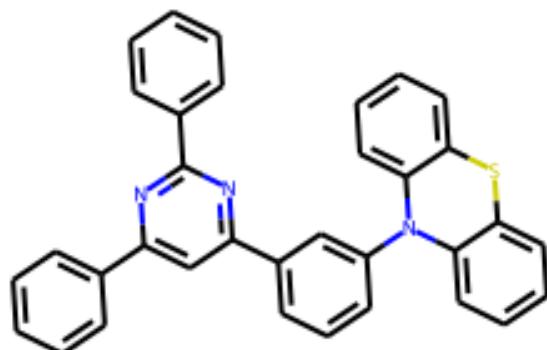
prob: 0.74



No.350

SMILES: c1ccc(-c2cc(-c3cccc(N4c5ccccc5Sc5ccccc54)c3)nc(-c3ccccc3)n2)cc1

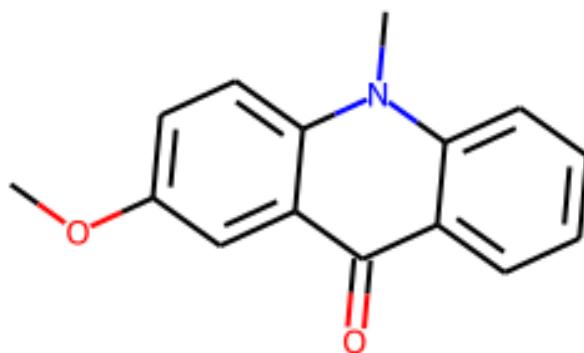
prob: 0.74



No.351

SMILES: C0c1ccc2c(c1)c(=O)c1ccccc1n2C

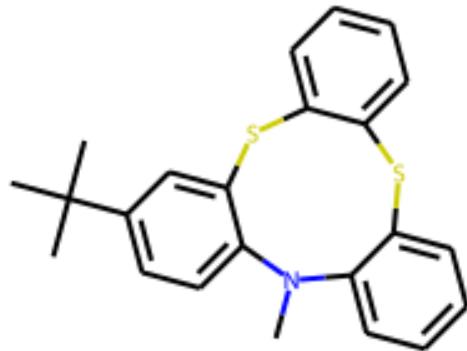
prob: 0.74



No.352

SMILES: CN1c2ccccc2Sc2ccccc2Sc2cc(C(C)(C)C)ccc21

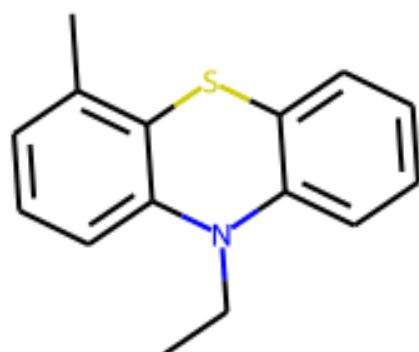
prob: 0.74



No.353

SMILES: CCN1c2ccccc2Sc2c(C)cccc21

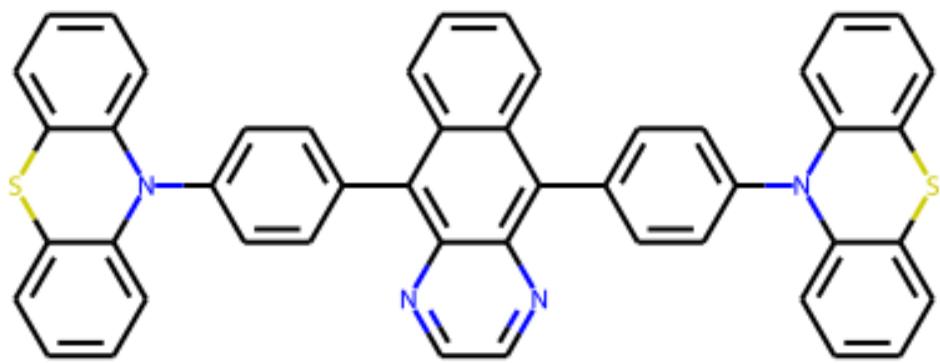
prob: 0.74



No.354

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2c3ccccc3c(-c3ccc(N4c5ccccc5Sc5ccccc54)cc3)c3nccnc23)cc1

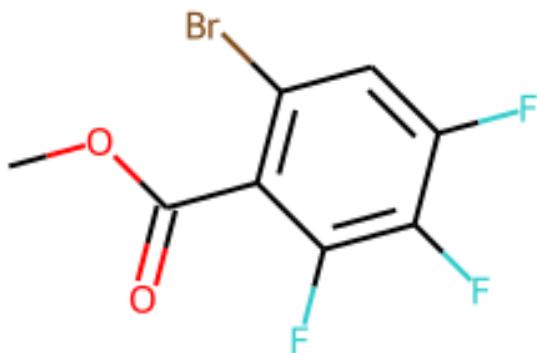
prob: 0.74



No.355

SMILES: COC(=O)c1c(Br)cc(F)c(F)c1F

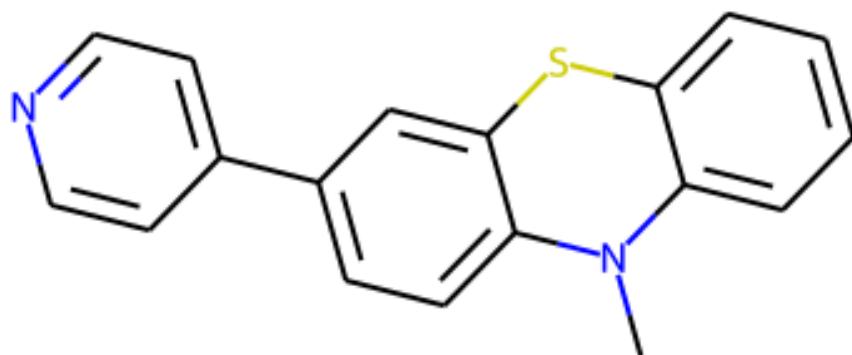
prob: 0.74



No.356

SMILES: CN1c2cccc2Sc2cc(-c3ccncc3)ccc21

prob: 0.74

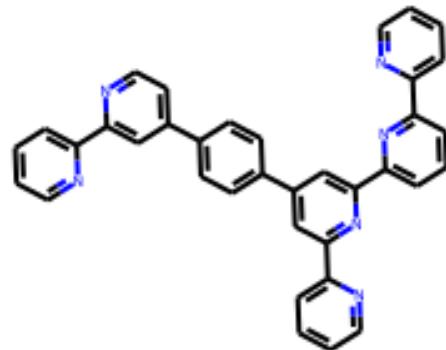


No.357

SMILES:

c1ccc(-c2cc(-c3ccc(-c4cc(-c5ccccn5)nc(-c5cccc(-c6ccccc6)n5)c4)cc3)ccn2)nc1

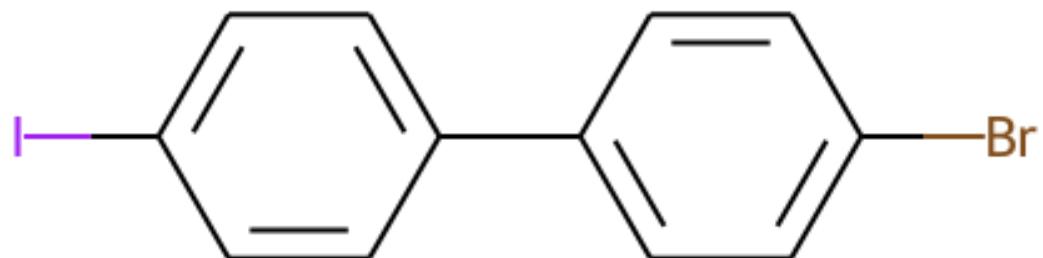
prob: 0.74



No.358

SMILES: Brc1ccc(-c2ccc(I)cc2)cc1

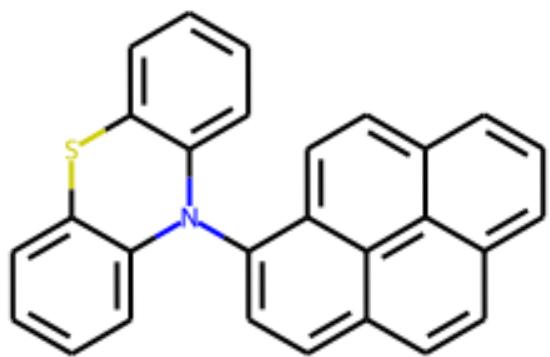
prob: 0.74



No.359

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2ccc3cccc4ccc1c2c34

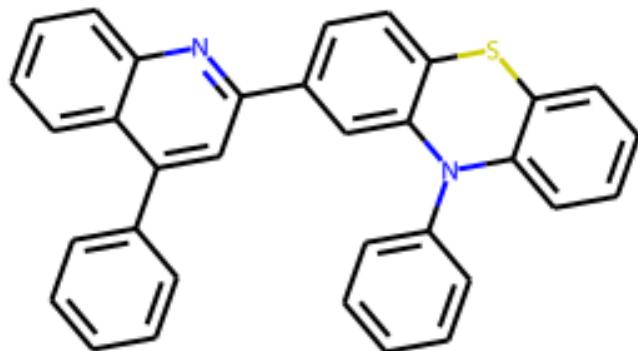
prob: 0.74



No.360

SMILES: c1ccc(-c2cc(-c3ccc4c(c3)N(c3cccc3)c3ccccc3S4)nc3cccc23)cc1

prob: 0.74



No.361

SMILES: Brc1ccc(-c2ccc(-c3ccc(I)cc3)cc2)cc1

prob: 0.74



No.362

SMILES: Cc1cc(N2c3cccc3Sc3cccc32)c(N2c3cccc3Sc3cccc32)cc1C

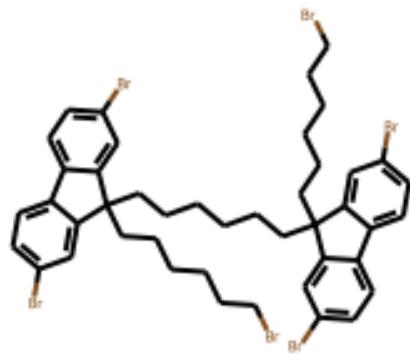
prob: 0.74



No.363

SMILES: BrCCCCCCC1(CCCCCC2(CCBr)cc3cc(Br)ccc3-c3ccc(Br)cc32)c2cc(Br)ccc2-c2cc(Br)cc21

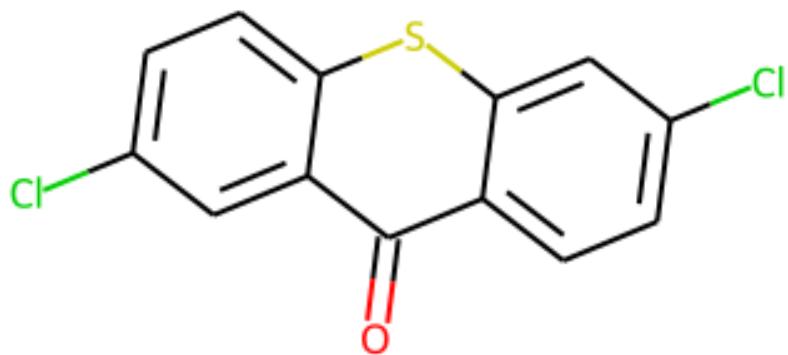
prob: 0.74



No.364

SMILES: O=c1c2ccc(Cl)cc2sc2ccc(Cl)cc12

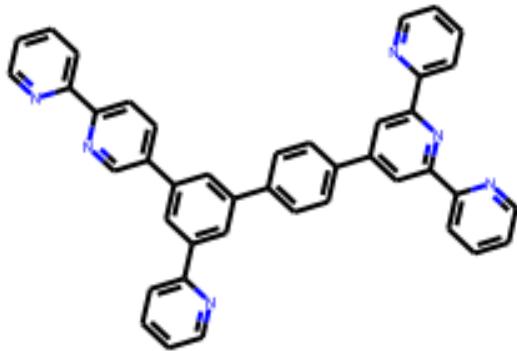
prob: 0.74



No. 365

SMILES: c1ccc(-c2cc(-c3ccc(-c4cc(-c5cccn5)nc(-c5cccn5)c4)cc3)cc(-c3ccc(-c4ccccn4)nc3)c2)nc1

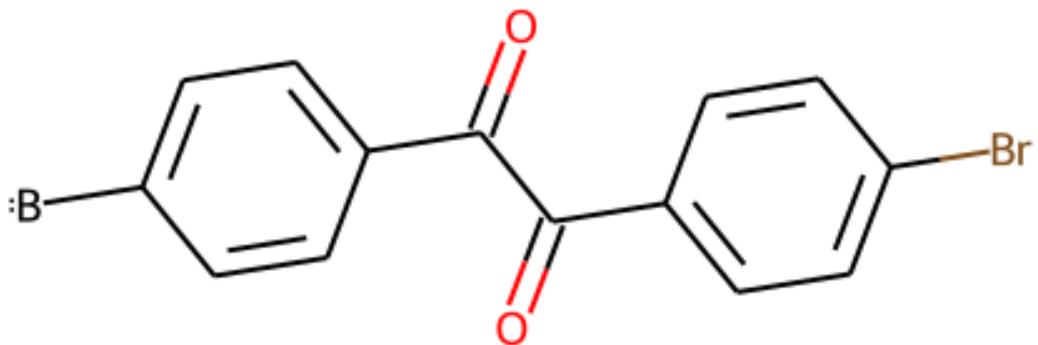
prob: 0.74



No. 366

SMILES: [B]c1ccc(C(=O)C(=O)c2ccc(Br)cc2)cc1

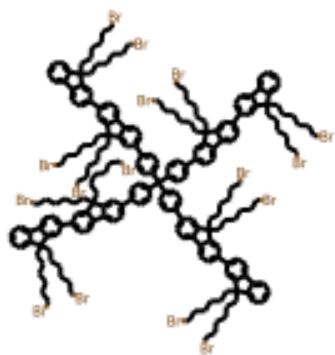
prob: 0.74



No. 367

SMILES: BrCCCCCCC1(CCCCCCBr)c2ccccc2-c2ccc(-c3ccc4c(c3)C(CCCCCCBr)(CCCCCCBr)c3cc(-c5ccc(C(c6ccc(-c7ccc8c(c7)C(CCCCCCBr)(CCCCCCBr)c7cc(-c9ccc%10c(c9)C(CCCCCCBr)(CCCCCCBr)c9cccc9-%10)ccc7-8)cc6)(c6ccc(-c7ccc8c(c7)C(CCCCCCBr)(CCCCCCBr)c7cc(-c9ccc%10c(c9)C(CCCCCCBr)(CCCCCCBr)c9cccc9-%10)ccc7-8)cc6)c6ccc(-c7ccc8c(c7)C(CCCBr)(CCCCCCBr)c7cc(-c9ccc%10c(c9)C(CCCCCCBr)(CCCCCCBr)c9cccc9-%10)ccc7-8)cc6)cc5)ccc3-4)cc21

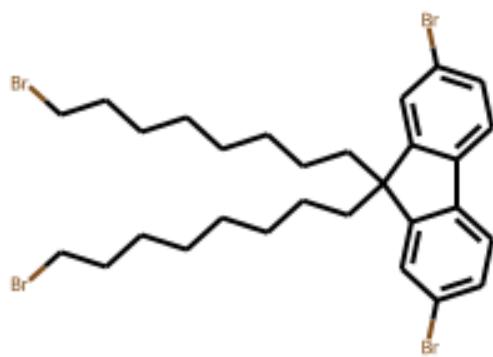
prob: 0.74



No. 368

SMILES: BrCCCCCCCCC1(CCCCCCCCBr)c2cc(Br)ccc2-c2ccc(Br)cc21

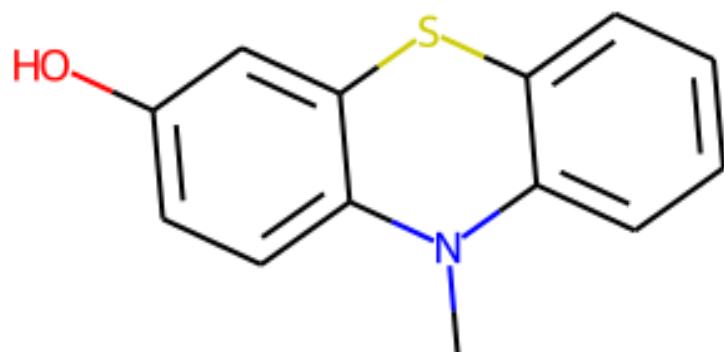
prob: 0.74



No.369

SMILES: CN1c2ccccc2Sc2cc(0)ccc21

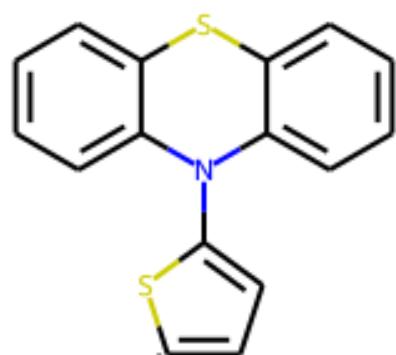
prob: 0.73



No.370

SMILES: [c]1ccc(N2c3ccccc3Sc3ccccc32)s1

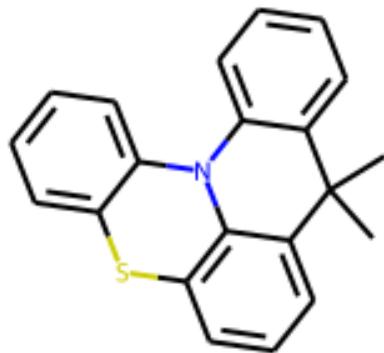
prob: 0.73



No.371

SMILES: CC1(C)c2ccccc2N2c3ccccc3Sc3cccc1c32

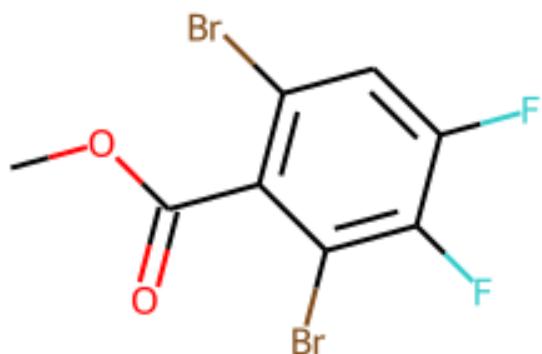
prob: 0.73



No.372

SMILES: COC(=O)c1c(Br)cc(F)c(F)c1Br

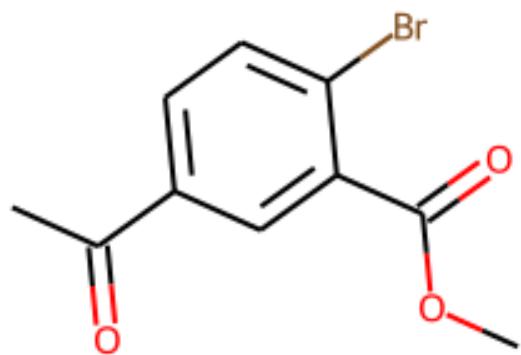
prob: 0.73



No.373

SMILES: COC(=O)c1cc(C(C)=O)ccc1Br

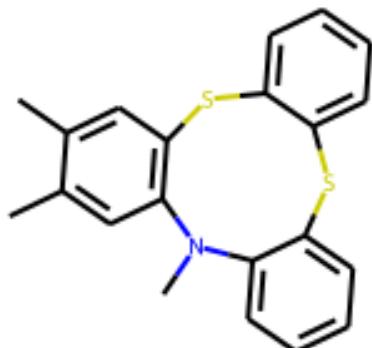
prob: 0.73



No.374

SMILES: Cc1cc2c(cc1C)N(C)c1ccccc1Sc1ccccc1S2

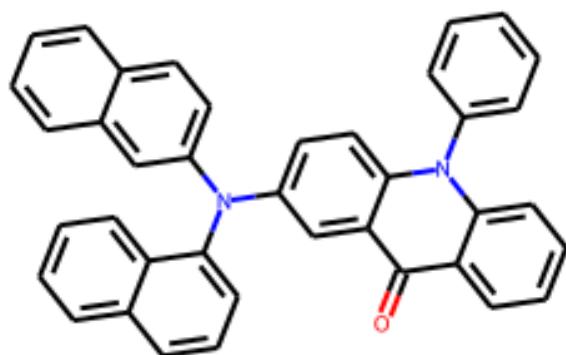
prob: 0.73



No.375

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2ccc(N(c3ccc4ccccc4c3)c3cccc4ccccc34)cc12

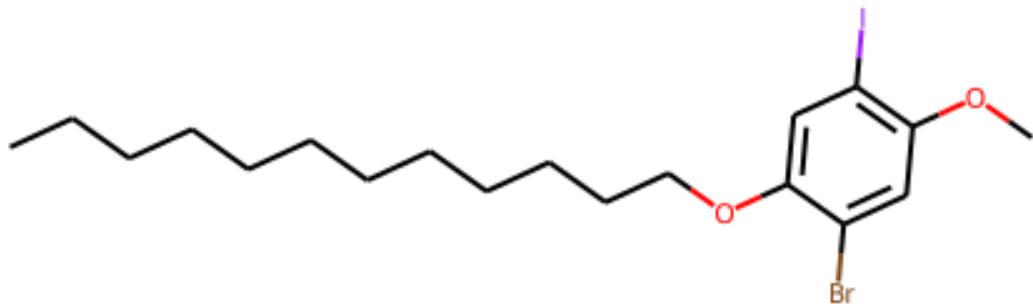
prob: 0.73



No.376

SMILES: CCCCCCCCCCCCCOc1cc(I)c(OC)cc1Br

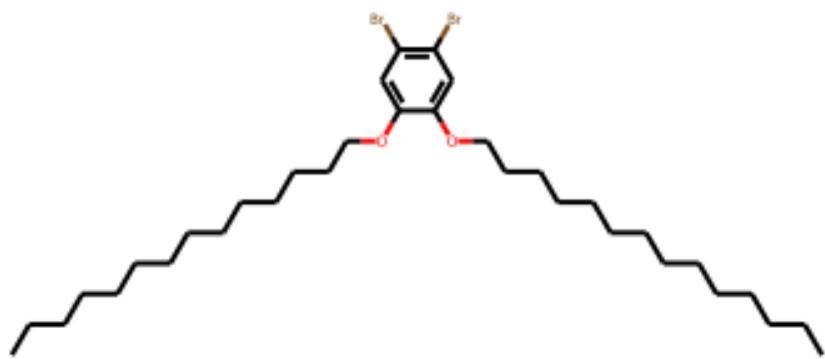
prob: 0.73



No.377

SMILES: CCCCCCCCCCCCCCOC1CC(Br)C(Br)CC1OCCCCCCCCCCCC

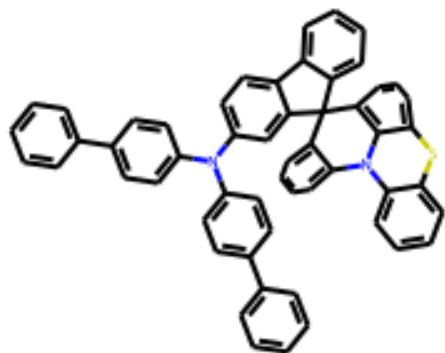
prob: 0.73



No.378

SMILES: c1ccc(-c2ccc(N(c3ccc(-c4ccccc4)cc3)c3cccc4c(c3)c3(c5ccccc5-4)c4ccccc4N4c5cccc5Sc5ccccc3c54)cc2)cc1

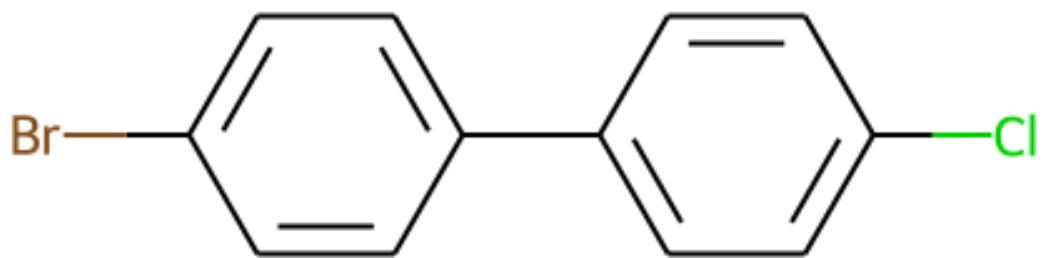
prob: 0.73



No.379

SMILES: Clc1ccc(-c2ccc(Br)cc2)cc1

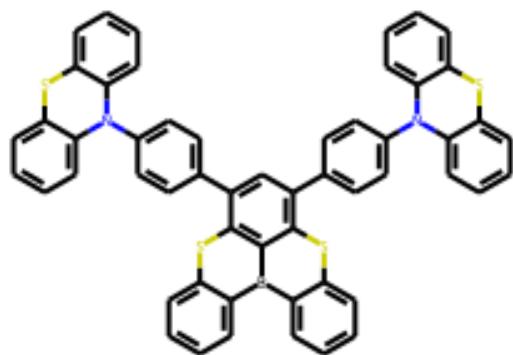
prob: 0.73



No.380

SMILES: c1ccc2c(c1)Sc1c(-c3ccc(N4c5cccc5Sc5cccc54)cc3)cc(-c3ccc(N4c5cccc5Sc5cccc54)cc3)c3c1B2c1cccc1S3

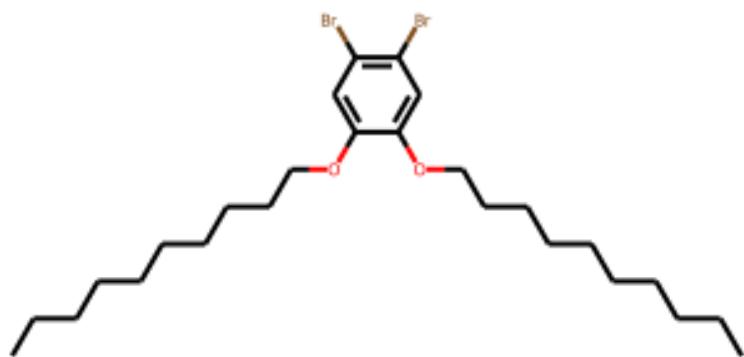
prob: 0.73



No.381

SMILES: CCCCCCCCCC0c1cc(Br)c(Br)cc10CCCCCCCC

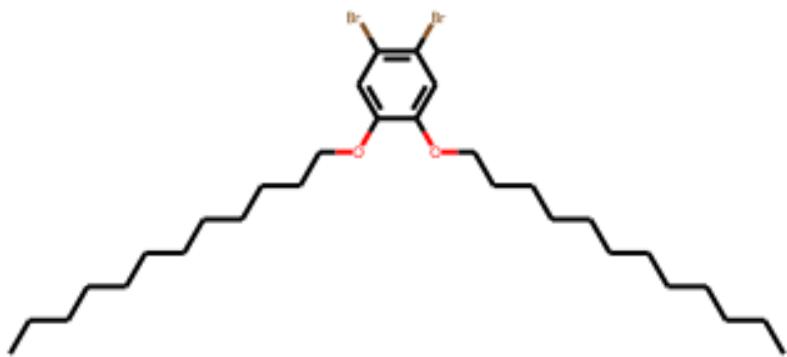
prob: 0.73



No.382

SMILES: CCCCCCCCCCCC0c1cc(Br)c(Br)cc10CCCCCCCC

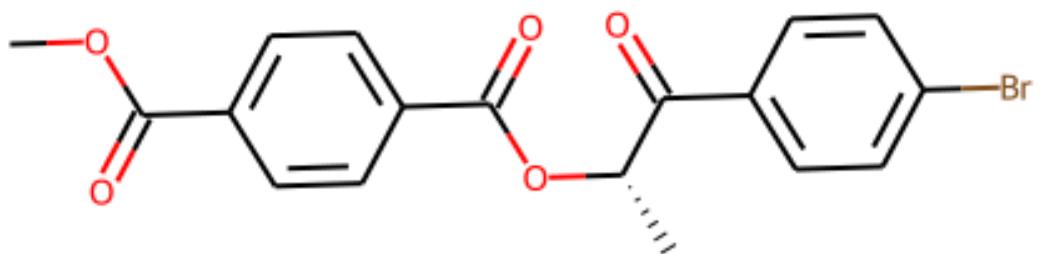
prob: 0.73



No.383

SMILES: COC(=O)c1ccc(C(=O)O[C@H](C)C(=O)c2ccc(Br)cc2)cc1

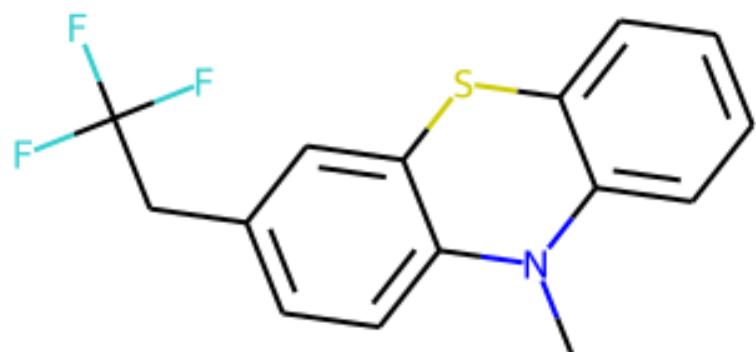
prob: 0.73



No.384

SMILES: CN1c2cccc2Sc2cc(CC(F)(F)F)ccc21

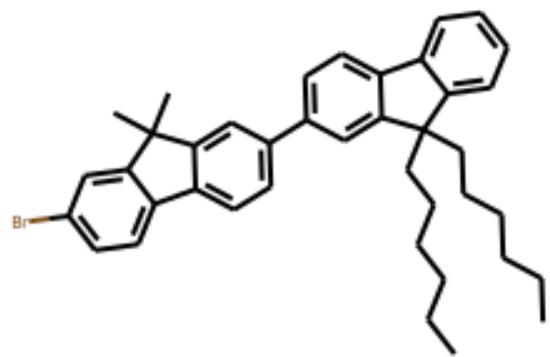
prob: 0.73



No.385

SMILES: CCCCCC1(CCCCC) c2cccc2-c2ccc(-c3ccc4c(c3)C(C)(C)c3cc(Br)ccc3-4)cc21

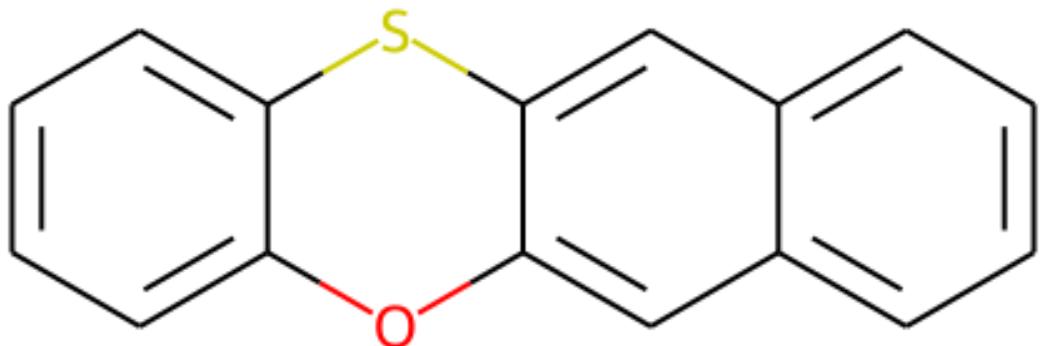
prob: 0.73



No.386

SMILES: c1ccc2c(c1)Oc1cc3cccc3cc1S2

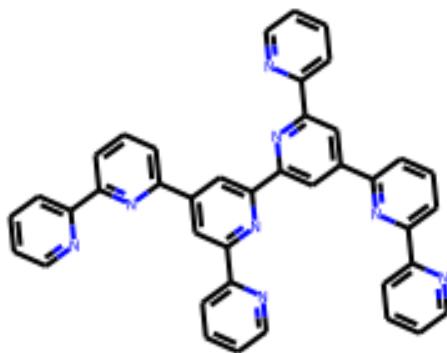
prob: 0.73



No.387

SMILES: c1ccc(-c2cccc(-c3cc(-c4cccn4)nc(-c4cc(-c5cccc(-c6cccn6)n5)cc(-c5cccn5)n4)c3)n2)nc1

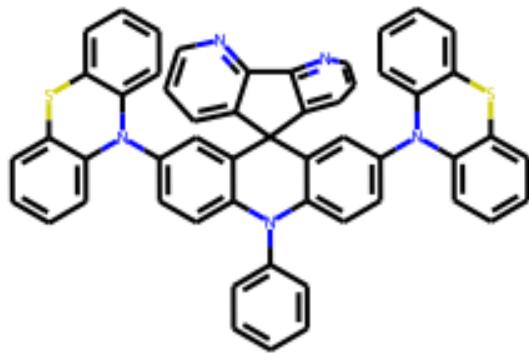
prob: 0.73



No.388

SMILES: c1ccc(N2c3ccc(N4c5cccc5Sc5ccccc54)cc3C3(c4cc(N5c6cccc6Sc6ccccc65)ccc42)c2cccnc2-c2ncccc23)cc1

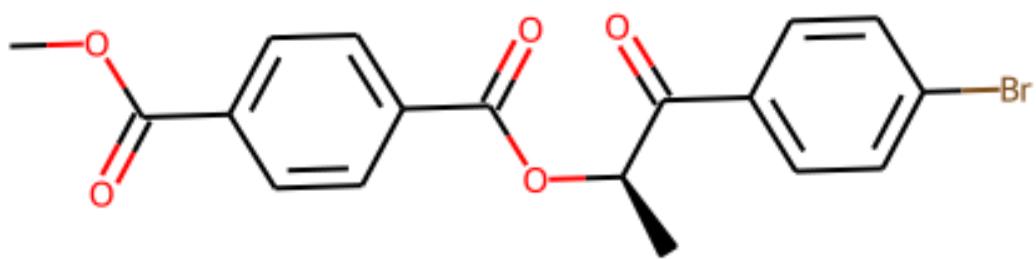
prob: 0.73



No.389

SMILES: COC(=O)c1ccc(C(=O)O[C@H](C)C(=O)c2ccc(Br)cc2)cc1

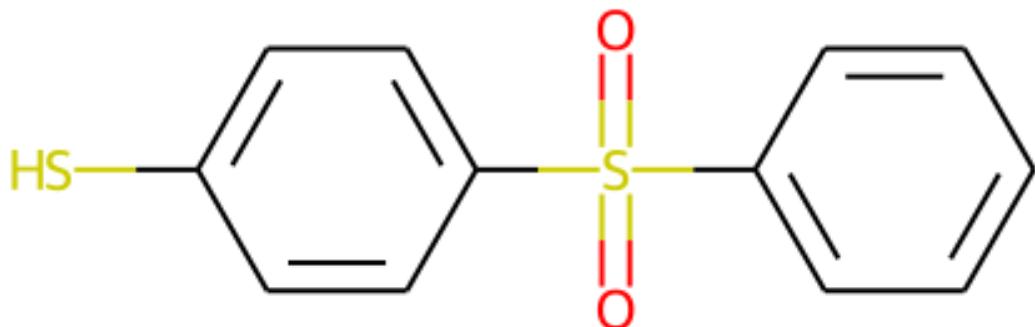
prob: 0.73



No.390

SMILES: O=S(=O)(c1ccccc1)c1ccc(S)cc1

prob: 0.73



No.391

SMILES: Fc1cncc(F)c1-c1cccc(C(F)(F)F)c1N1c2ccccc2Sc2ccccc21

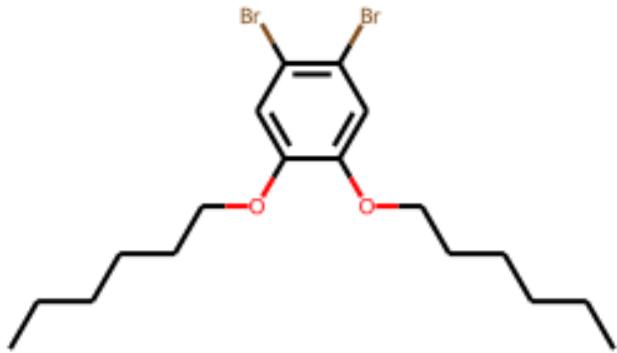
prob: 0.73



No.392

SMILES: CCCCCC0c1cc(Br)c(Br)cc1OCCCCCC

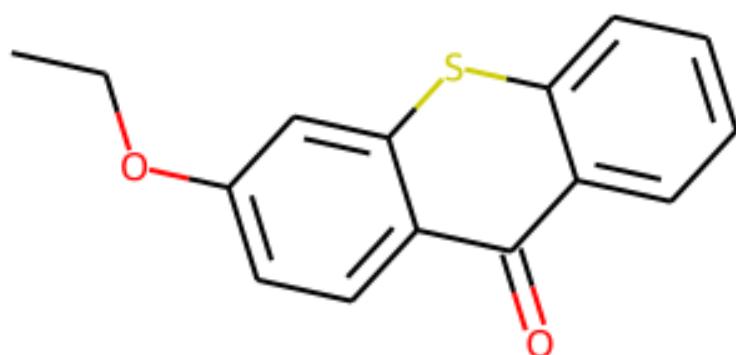
prob: 0.73



No.393

SMILES: CC0c1ccc2c(=O)c3ccccc3sc2c1

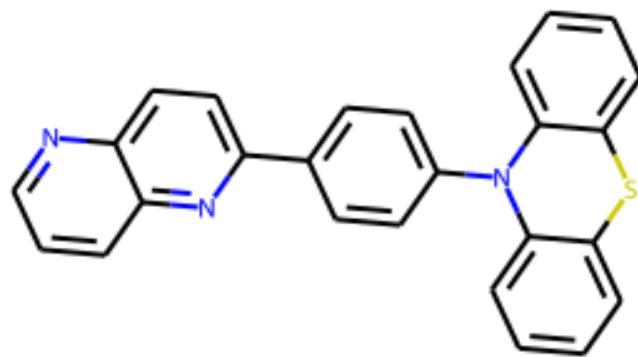
prob: 0.73



No.394

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2ccc3ncccc3n2)cc1

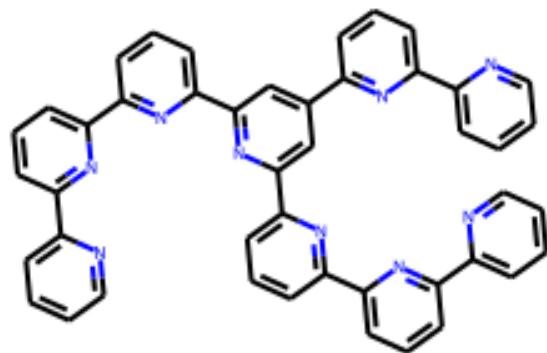
prob: 0.73



No.395

SMILES: c1ccc(-c2cccc(-c3cc(-c4cccc(-c5cccc(-c6cccn6)n5)n4)nc(-c4cccc(-c5cccc(-c6cccn6)n5)n4)c3)n2)nc1

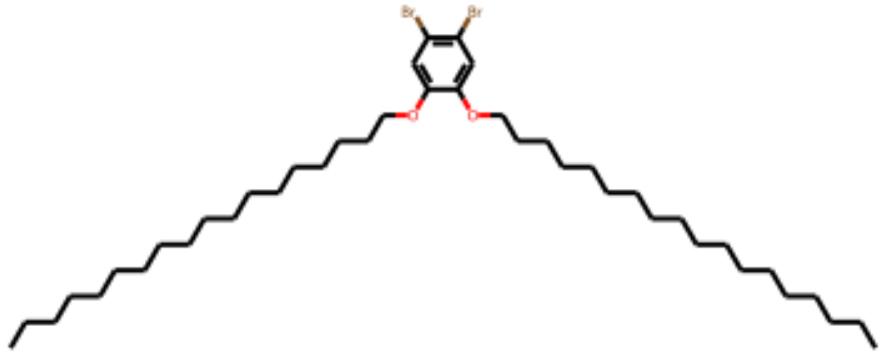
prob: 0.73



No.396

SMILES: CCCCCCCCCCCCCCCCCC0c1cc(Br)c(Br)cc10CCCCCCCCCCCCCCCCCCC

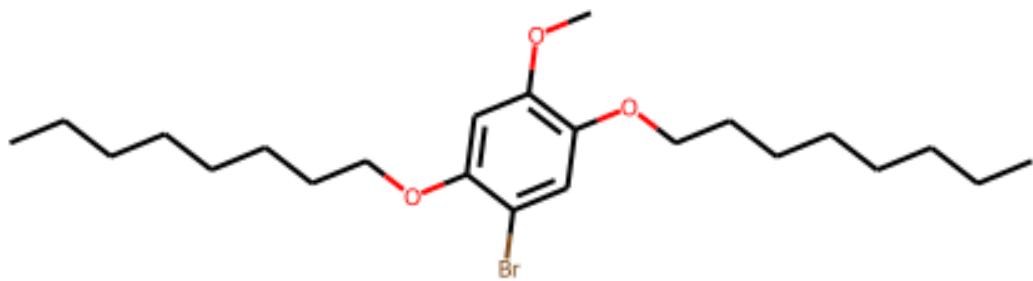
prob: 0.73



No.397

SMILES: CCCCCCCCOC1CC(OC)C(OCCCCCC)CC1Br

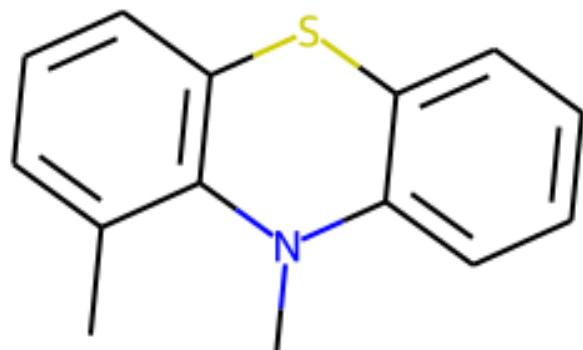
prob: 0.73



No.398

SMILES: Cc1ccccc2c1N(C)c1ccccc1S2

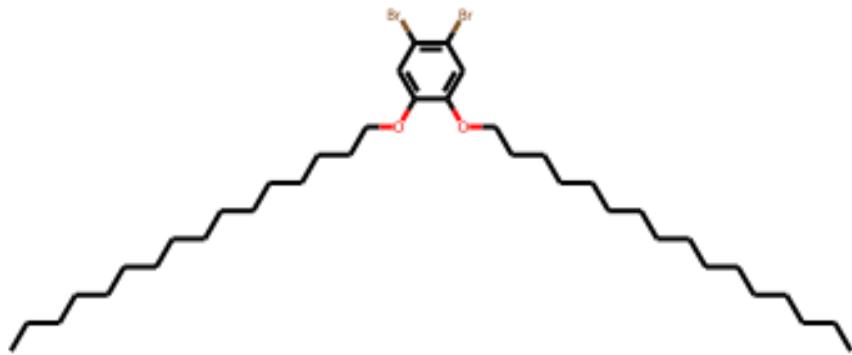
prob: 0.73



No.399

SMILES: CCCCCCCCCCCCCCCCC0c1cc(Br)c(Br)cc10CCCCCCCCCCCCCCCC

prob: 0.73

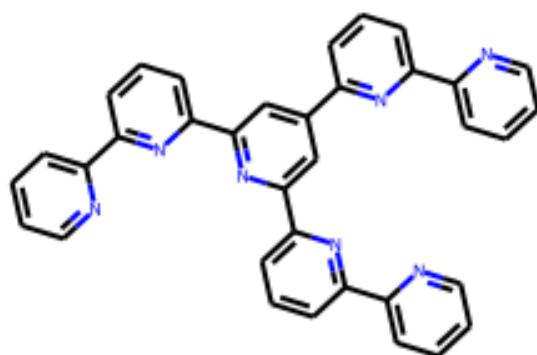


No.400

SMILES:

c1cccc(-c2cccc(-c3cc(-c4cccc(-c5cccn5)n4)nc(-c4cccc(-c5cccn5)n4)c3)n2)nc1

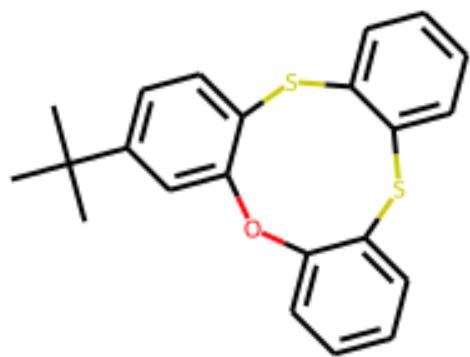
prob: 0.73



No.401

SMILES: CC(C)(C)c1ccc2c(c1)0c1ccccc1Sc1ccccc1S2

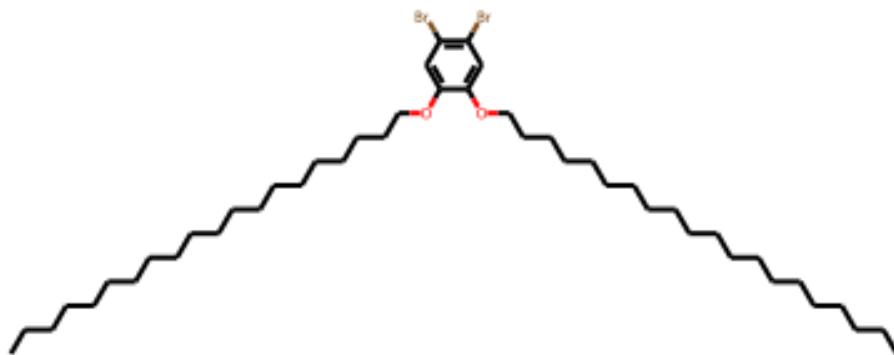
prob: 0.73



No.402

SMILES: CCCCCCCCCCCCCCCCCCCC0c1cc(Br)c(Br)cc10CCCCCCCCCCCCCCCCCCC

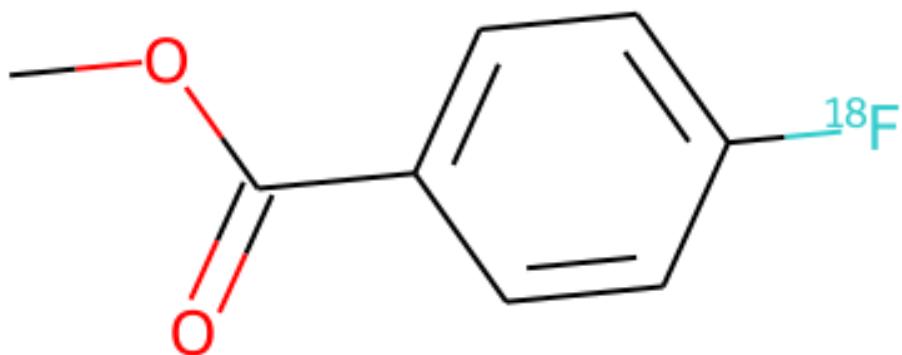
prob: 0.73



No.403

SMILES: COC(=O)c1ccc([18F])cc1

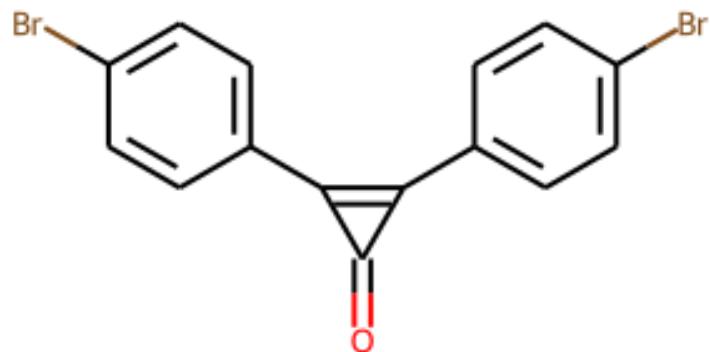
prob: 0.73



No.404

SMILES: O=c1c(-c2ccc(Br)cc2)c1-c1ccc(Br)cc1

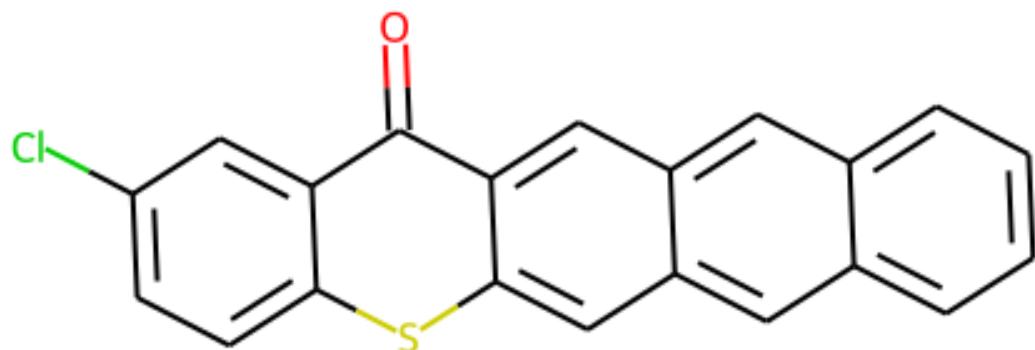
prob: 0.73



No.405

SMILES: O=c1c2cc(Cl)ccc2sc2cc3cc4cccc4cc3cc12

prob: 0.73

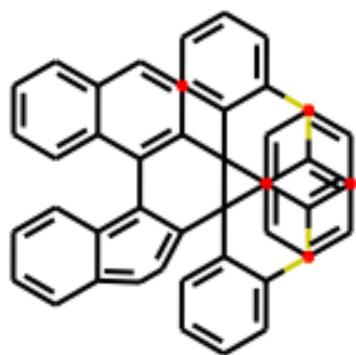


No.406

SMILES:

c1cccc2c(c1)Sc1ccccc1C21c2ccc3ccccc3c2-c2c(ccc3ccccc23)C12c1ccccc1Sc1ccccc12

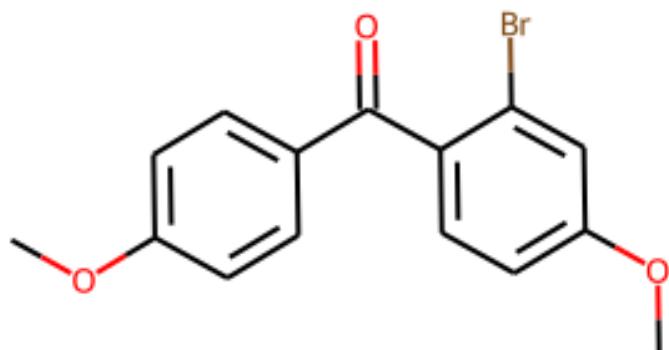
prob: 0.73



No.407

SMILES: C0c1ccc(C(=O)c2ccc(OC)cc2Br)cc1

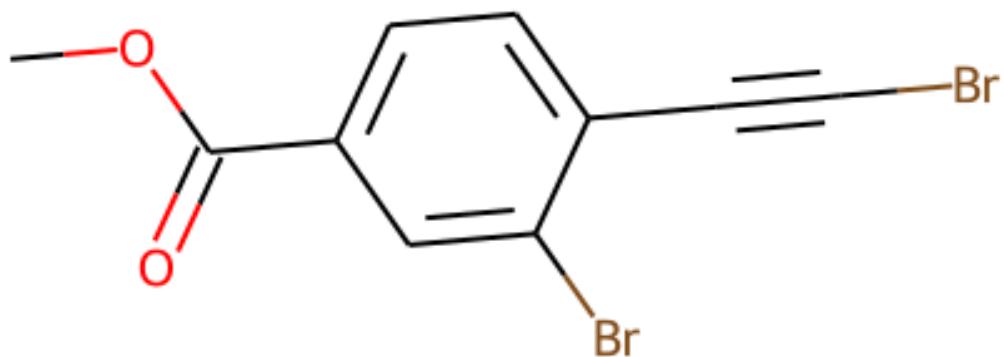
prob: 0.73



No.408

SMILES: COC(=O)c1ccc(C#CBr)c(Br)c1

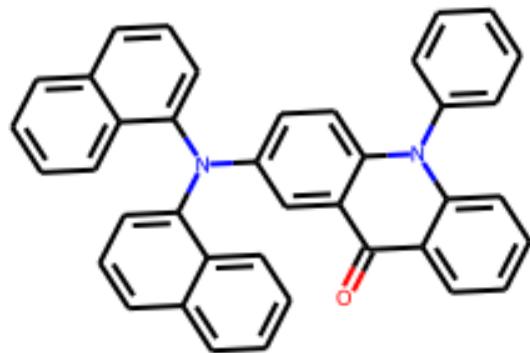
prob: 0.73



No.409

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2ccc(N(c3cccc4cccc34)c3cccc4cccc34)cc12

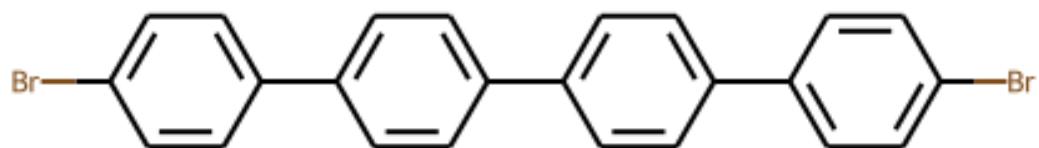
prob: 0.73



No.410

SMILES: Brc1ccc(-c2ccc(-c3ccc(-c4ccc(Br)cc4)cc3)cc2)cc1

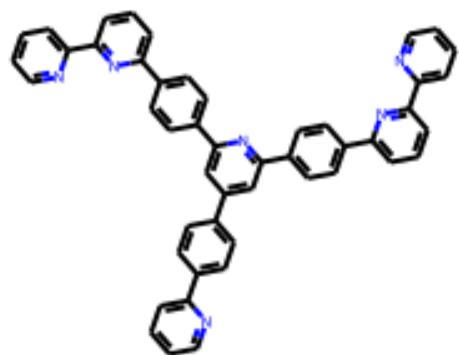
prob: 0.73



No.411

SMILES: c1ccc(-c2ccc(-c3cc(-c4ccc(-c5cccc(-c6cccn6)n5)cc4)nc(-c4ccc(-c5cccc(-c6cccn6)n5)cc4)c3)cc2)nc1

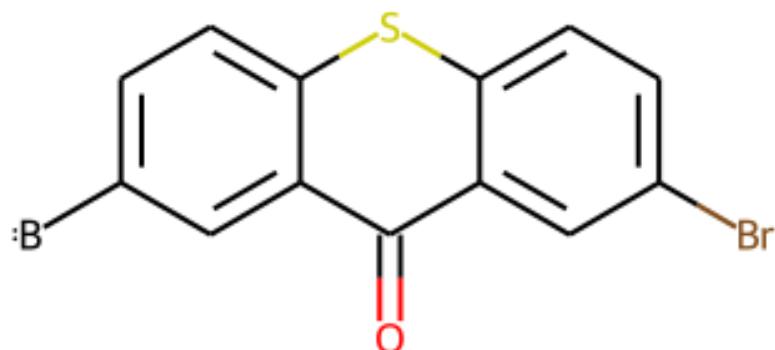
prob: 0.73



No.412

SMILES: [B]c1ccc2sc3cccc(Br)cc3c(=O)c2c1

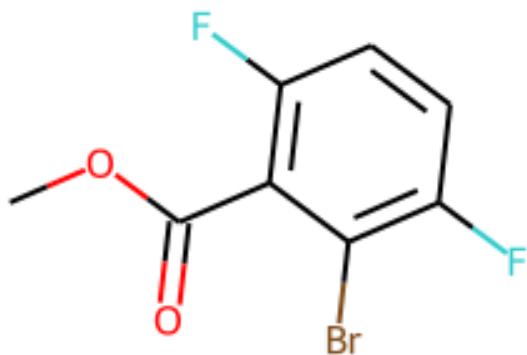
prob: 0.73



No.413

SMILES: COC(=O)c1c(F)ccc(F)c1Br

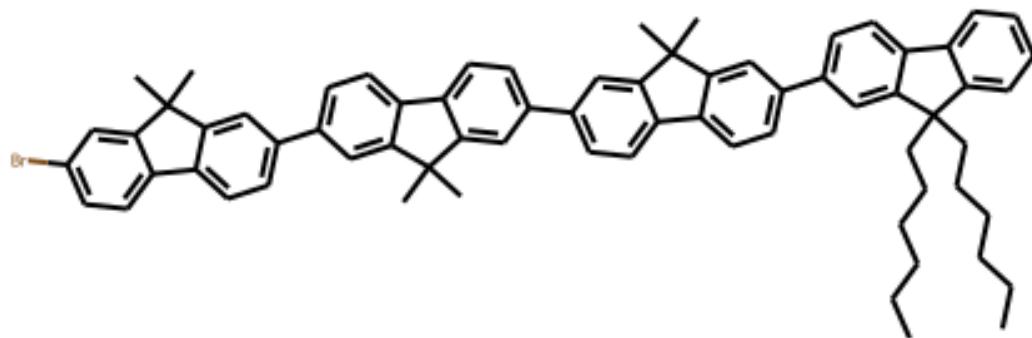
prob: 0.73



No.414

SMILES: CCCCCCC1(CCCCCC)c2cccc2-c2ccc(-c3ccc4c(c3)C(C)(C)c3cc(-c5ccc6c(c5)C(C)(C)c5cc(-c7ccc8c(c7)C(C)(C)c7cc(Br)ccc7-8)ccc5-6)ccc3-4)cc21

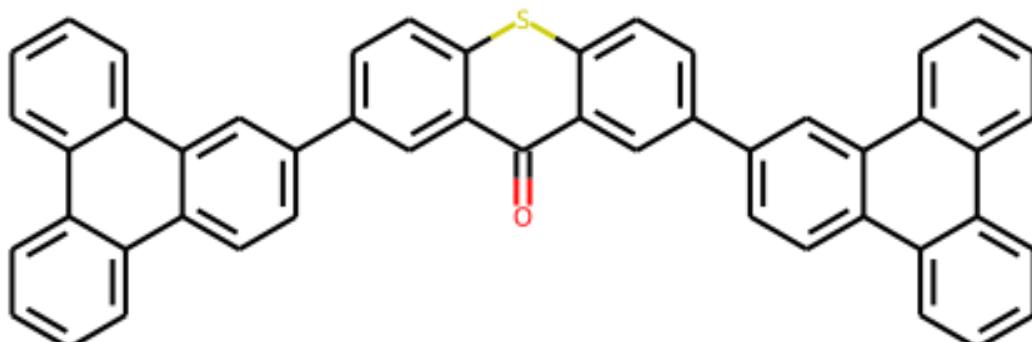
prob: 0.73



No.415

SMILES:

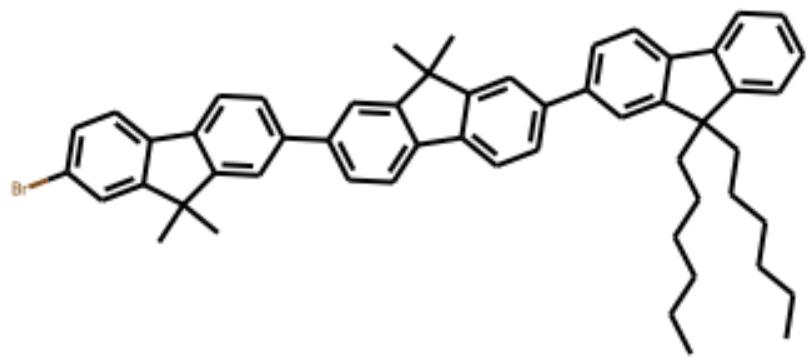
O=c1c2cc(-c3ccc4c5cccc5c5cccc5c4c3)ccc2sc2ccc(-c3ccc4c5cccc5c5cccc5c4c3)cc12
prob: 0.73



No.416

SMILES: CCCCCCC1(CCCCCC)c2cccc2-c2ccc(-c3ccc4c(c3)C(C)(C)c3cc(-c5ccc6c(c5)C(C)(C)c5cc(Br)ccc5-6)ccc3-4)cc21

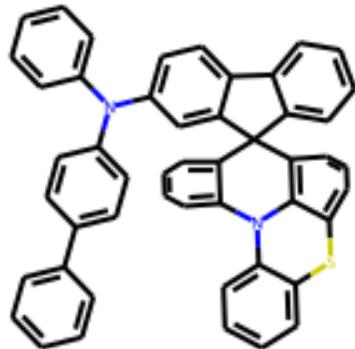
prob: 0.73



No. 417

SMILES: c1ccc(-c2ccc(N(c3ccccc3)c3ccc4c(c3)C3(c5ccccc5-4)c4ccccc4N4c5ccccc5Sc5cc cc3c54)cc2)cc1

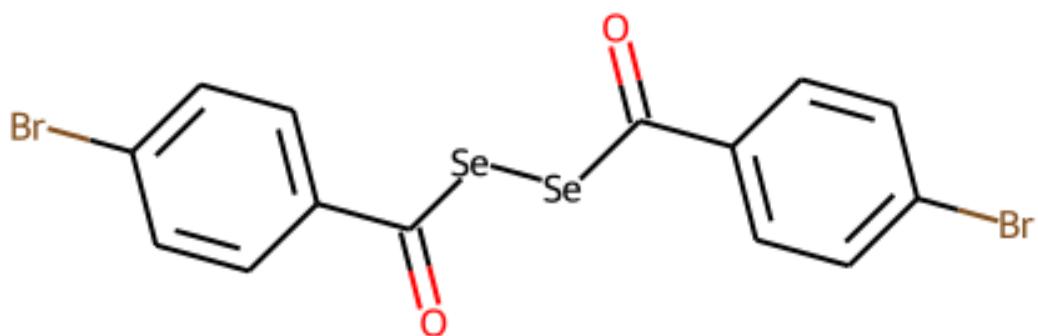
prob: 0.73



No. 418

SMILES: O=C([Se][Se]C(=O)c1ccc(Br)cc1)c1ccc(Br)cc1

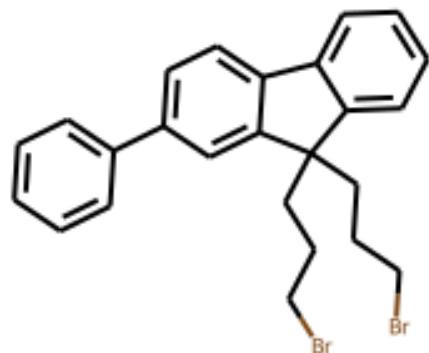
prob: 0.73



No.419

SMILES: BrCCCC1(CCCBr)c2ccccc2-c2ccc(-c3ccccc3)cc21

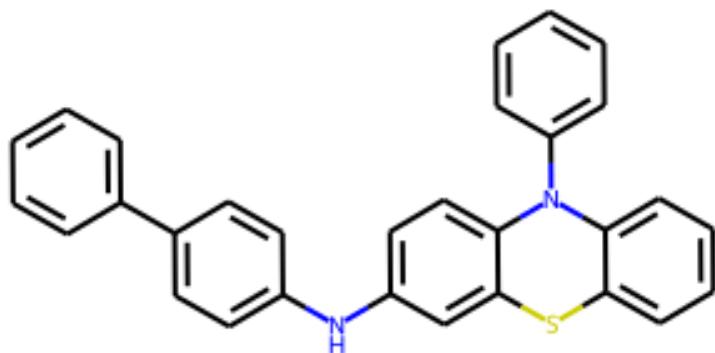
prob: 0.73



No.420

SMILES: c1ccc(-c2ccc(Nc3ccc4c(c3)Sc3ccccc3N4c3ccccc3)cc2)cc1

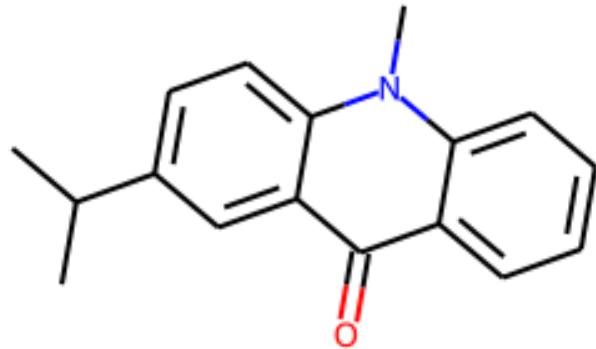
prob: 0.73



No. 421

SMILES: CC(C)c1ccc2c(c1)c(=O)c1cccc1n2C

prob: 0.73



No. 422

SMILES: Brcc1ccc(-c2ccc(-c3ccc(Br)cc3)cc2)cc1

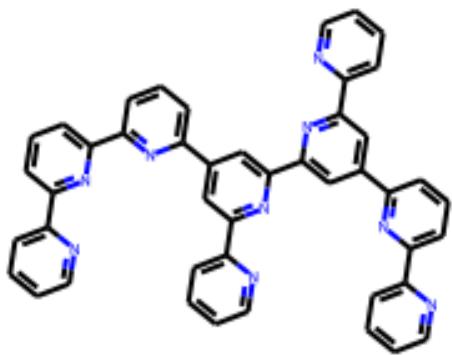
prob: 0.73



No. 423

SMILES: c1ccc(-c2cccc(-c3cc(-c4cccn4)nc(-c4cc(-c5cccc(-c6cccc(-c7cccn7)n6)n5)c(-c5cccn5)n4)c3)n2)nc1

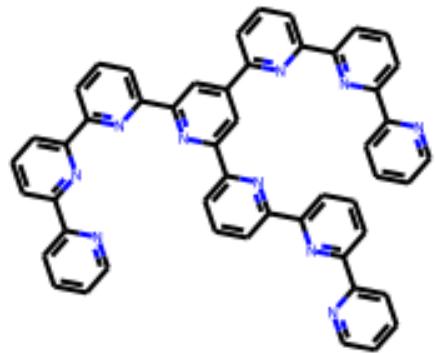
prob: 0.73



No.424

SMILES: c1ccc(-c2cccc(-c3cccc(-c4cc(-c5cccc(-c6cccc(-c7ccccc7)n6)n5)nc(-c5cccc(-c6cccc(-c7ccccc7)n6)n5)c4)n3)n2)nc1

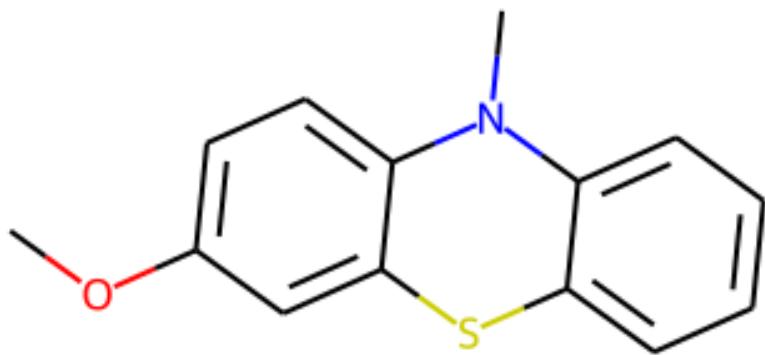
prob: 0.73



No.425

SMILES: C0c1ccc2c(c1)Sc1ccccc1N2C

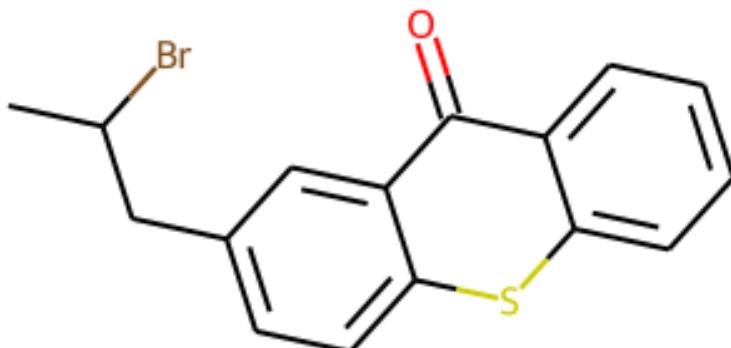
prob: 0.73



No.426

SMILES: CC(Br)Cc1ccc2sc3ccccc3c(=O)c2c1

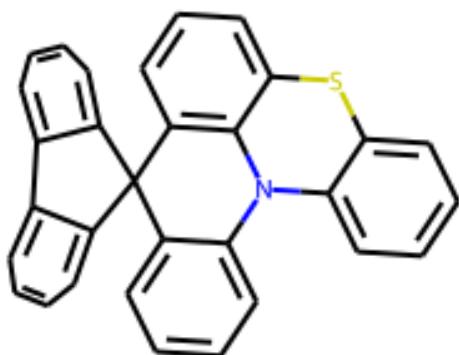
prob: 0.73



No.427

SMILES: c1ccc2c(c1)Sc1ccccc3c1N2c1ccccc1C31c2ccccc2-c2ccccc21

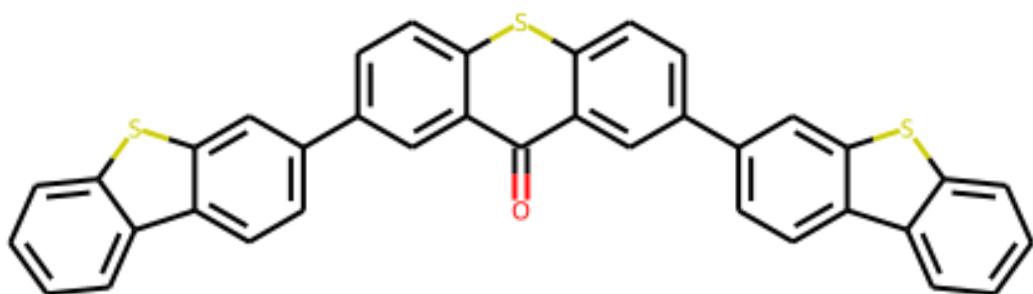
prob: 0.73



No.428

SMILES: O=c1c2cc(-c3ccc4c(c3)sc3cccc34)ccc2sc2ccc(-c3ccc4c(c3)sc3cccc34)cc12

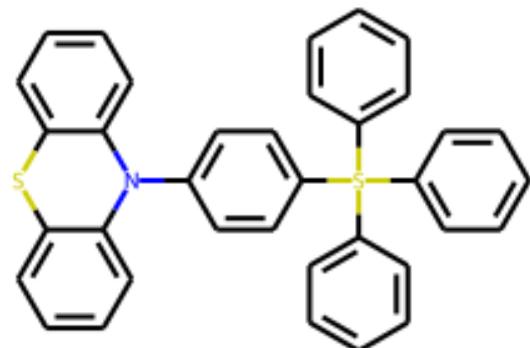
prob: 0.73



No.429

SMILES: c1ccc(S(c2cccc2)(c2cccc2)c2ccc(N3c4cccc4Sc4cccc43)cc2)cc1

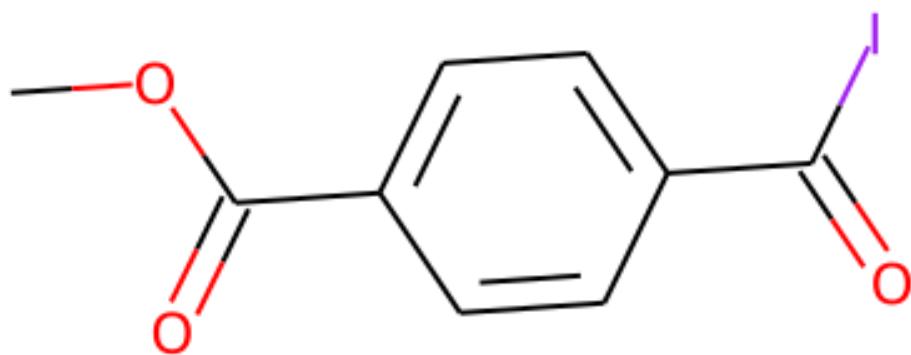
prob: 0.73



No.430

SMILES: COC(=O)c1ccc(C(=O)I)cc1

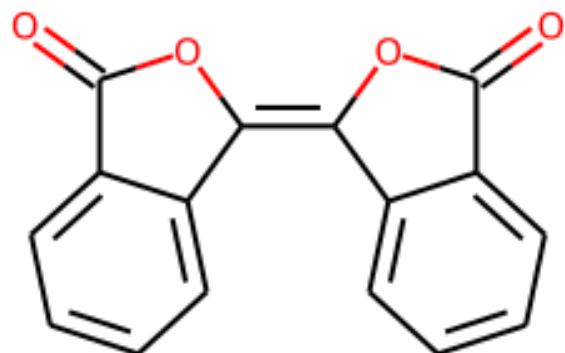
prob: 0.73



No.431

SMILES: O=C1O/C(=C2\OC(=O)c3ccccc32)c2ccccc21

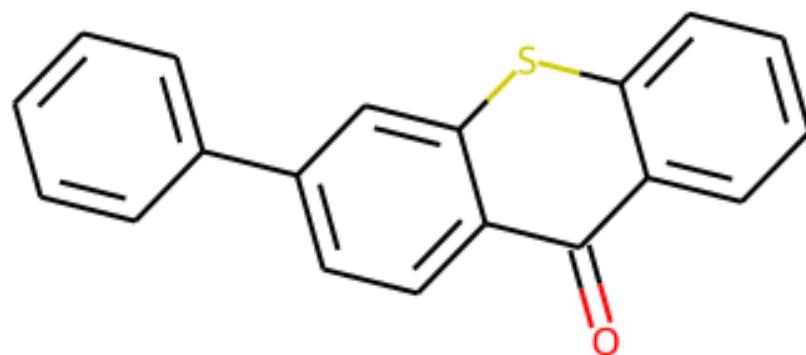
prob: 0.73



No.432

SMILES: O=c1c2ccccc2sc2cc(-c3ccccc3)ccc12

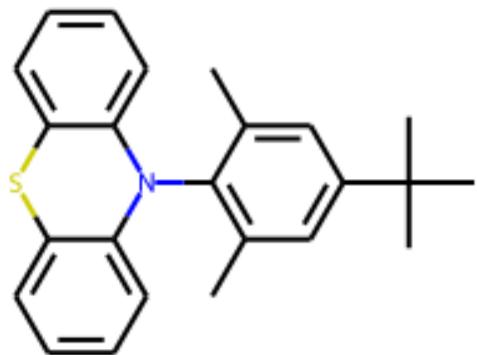
prob: 0.73



No.433

SMILES: Cc1cc(C(C)(C)C)cc(C)c1N1c2ccccc2Sc2ccccc21

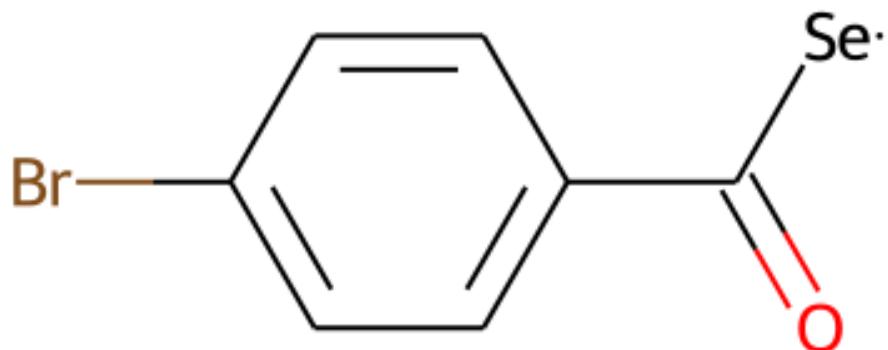
prob: 0.73



No.434

SMILES: O=C([Se])c1ccc(Br)cc1

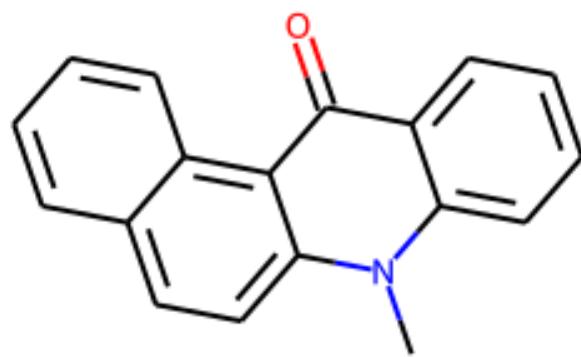
prob: 0.73



No.435

SMILES: Cn1c2ccccc2c(=O)c2c3ccccc3ccc21

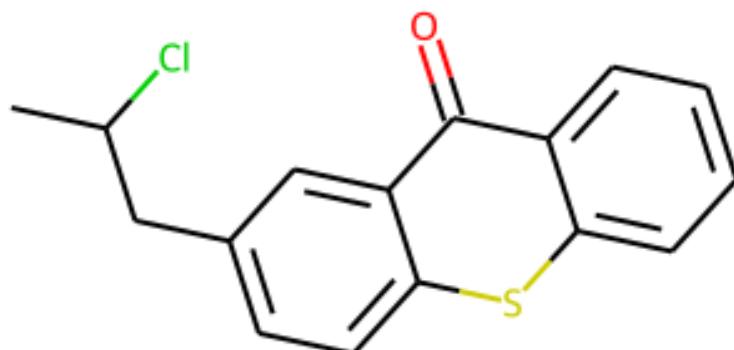
prob: 0.73



No.436

SMILES: CC(C1)Cc1ccc2sc3ccccc3c(=O)c2c1

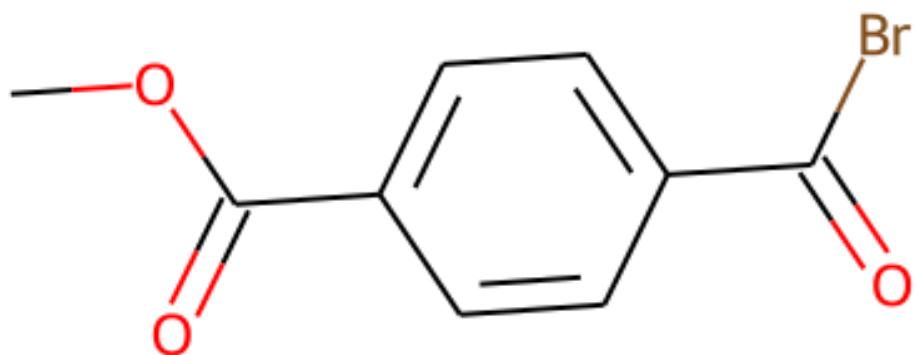
prob: 0.73



No.437

SMILES: COC(=O)c1ccc(C(=O)Br)cc1

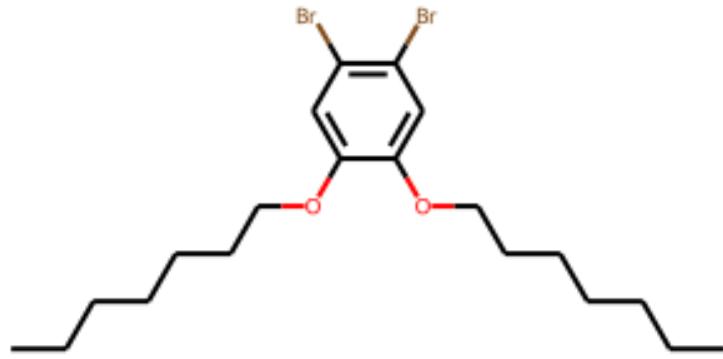
prob: 0.73



No. 438

SMILES: CCCCCCBrcc(Br)cc(Br)cc10CCCCCCC

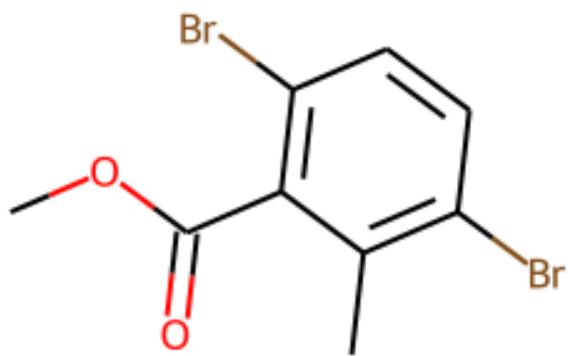
prob: 0.73



No. 439

SMILES: COC(=O)c1c(Br)ccc(Br)c1C

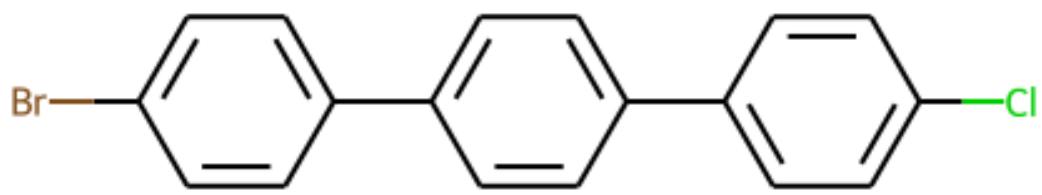
prob: 0.73



No. 440

SMILES: Clc1ccc(-c2ccc(-c3ccc(Br)cc3)cc2)cc1

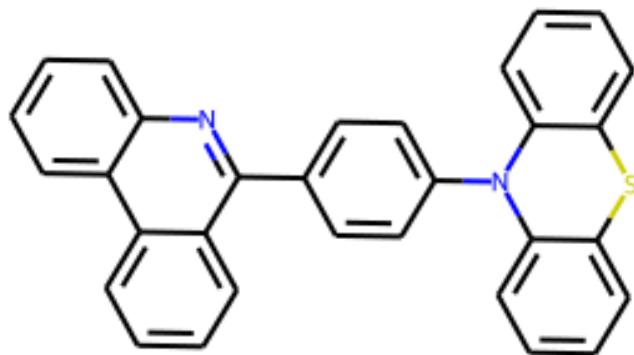
prob: 0.73



No. 441

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2nc3cccccc3c3cccccc23)cc1

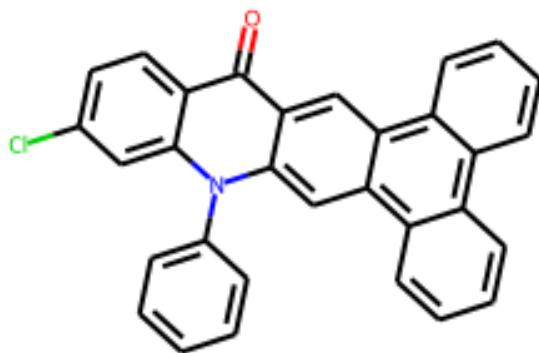
prob: 0.73



No. 442

SMILES: O=c1c2ccc(C1)cc2n(-c2cccc2)c2cc3c4cccc4c4cccc4c3cc12

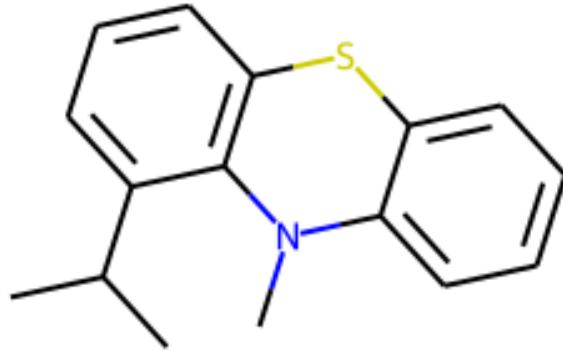
prob: 0.73



No.443

SMILES: CC(C)c1ccccc2c1N(C)c1ccccc1S2

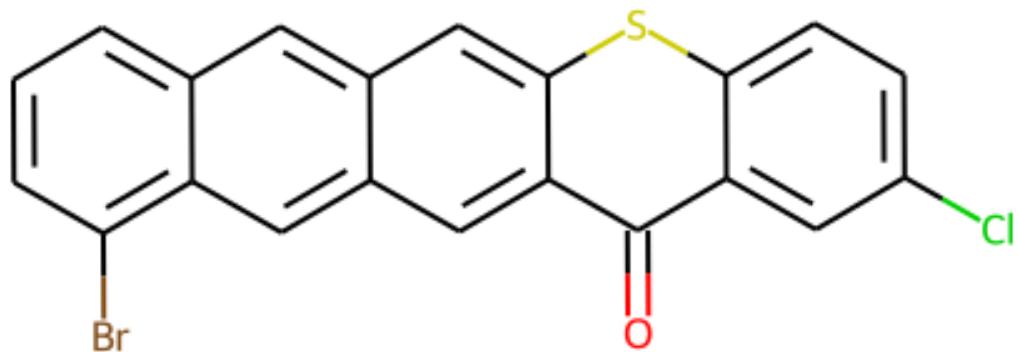
prob: 0.73



No.444

SMILES: O=c1c2cc(Cl)ccc2sc2cc3cc4cccc(Br)c4cc3cc12

prob: 0.72



No.445

SMILES:

Cc1cc(C)c(P(c2c(C)cc(C)cc2C)c2c(C)c(C)c(N3c4cccc4Sc4cccc43)c(C)c2C)c(C)c1

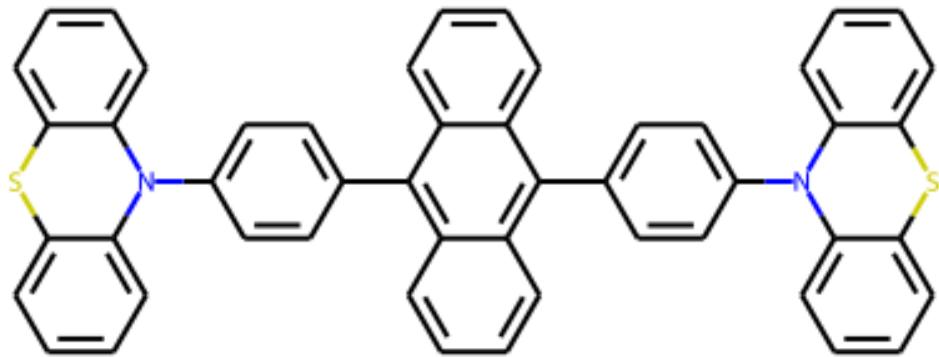
prob: 0.72



No.446

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc(-c2c3ccccc3c(-c3ccc(N4c5ccccc5Sc5ccccc54)cc3)c3cccc23)cc1

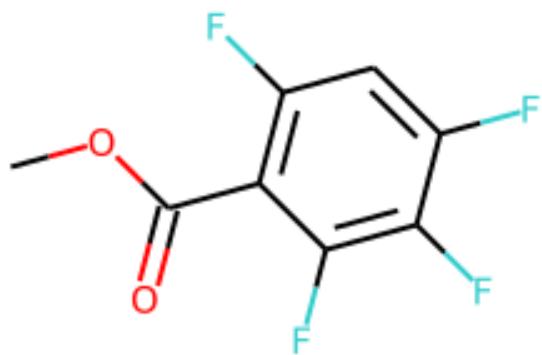
prob: 0.72



No.447

SMILES: COC(=O)c1c(F)cc(F)c(F)c1F

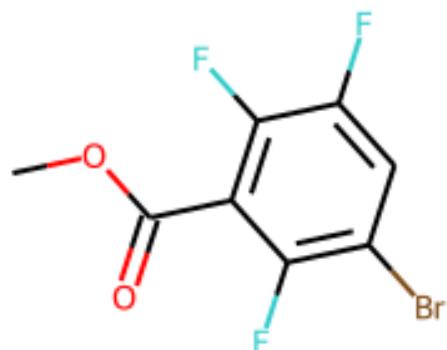
prob: 0.72



No.448

SMILES: COC(=O)c1c(F)c(F)cc(Br)c1F

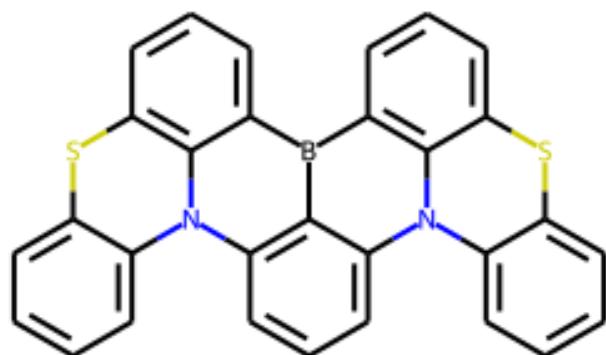
prob: 0.72



No.449

SMILES: c1ccc2c(c1)Sc1cccc3c1N2c1cccc2c1B3c1cccc3c1N2c1ccccc1S3

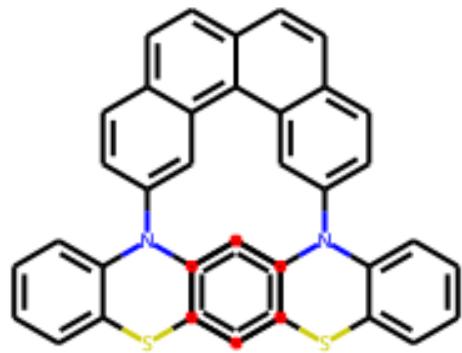
prob: 0.72



No.450

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2ccc3ccc4ccc(N5c6ccccc6Sc6ccccc65)cc4c3c2c1

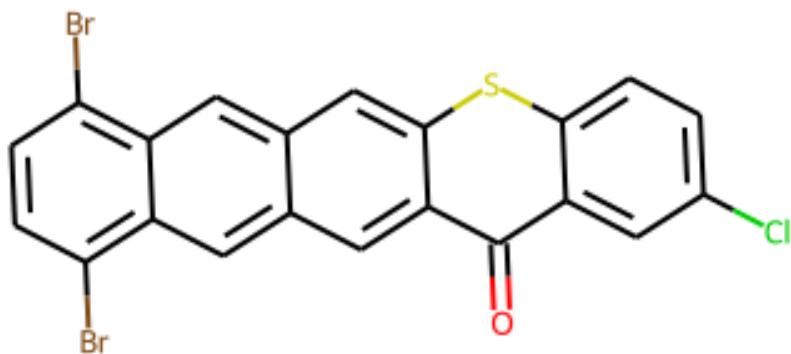
prob: 0.72



No.451

SMILES: O=c1c2cc(Cl)ccc2sc2cc3cc4c(Br)ccc(Br)c4cc3cc12

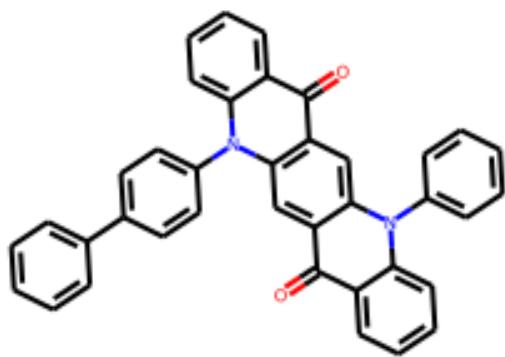
prob: 0.72



No.452

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2cc3c(=O)c4ccccc4n(-c4ccc(-c5ccccc5)cc4)c3cc12

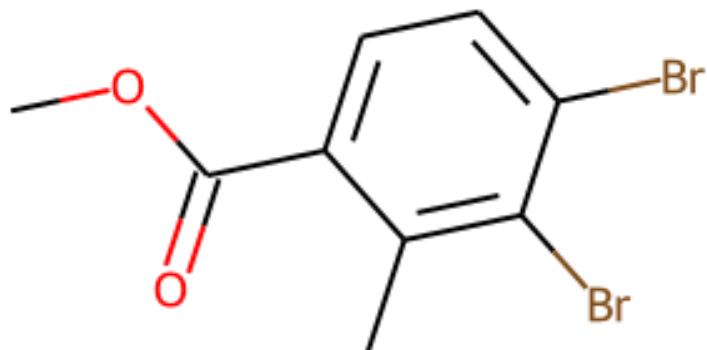
prob: 0.72



No.453

SMILES: COC(=O)c1ccc(Br)c(Br)c1C

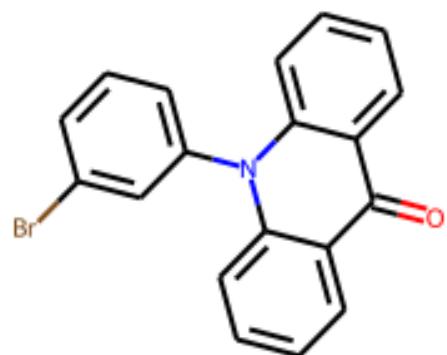
prob: 0.72



No.454

SMILES: O=c1c2ccccc2n(-c2cccc(Br)c2)c2ccccc12

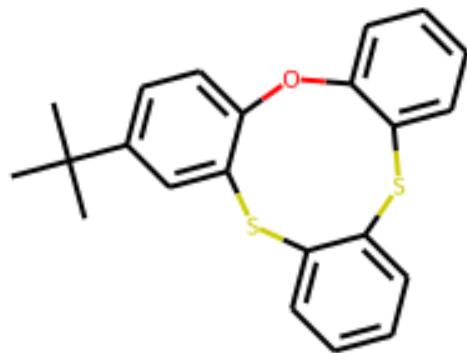
prob: 0.72



No. 455

SMILES: CC(C)(C)c1ccc2c(c1)Sc1ccccc1Sc1ccccc1O2

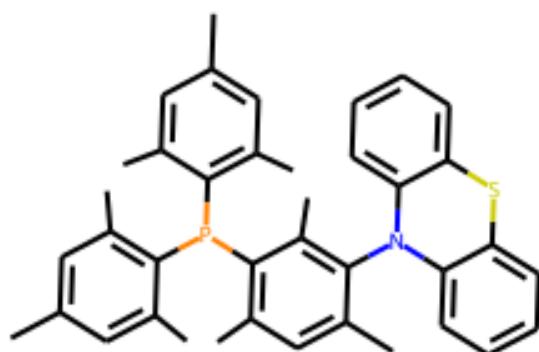
prob: 0.72



No. 456

SMILES: Cc1cc(C)c(P(c2c(C)cc(C)cc2C)c2c(C)cc(C)c(N3c4ccccc4Sc4ccccc43)c2C)c(C)c1

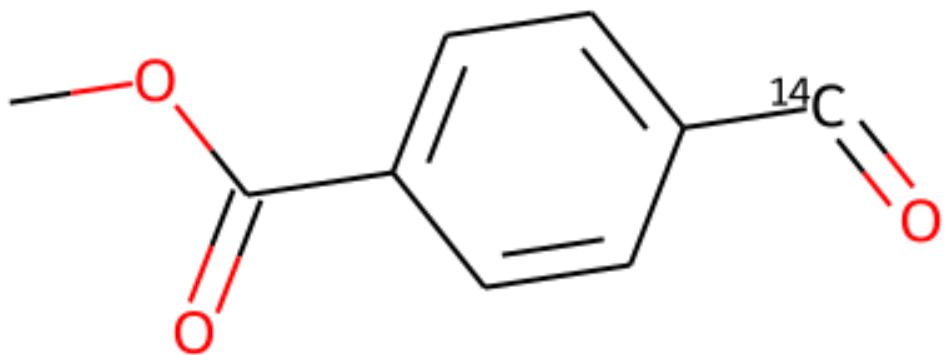
prob: 0.72



No. 457

SMILES: COC(=O)c1ccc([14CH]=O)cc1

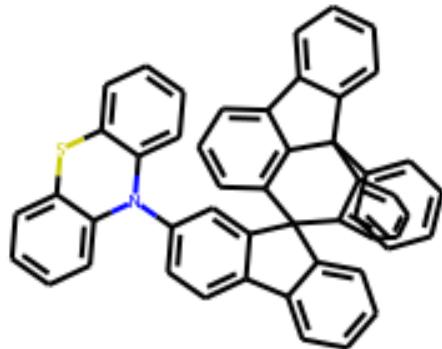
prob: 0.72



No. 458

SMILES: c1ccc(C23c4ccccc4-c4cccc(c42)C2(c4ccccc4-c4ccc(N5c6ccccc6Sc6ccccc65)cc42)c2ccccc23)cc1

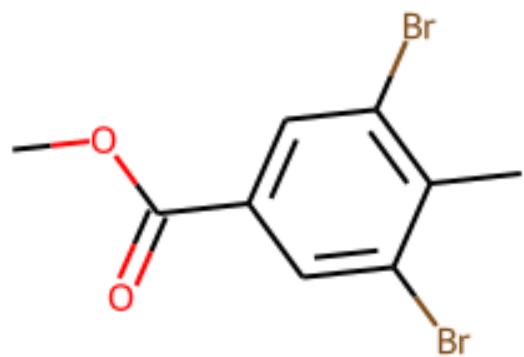
prob: 0.72



No. 459

SMILES: COC(=O)c1cc(Br)c(C)c(Br)c1

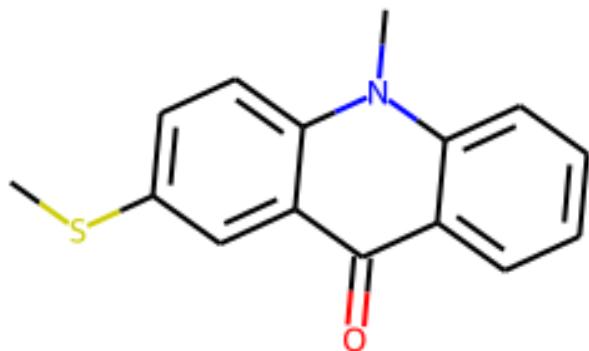
prob: 0.72



No.460

SMILES: CSc1ccc2c(c1)c(=O)c1ccccc1n2C

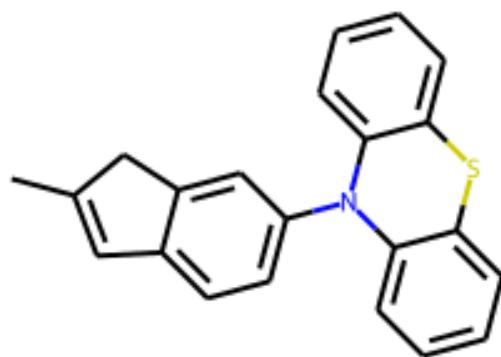
prob: 0.72



No.461

SMILES: CC1=Cc2ccc(N3c4ccccc4Sc4ccccc43)cc2C1

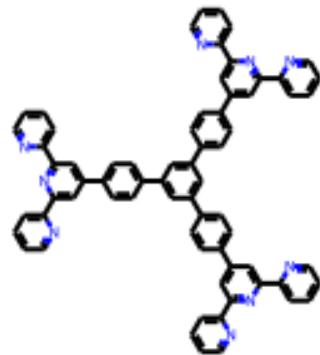
prob: 0.72



No.462

SMILES: c1ccc(-c2cc(-c3ccc(-c4cc(-c5ccc(-c6cc(-c7ccccn7)nc(-c7ccccn7)c6)cc5)cc(-c5ccc(-c6cc(-c7ccccn7)nc(-c7ccccn7)c6)cc5)c4)cc3)cc(-c3ccccn3)n2)nc1

prob: 0.72



No.463

SMILES: COC(=O)c1ccc(F)c(C)c1Br

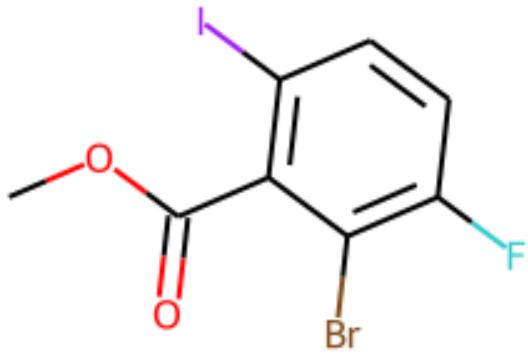
prob: 0.72



No.464

SMILES: COC(=O)c1c(I)ccc(F)c1Br

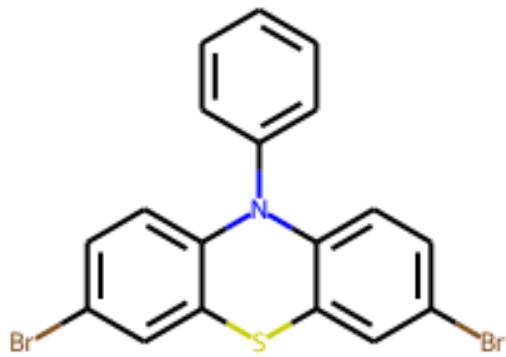
prob: 0.72



No.465

SMILES: Brcc1ccc2c(c1)Sc1cc(Br)ccc1N2c1cccc1

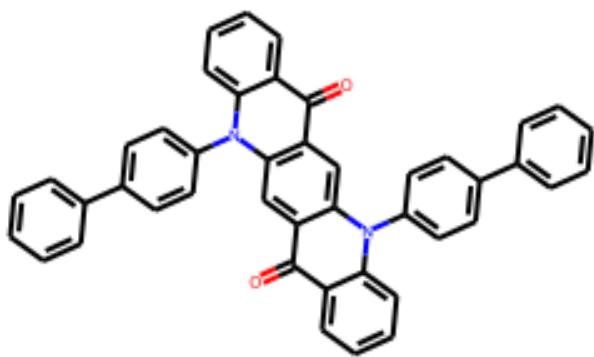
prob: 0.72



No.466

SMILES: O=c1c2ccccc2n(-c2ccc(-c3ccccc3)cc2)c2cc3c(=O)c4ccccc4n(-c4ccc(-c5ccccc5)cc4)c3cc12

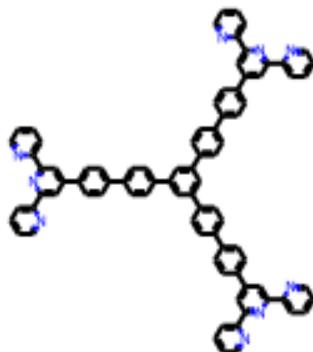
prob: 0.72



No. 467

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccc(-c5cc(-c6ccc(-c7ccc(-c8cc(-c9ccccn9)nc(-c9ccccn9)c8)cc7)cc6)cc(-c6ccc(-c7ccc(-c8cc(-c9ccccn9)nc(-c9ccccn9)c8)cc7)cc6)c5)cc4)cc3)cc(-c3ccccn3)n2)nc1

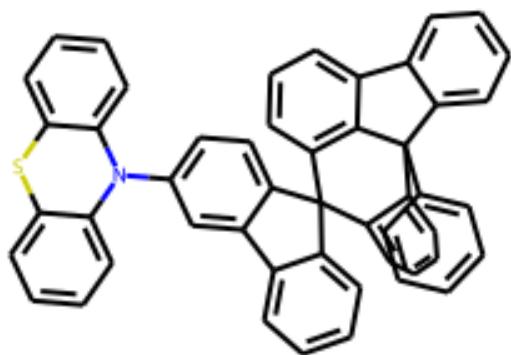
prob: 0.72



No. 468

SMILES: c1ccc(C23c4cccc4-c4cccc(c42)C2(c4cccc4-c4cc(N5c6cccc6Sc6cccc65)ccc42)c2cccc23)cc1

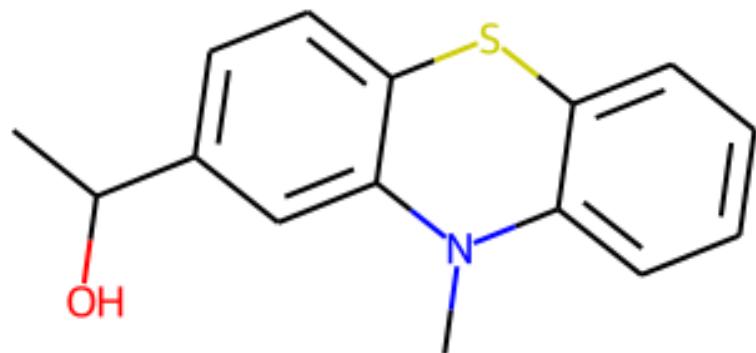
prob: 0.72



No.469

SMILES: CC(=O)c1ccc2c(c1)N(C)c1ccccc1S2

prob: 0.72



No.470

SMILES:

Cc1cc(C)c([As])(c2cc(C)cc(C)cc2C)c2cc(C)c(C)c(N3c4ccccc4Sc4ccccc43)c(C)c2Cc(C)c1

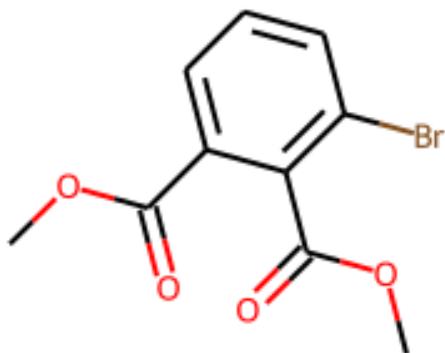
prob: 0.72



No.471

SMILES: COC(=O)c1ccccc(Br)c1C(=O)OC

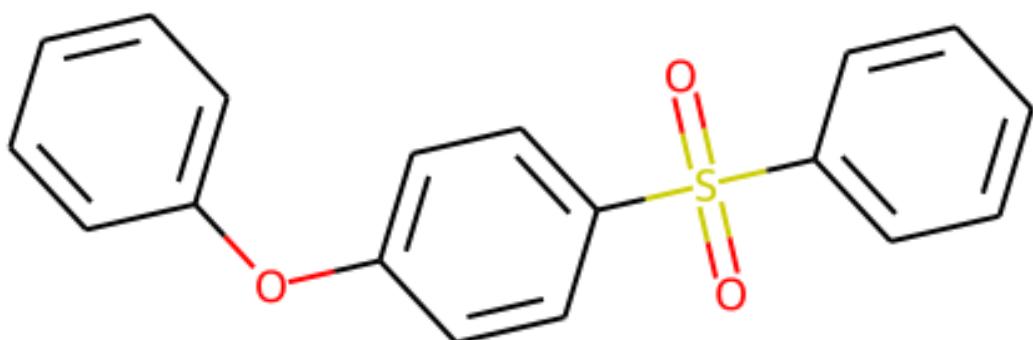
prob: 0.72



No.472

SMILES: O=S(=O)(c1ccccc1)c1ccc(Oc2ccccc2)cc1

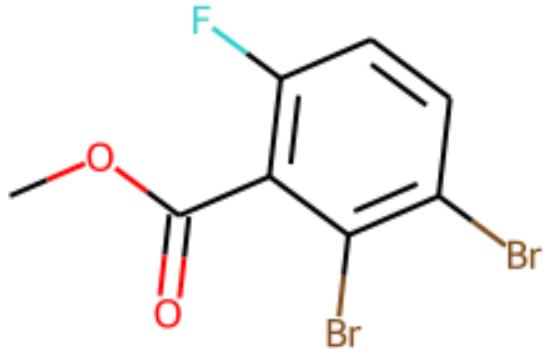
prob: 0.72



No. 473

SMILES: COC(=O)c1c(F)ccc(Br)c1Br

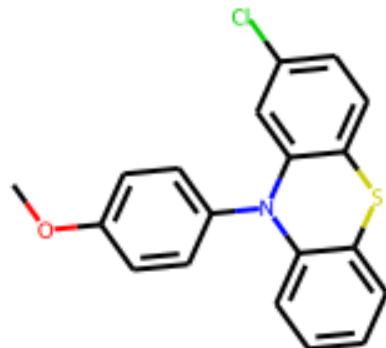
prob: 0.72



No. 474

SMILES: C0c1ccc(N2c3cccc3Sc3ccc(C1)cc32)cc1

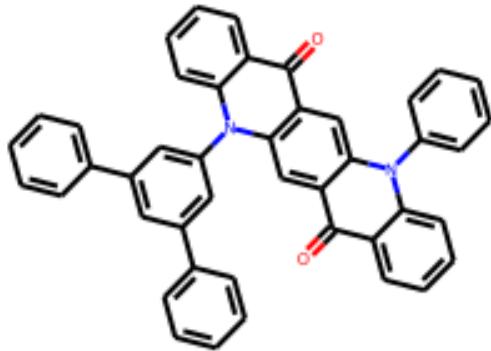
prob: 0.72



No. 475

SMILES: O=c1c2cccccc2n(-c2cccccc2)c2cc3c(=O)c4cccccc4n(-c4cc(-c5cccccc5)cc(-c5cccccc5)c4)c3cc12

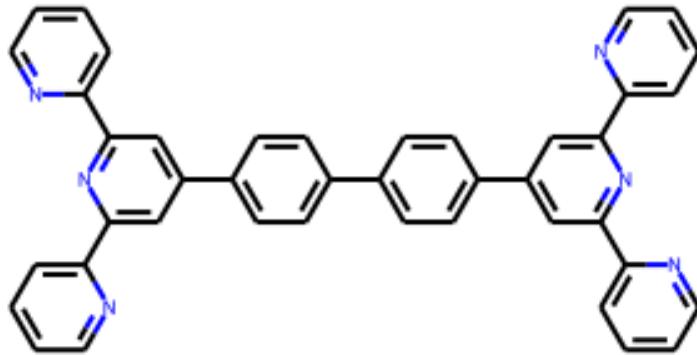
prob: 0.72



No.476

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccc(-c5cc(-c6ccccc6)nc(-c6ccccc6)c5)cc4)cc3)cc(-c3ccccn3)n2)nc1

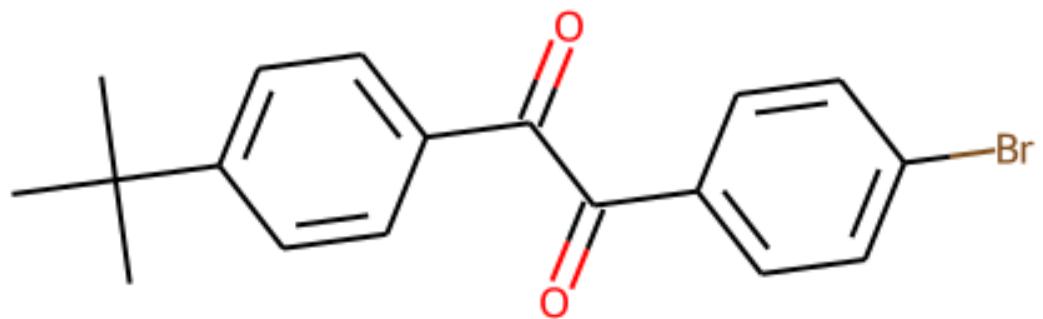
prob: 0.72



No.477

SMILES: CC(C)(C)c1ccc(C(=O)C(=O)c2ccc(Br)cc2)cc1

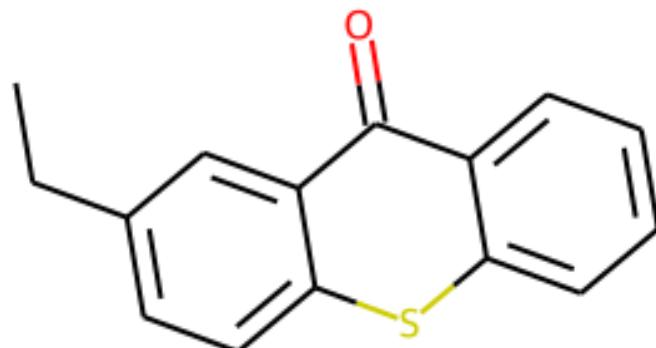
prob: 0.72



No.478

SMILES: CCc1ccc2sc3ccccc3c(=O)c2c1

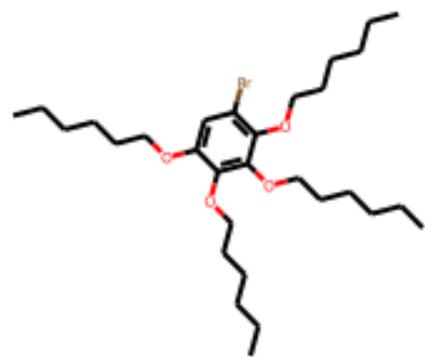
prob: 0.72



No.479

SMILES: CCCCCC0c1cc(Br)c(OCCCCCC)c(OCCCCCC)c1OCCCCCC

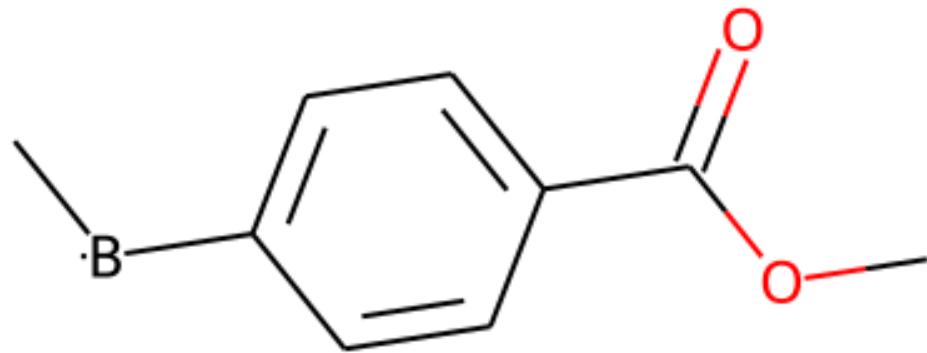
prob: 0.72



No. 480

SMILES: C[B]c1ccc(C(=O)OC)cc1

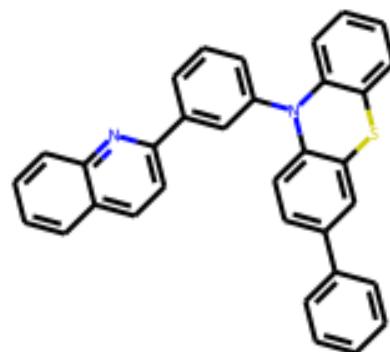
prob: 0.72



No. 481

SMILES: c1ccc(-c2ccc3c(c2)Sc2cccc2N3c2cccc(-c3ccc4cccc4n3)c2)cc1

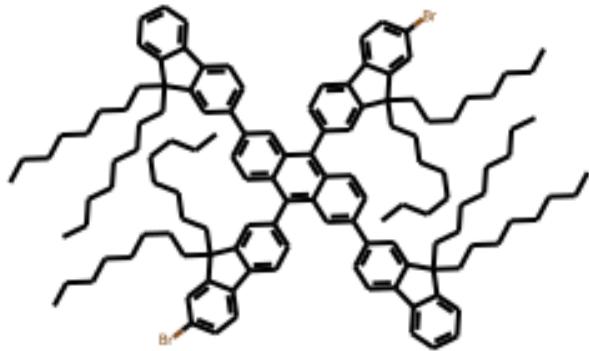
prob: 0.72



No. 482

SMILES: CCCCCCCC1(CCCCCCCC)c2cccc2-c2ccc(-c3ccc4c(-c5ccc6c(c5)C(CCCCCCCC)(CCCC)C5cc(Br)ccc5-6)c5cc(-c6ccc7c(c6)C(CCCCCCCC)(CCCC)C6cccc6-7)ccc5c(-c5cc6c(c5)C(CCCCCCCC)(CCCC)C5cc(Br)ccc5-6)c4c3)cc21

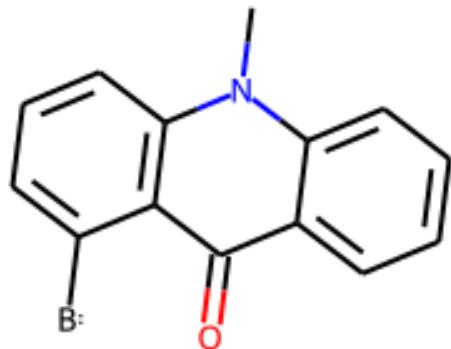
prob: 0.72



No.483

SMILES: [B]c1cccc2c1c(=O)c1ccccc1n2C

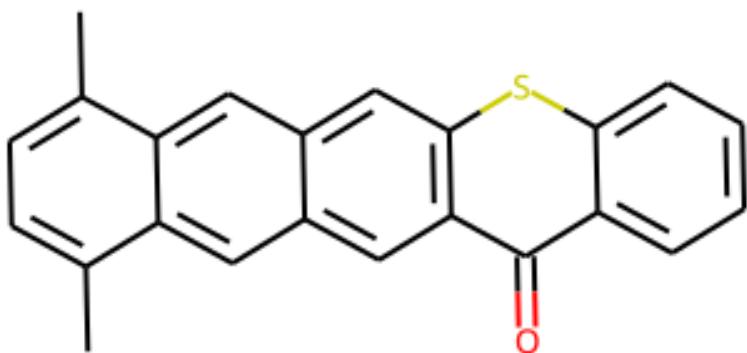
prob: 0.72



No.484

SMILES: Cc1ccc(C)c2cc3cc4c(=O)c5ccccc5sc4cc3cc12

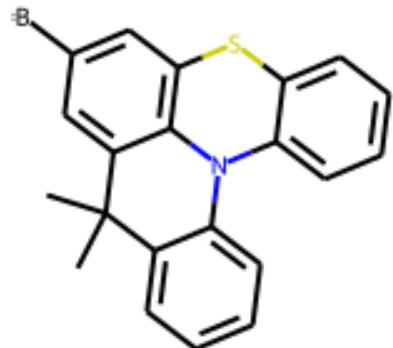
prob: 0.72



No.485

SMILES: [B]c1cc2c3c(c1)C(C)(C)c1ccccc1N3c1ccccc1S2

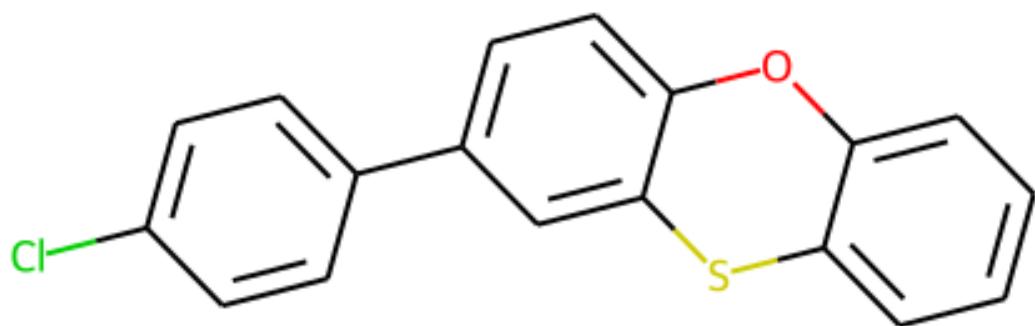
prob: 0.72



No.486

SMILES: Clc1ccc(-c2ccc3c(c2)Sc2ccccc2O)cc1

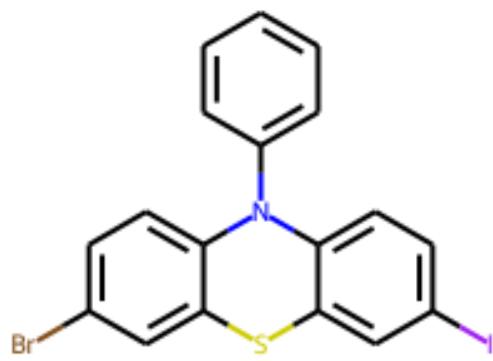
prob: 0.72



No.487

SMILES: Brcc1ccc2c(c1)Sc1cc(I)ccc1N2c1ccccc1

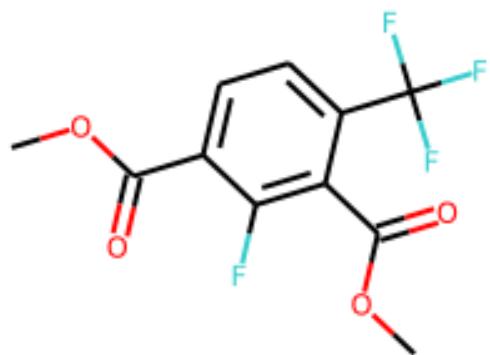
prob: 0.72



No.488

SMILES: COC(=O)c1ccc(C(F)(F)F)c(C(=O)OC)c1F

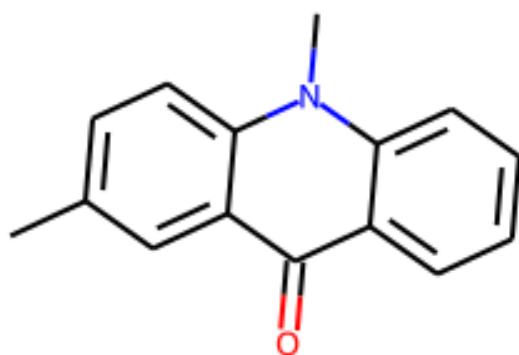
prob: 0.72



No.489

SMILES: Cc1ccc2c(c1)c(=O)c1ccccc1n2C

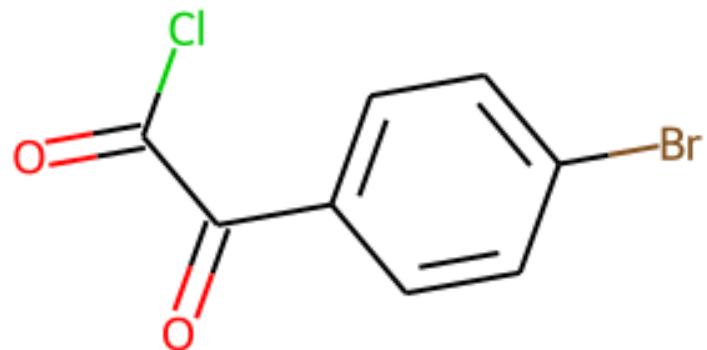
prob: 0.72



No.490

SMILES: O=C(Cl)C(=O)c1ccc(Br)cc1

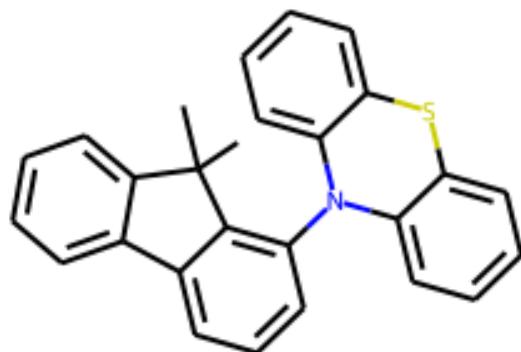
prob: 0.72



No.491

SMILES: CC1(C)c2ccccc2-c2cccc(N3c4ccccc4Sc4ccccc43)c21

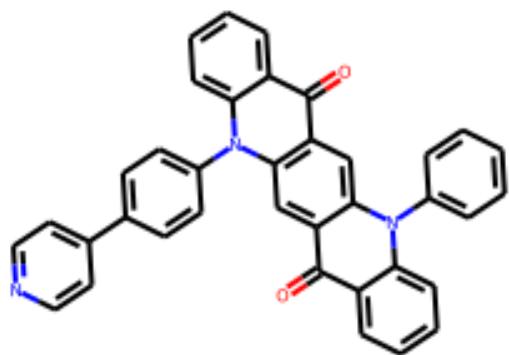
prob: 0.72



No.492

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2cc3c(=O)c4ccccc4n(-c4ccc(-c5ccncc5)cc4)c3cc12

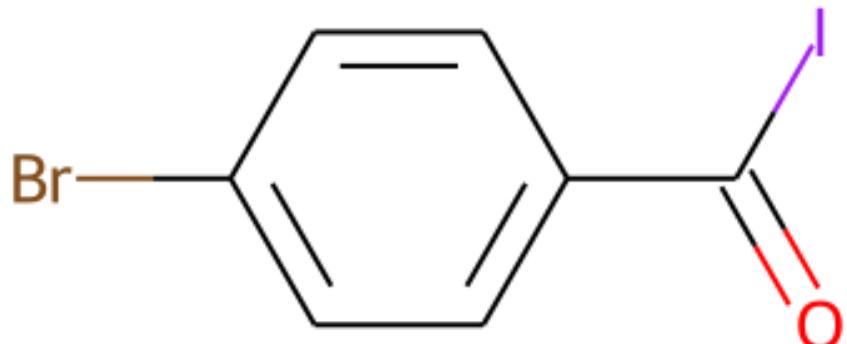
prob: 0.72



No.493

SMILES: O=C(I)c1ccc(Br)cc1

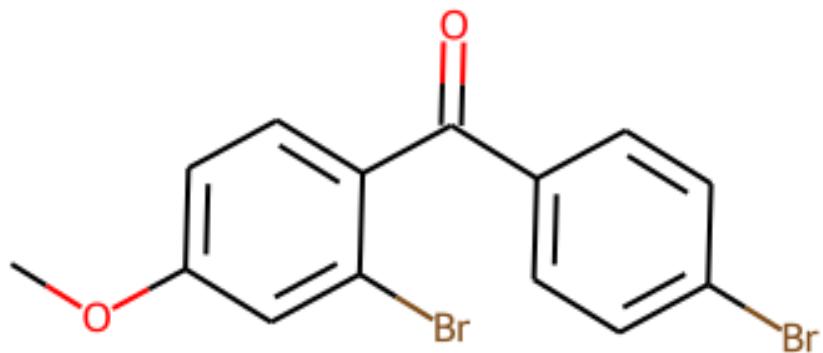
prob: 0.72



No.494

SMILES: C0c1ccc(C(=O)c2ccc(Br)cc2)c(Br)c1

prob: 0.72

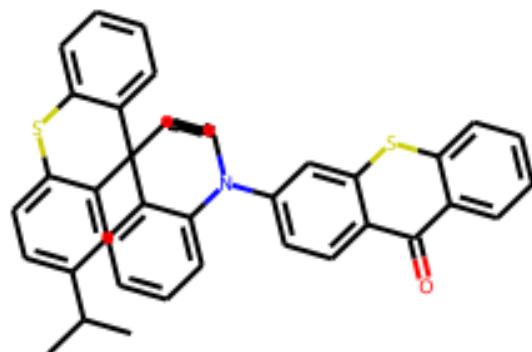


No.495

SMILES:

CC(C)c1ccc2c(c1)C1(c3cccc3S2)c2ccccc2N(c2ccc3c(=O)c4cccc4sc3c2)c2ccccc21

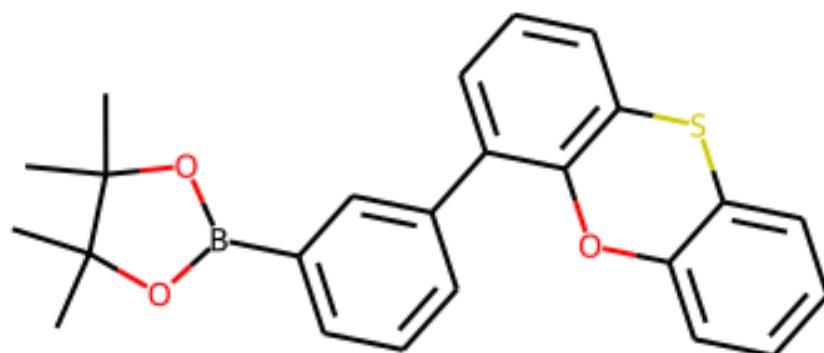
prob: 0.72



No.496

SMILES: CC1(C)OB(c2ccccc(-c3cccc4c30c3ccccc3S4)c2)OC1(C)C

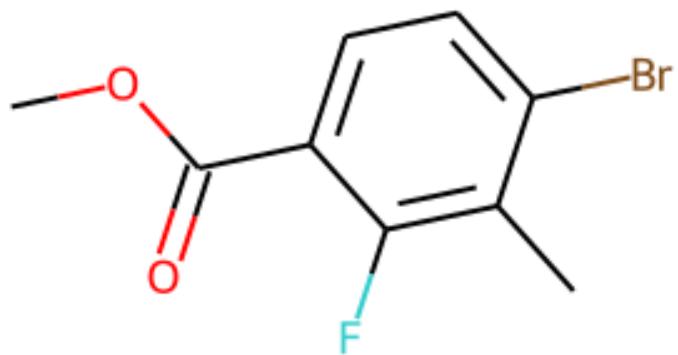
prob: 0.72



No.497

SMILES: COC(=O)c1ccc(Br)c(C)c1F

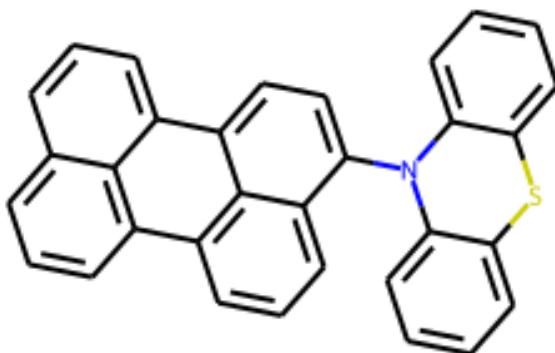
prob: 0.72



No.498

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1ccc2c3cccc4cccc(c5cccc1c52)c43

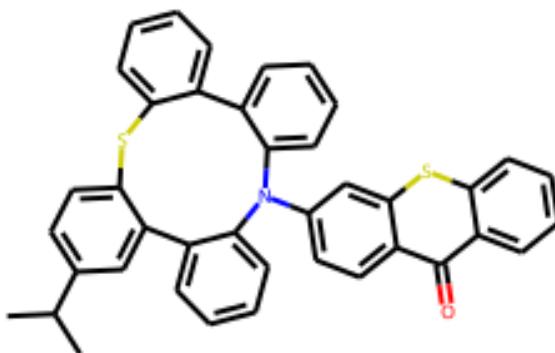
prob: 0.72



No.499

SMILES: CC(C)c1ccc2c(c1)-c1ccccc1N(c1ccc3c(=O)c4ccccc4sc3c1)c1ccccc1-c1ccccc1S2

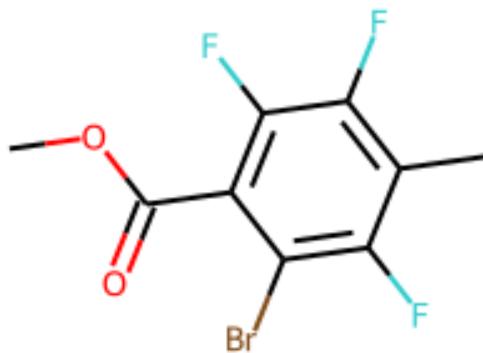
prob: 0.72



No.500

SMILES: COC(=O)c1c(F)c(F)c(C)c(F)c1Br

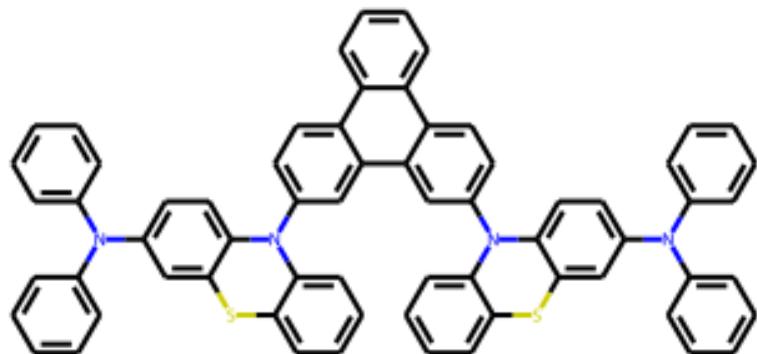
prob: 0.72



No.501

SMILES: c1ccc(N(c2ccccc2)c2ccc3c(c2)Sc2ccccc2N3c2ccc3c4ccccc4c4ccc(N5c6ccccc6Sc6cc(N(c7ccccc7)c7ccccc7)ccc65)cc4c3c2)cc1

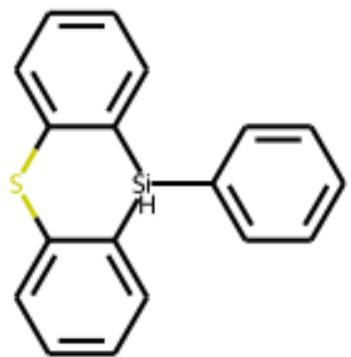
prob: 0.72



No.502

SMILES: c1ccc([SiH]2c3ccccc3Sc3ccccc32)cc1

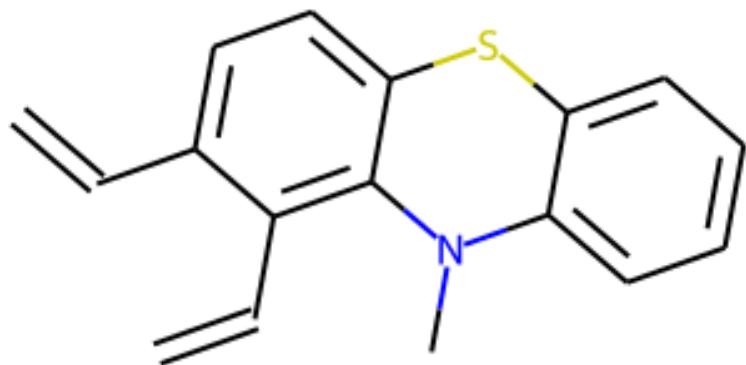
prob: 0.72



No.503

SMILES: C=Cc1ccc2c(c1C=C)N(C)c1ccccc1S2

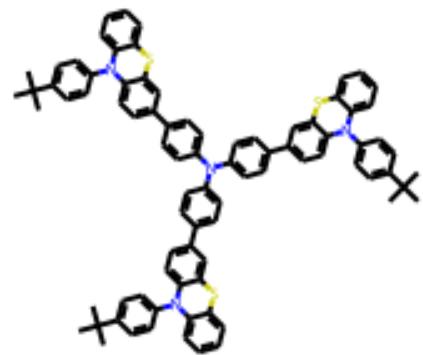
prob: 0.72



No.504

SMILES: CC(C)(C)c1cccc(N2c3cccc3Sc3cc(-c4ccc(N(c5ccc(-c6ccc7c(c6)Sc6ccccc6N7c6cc c(C(C)(C)C)cc6)cc5)c5ccc(-c6ccc7c(c6)Sc6ccccc6N7c6ccc(C(C)(C)C)cc6)cc5)cc4)ccc32)cc1

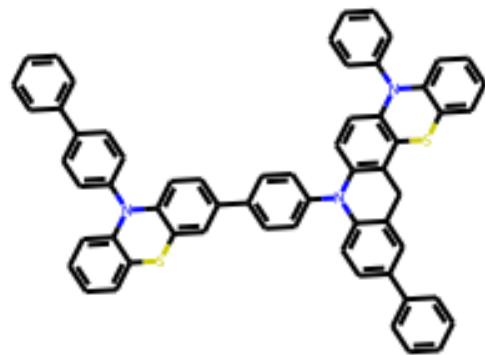
prob: 0.72



No.505

SMILES: c1ccc(-c2ccc(N3c4cccc4Sc4cc(-c5ccc(N6c7ccc(-c8cccc8)cc7Cc7c6ccc6c7Sc7cccc7N6c6cccc6)cc5)ccc43)cc2)cc1

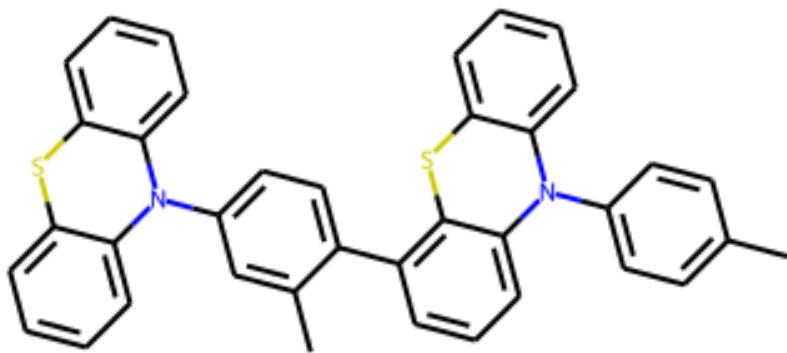
prob: 0.72



No.506

SMILES: Cc1ccc(N2c3cccc3Sc3c(-c4ccc(N5c6cccc6Sc6cccc65)cc4C)cccc32)cc1

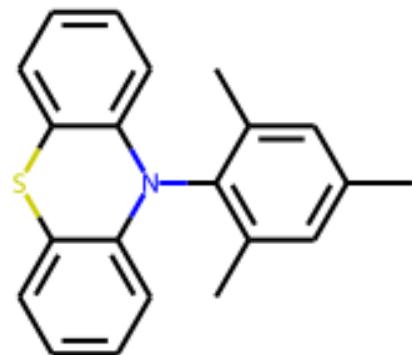
prob: 0.72



No.507

SMILES: Cc1cc(C)c(N2c3cccc3Sc3cccc32)c(C)c1

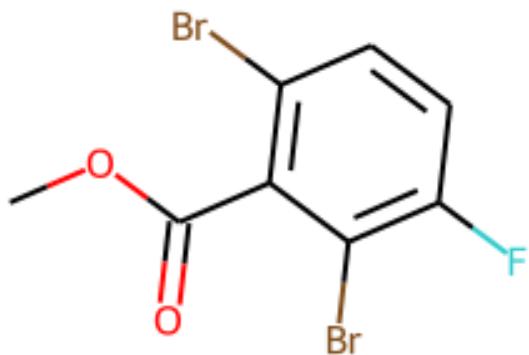
prob: 0.72



No.508

SMILES: COC(=O)c1c(Br)ccc(F)c1Br

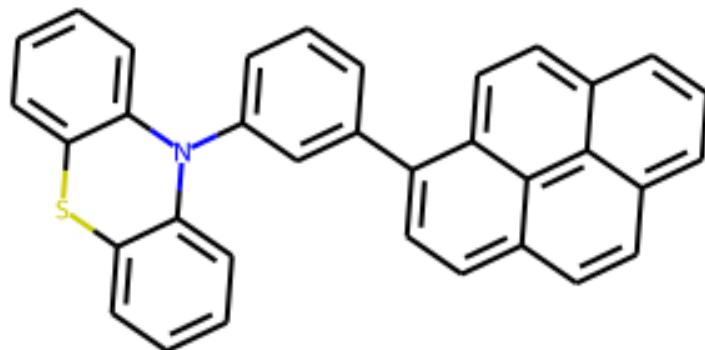
prob: 0.72



No.509

SMILES: c1cc(-c2ccc3ccc4cccc5ccc2c3c45)cc(N2c3ccccc3Sc3ccccc32)c1

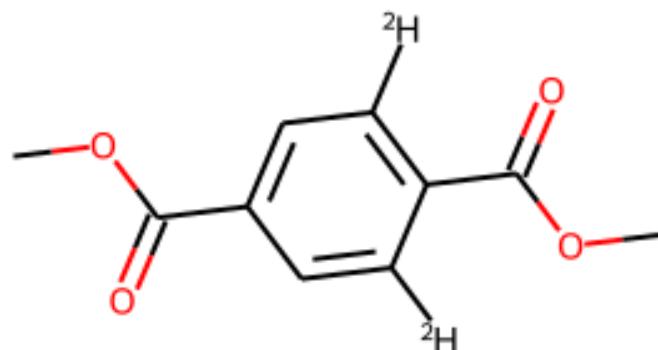
prob: 0.72



No.510

SMILES: [2H]c1cc(C(=O)OC)cc([2H])c1C(=O)OC

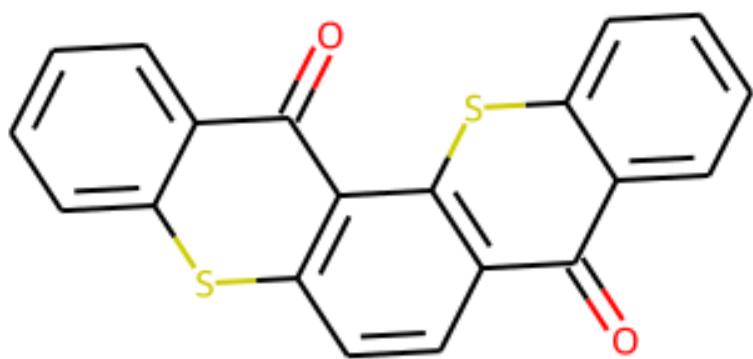
prob: 0.72



No.511

SMILES: O=c1c2ccccc2sc2c1ccc1sc3ccccc3c(=O)c12

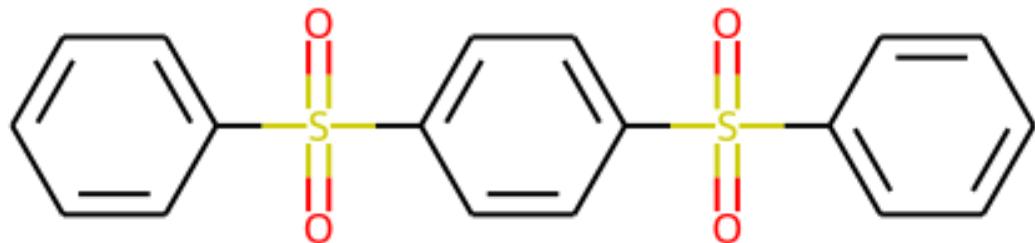
prob: 0.72



No.512

SMILES: O=S(=O)(c1ccccc1)c1ccc(S(=O)(=O)c2ccccc2)cc1

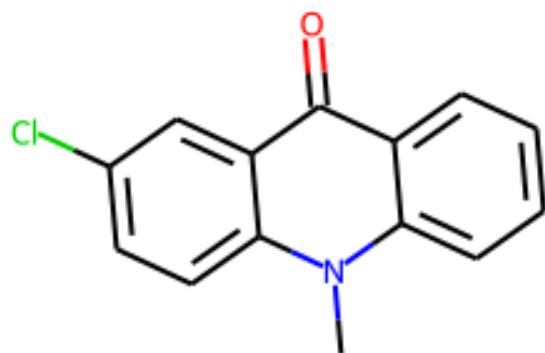
prob: 0.72



No.513

SMILES: Cn1c2ccccc2c(=O)c2cc(Cl)ccc21

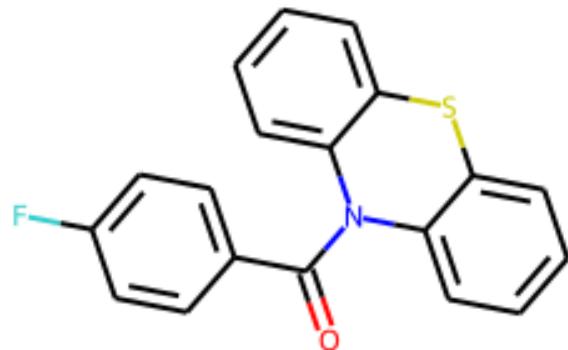
prob: 0.72



No.514

SMILES: O=C(c1ccc(F)cc1)N1c2cccc2Sc2cccc21

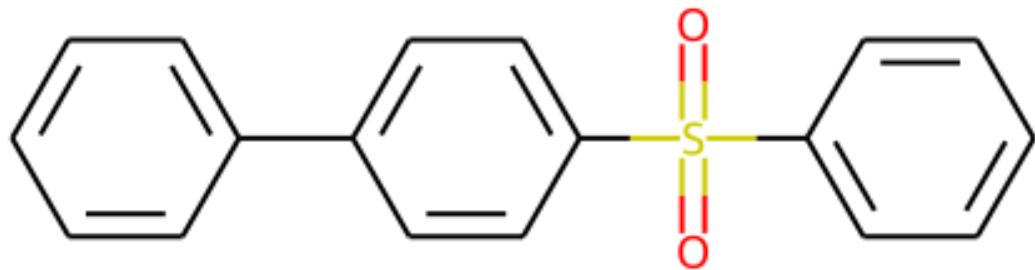
prob: 0.72



No.515

SMILES: O=S(=O)(c1ccccc1)c1ccc(-c2ccccc2)cc1

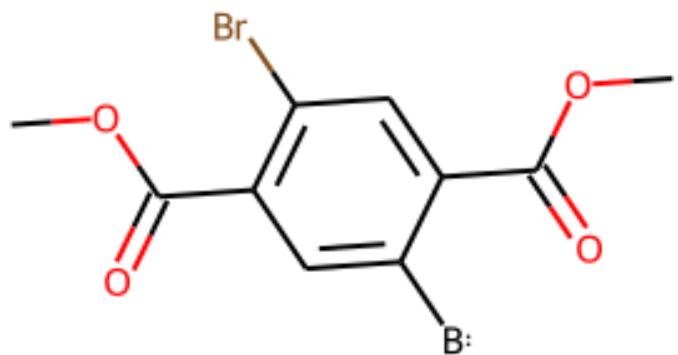
prob: 0.72



No.516

SMILES: [B]c1cc(C(=O)OC)c(Br)cc1C(=O)OC

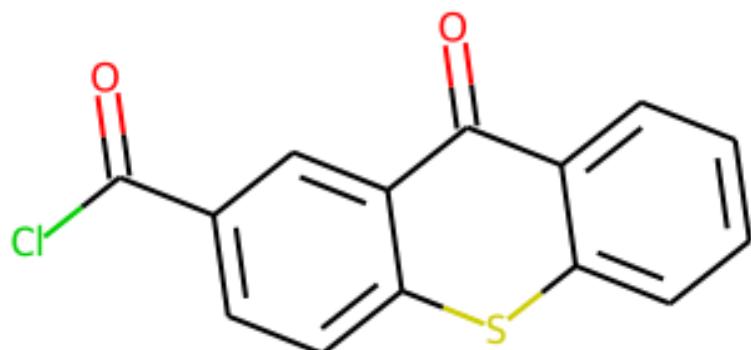
prob: 0.72



No.517

SMILES: O=C(Cl)c1ccc2sc3ccccc3c(=O)c2c1

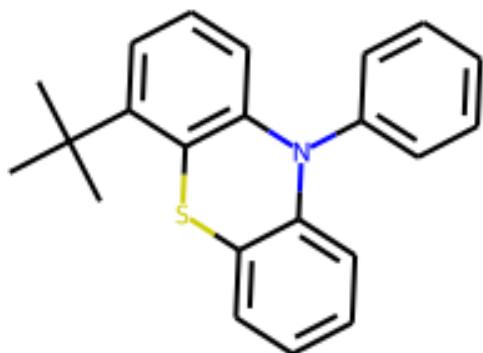
prob: 0.72



No.518

SMILES: CC(C)(C)c1ccccc2c1Sc1ccccc1N2c1ccccc1

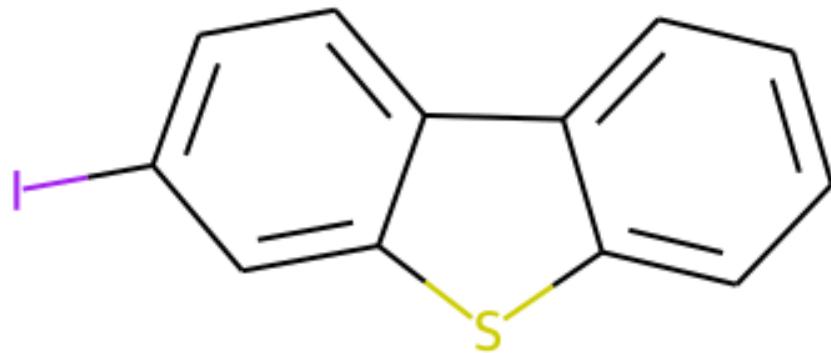
prob: 0.72



No.519

SMILES: Ic1ccc2c(c1)sc1ccccc12

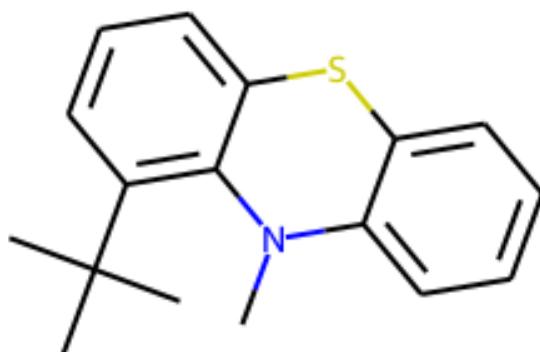
prob: 0.72



No.520

SMILES: CN1c2cccc2Sc2cccc(C(C)(C)C)c21

prob: 0.72

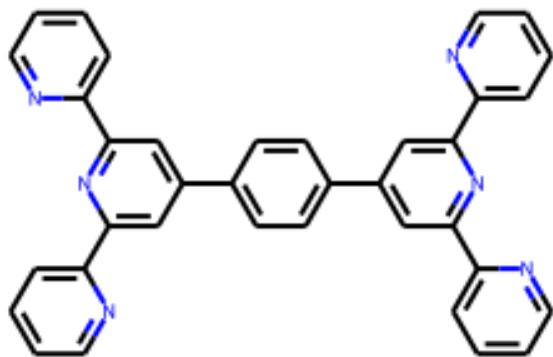


No.521

SMILES:

c1cccc(-c2cc(-c3ccc(-c4cc(-c5cccn5)nc(-c5cccn5)c4)cc3)cc(-c3cccn3)n2)nc1

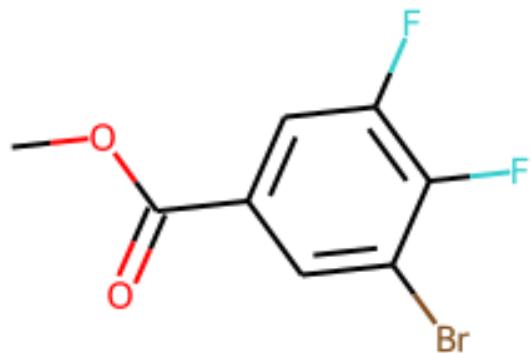
prob: 0.72



No.522

SMILES: COC(=O)c1cc(F)c(F)c(Br)c1

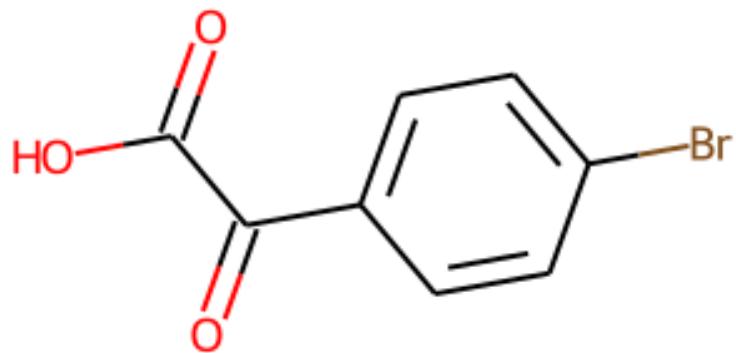
prob: 0.71



No.523

SMILES: O=C(O)C(=O)c1ccc(Br)cc1

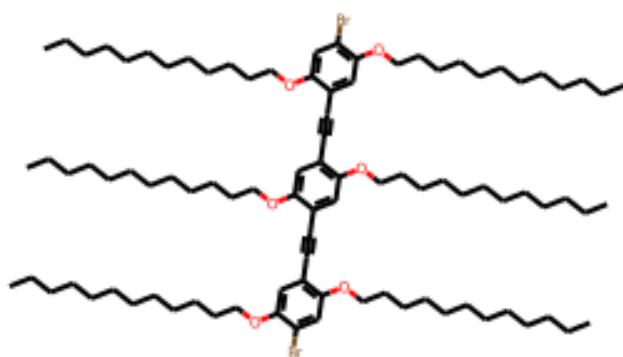
prob: 0.71



No. 524

SMILES: CCCCCCCCCCCC0c1cc(C#Cc2cc(0CCCCCCCCCCCC)cc(C#Cc3cc(0CCCCCCCCCCCC)c(Br)cc30CCCCCCCCCCCC)cc20CCCCCCCCCCCC)cc(0CCCCCCCCCCCC)cc1Br

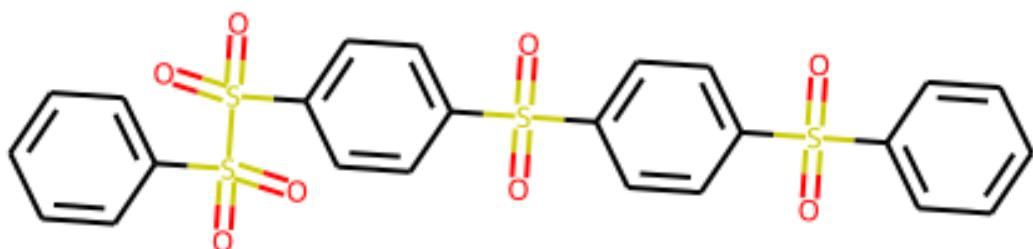
prob: 0.71



No. 525

SMILES: O=S(=O)(c1ccccc1)c1ccc(S(=O)(=O)c2ccc(S(=O)(=O)S(=O)(=O)c3ccccc3)cc2)cc1

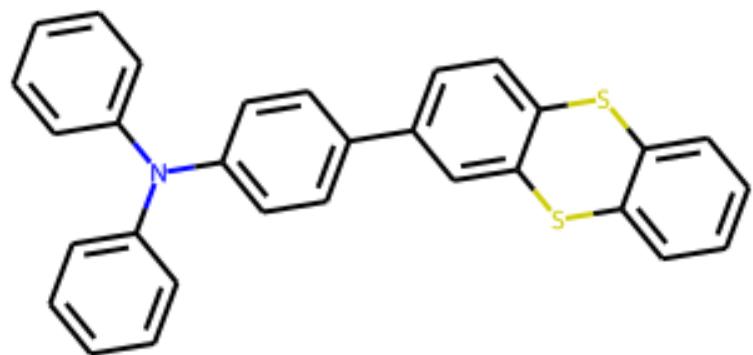
prob: 0.71



No. 526

SMILES: c1ccc(N(c2ccccc2)c2ccc(-c3ccc4c(c3)Sc3ccccc3S4)cc2)cc1

prob: 0.71



No.527

SMILES: CC(C)c1cc(N2c3ccccc3Sc3ccccc32)cc(C(C)C)c1Br

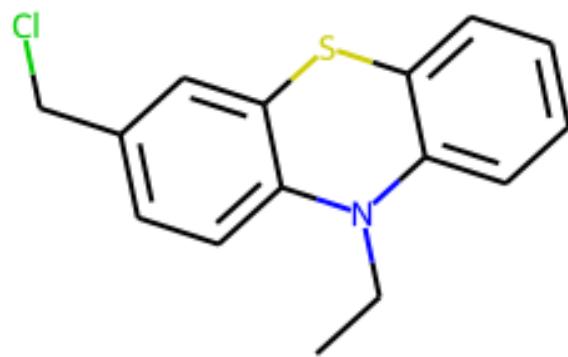
prob: 0.71



No.528

SMILES: CCN1c2ccccc2Sc2cc(CCl)ccc21

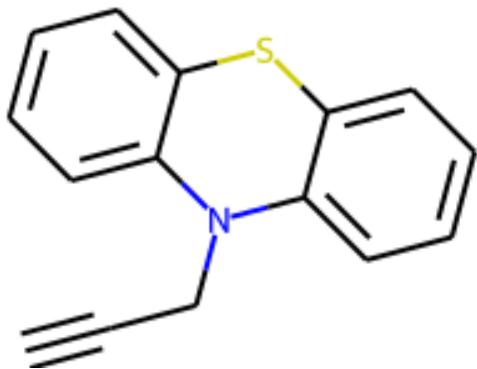
prob: 0.71



No.529

SMILES: C#CCN1c2ccccc2Sc2ccccc21

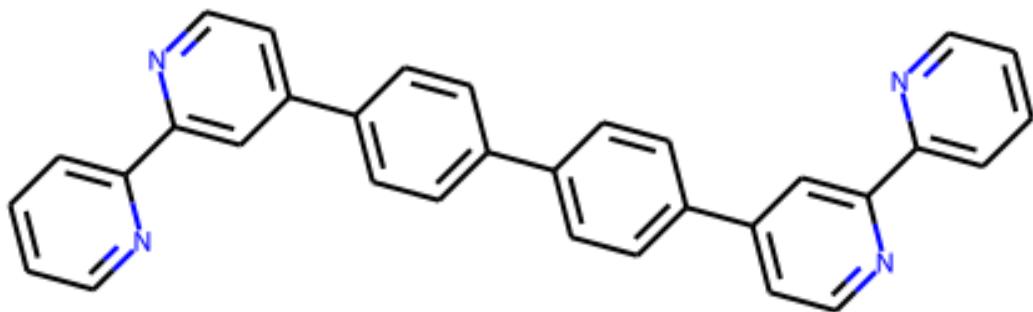
prob: 0.71



No.530

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccc(-c5ccnc(-c6cccn6)c5)cc4)cc3)ccn2)nc1

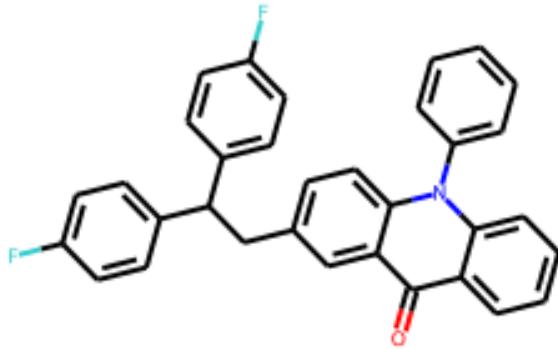
prob: 0.71



No.531

SMILES: O=c1c2ccccc2n(-c2ccccc2)c2ccc(CC(c3ccc(F)cc3)c3ccc(F)cc3)cc12

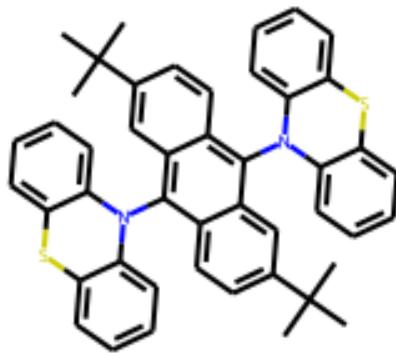
prob: 0.71



No.532

SMILES: CC(C)(C)c1ccc2c(N3c4ccccc4Sc4ccccc43)c3cc(C(C)(C)C)ccc3c(N3c4ccccc4Sc4ccc43)c2c1

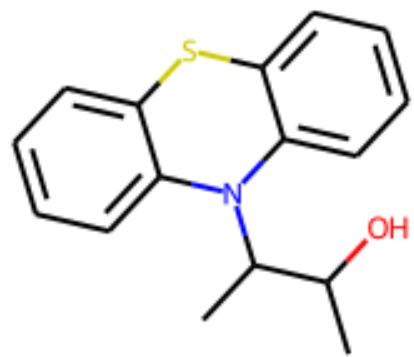
prob: 0.71



No.533

SMILES: CC(O)C(C)N1c2ccccc2Sc2ccccc21

prob: 0.71



No.534

SMILES: CC(C)N1c2ccccc2C2(c3ccccc3Sc3ccccc32)c2ccccc21

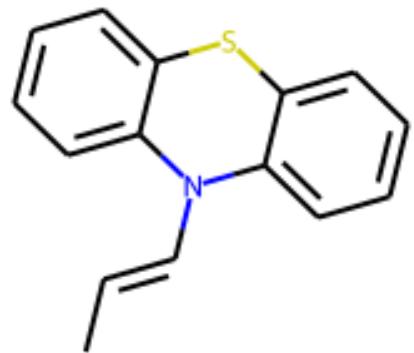
prob: 0.71



No.535

SMILES: C/C=C/N1c2ccccc2Sc2ccccc21

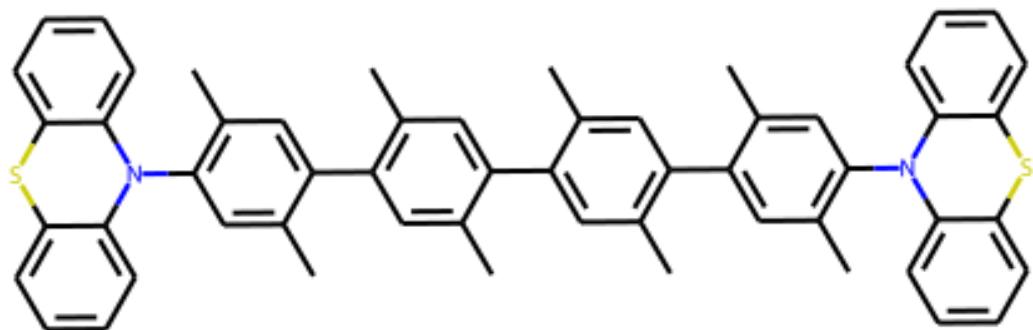
prob: 0.71



No. 536

SMILES: Cc1cc(-c2cc(C)c(N3c4cccc4Sc4cccc43)cc2C)c(C)cc1-c1cc(C)c(-c2cc(C)c(N3c4cccc4Sc4cccc43)cc2C)cc1C

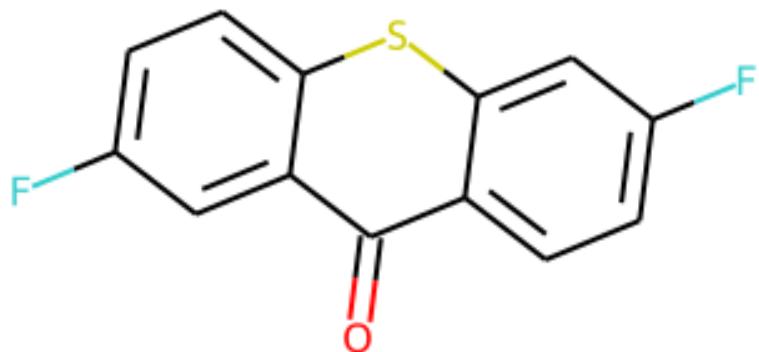
prob: 0.71



No. 537

SMILES: O=c1c2ccc(F)cc2sc2ccc(F)cc12

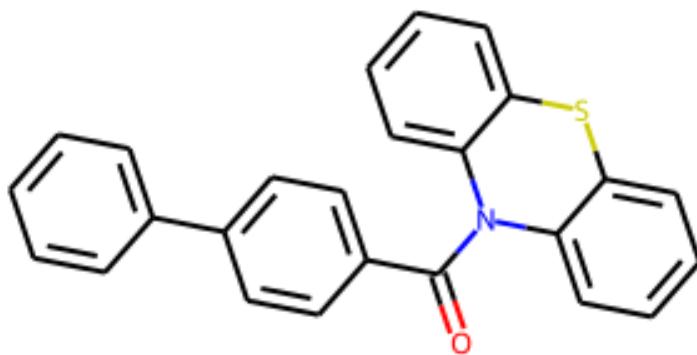
prob: 0.71



No. 538

SMILES: O=C(c1ccc(-c2ccccc2)cc1)N1c2ccccc2Sc2ccccc21

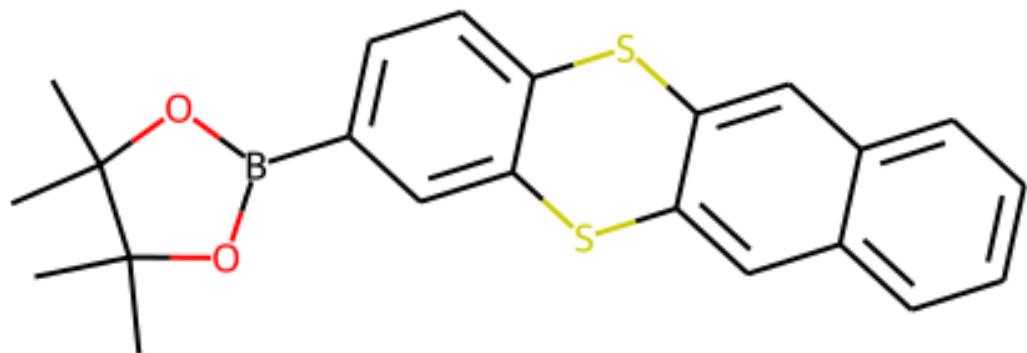
prob: 0.71



No.539

SMILES: CC1(C)OB(c2ccc3c(c2)Sc2cc4cccc4cc2S3)OC1(C)C

prob: 0.71

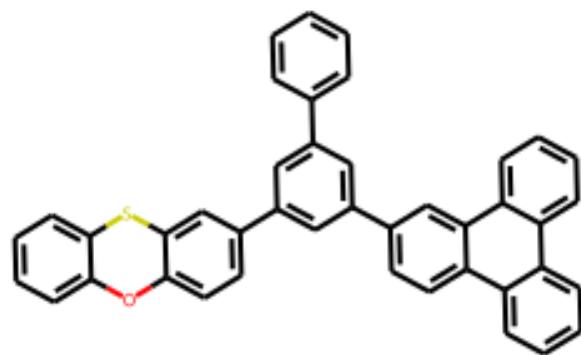


No.540

SMILES:

c1ccc(-c2cc(-c3ccc4c(c3)Sc3cccc3O)cc(-c3ccc4c5cccc5c5cccc5c4c3)c2)cc1

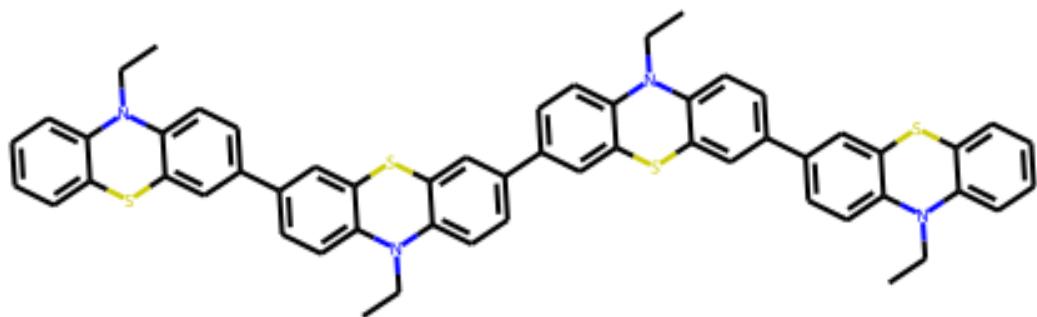
prob: 0.71



No.541

SMILES: CCN1c2ccccc2Sc2cc(-c3ccc4c(c3)Sc3cc(-c5ccc6c(c5)Sc5cc(-c7ccc8c(c7)Sc7ccc
cc7N8CC)ccc5N6CC)ccc3N4CC)ccc21

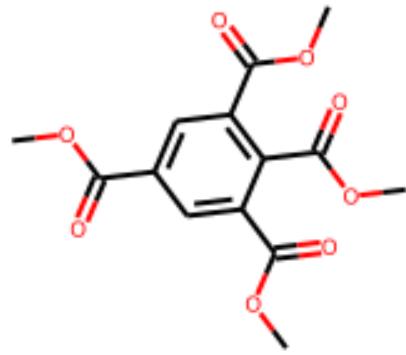
prob: 0.71



No.542

SMILES: COC(=O)c1cc(C(=O)OC)c(C(=O)OC)c(C(=O)OC)c1

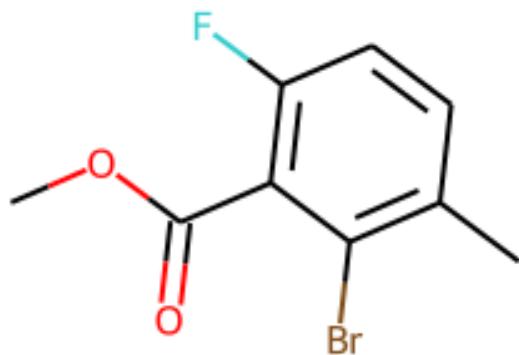
prob: 0.71



No.543

SMILES: COC(=O)c1c(F)ccc(C)c1Br

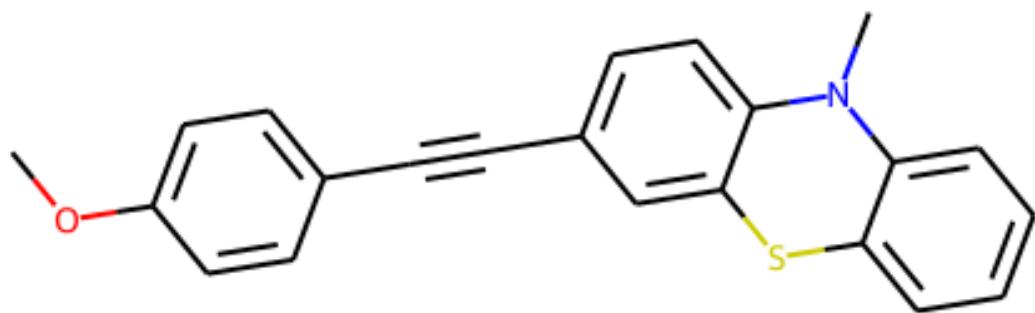
prob: 0.71



No.544

SMILES: COc1cccc(C#Cc2ccc3c(c2)Sc2ccccc2N3C)cc1

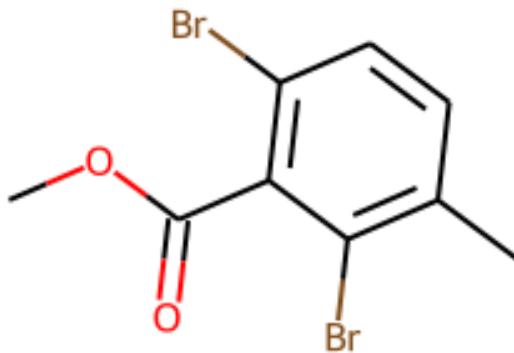
prob: 0.71



No.545

SMILES: COC(=O)c1c(Br)ccc(C)c1Br

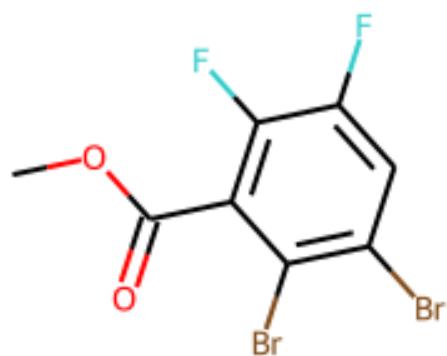
prob: 0.71



No.546

SMILES: COC(=O)c1c(F)c(F)cc(Br)c1Br

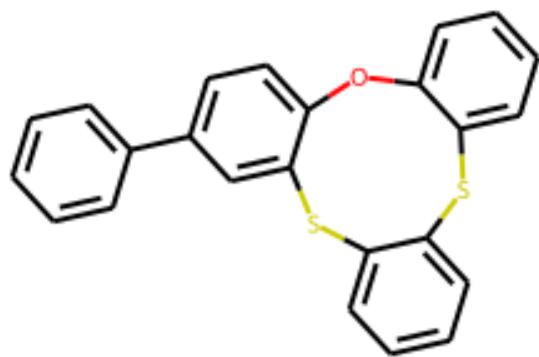
prob: 0.71



No.547

SMILES: c1ccc(-c2ccc3c(c2)Sc2cccc2Sc2cccc2O3)cc1

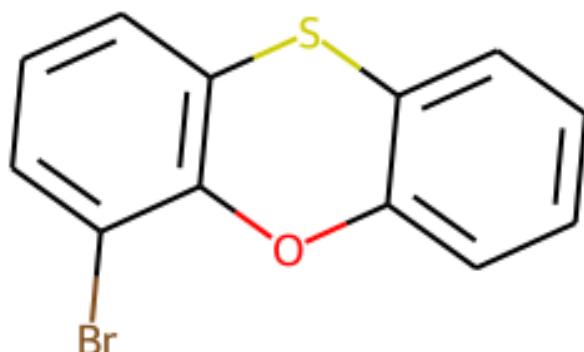
prob: 0.71



No.548

SMILES: Brcccc2c10c1ccccc1S2

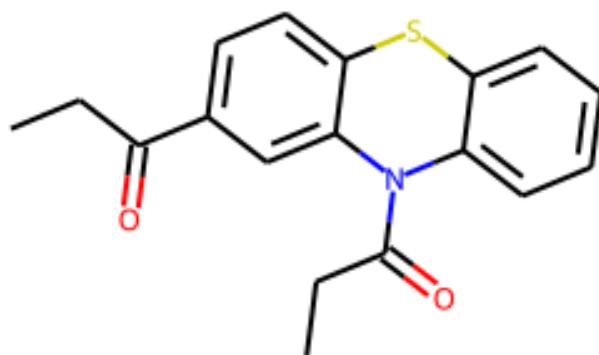
prob: 0.71



No.549

SMILES: CCC(=O)c1ccc2c(c1)N(C(=O)CC)c1ccccc1S2

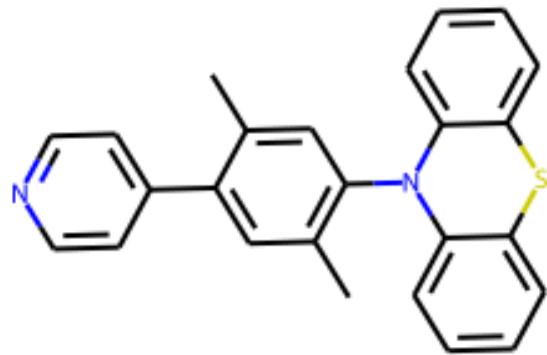
prob: 0.71



No.550

SMILES: Cc1cc(N2c3cccc3Sc3cccc32)c(C)cc1-c1ccncc1

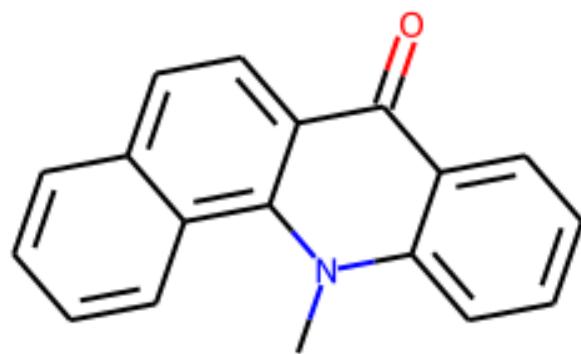
prob: 0.71



No.551

SMILES: Cn1c2ccccc2c(=O)c2ccc3ccccc3c21

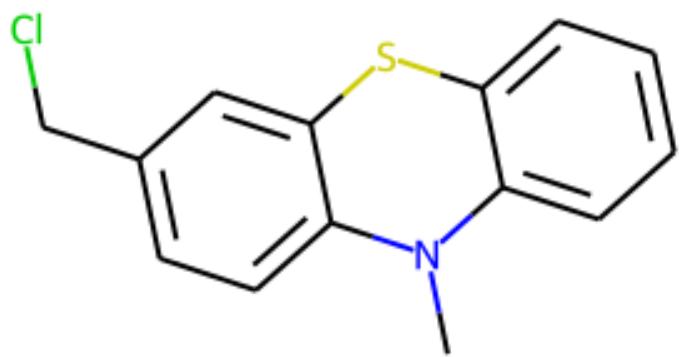
prob: 0.71



No.552

SMILES: CN1c2ccccc2Sc2cc(CCl)ccc21

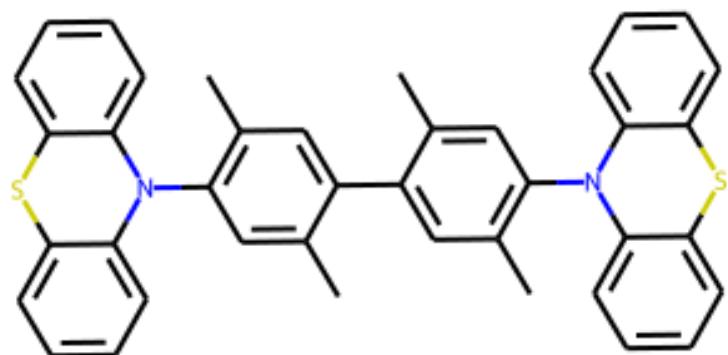
prob: 0.71



No.553

SMILES: Cc1cc(N2c3cccc3Sc3cccc32)c(C)cc1-c1cc(C)c(N2c3cccc3Sc3cccc32)cc1C

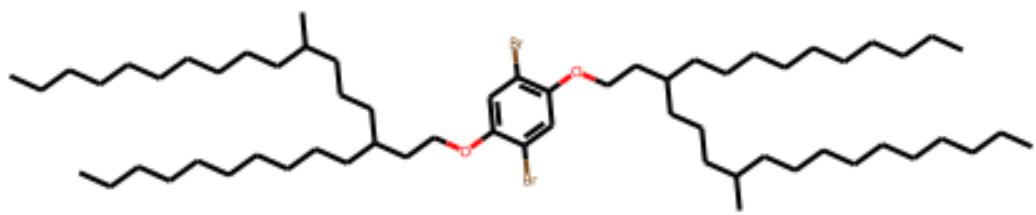
prob: 0.71



No.554

SMILES: CCCCCCCCCC(C)CCCC(CCCCCCCCC)CCOc1cc(Br)c(OCCC(CCCCCCCCC)CCCC(C)CCCCCCCC)cc1Br

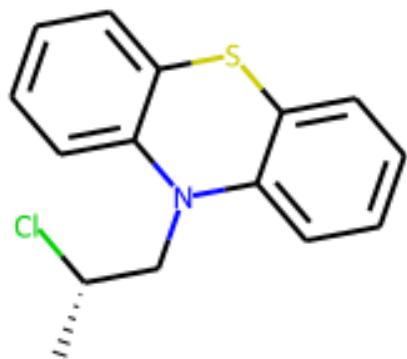
prob: 0.71



No.555

SMILES: C[C@H] (C1)CN1c2ccccc2Sc2ccccc21

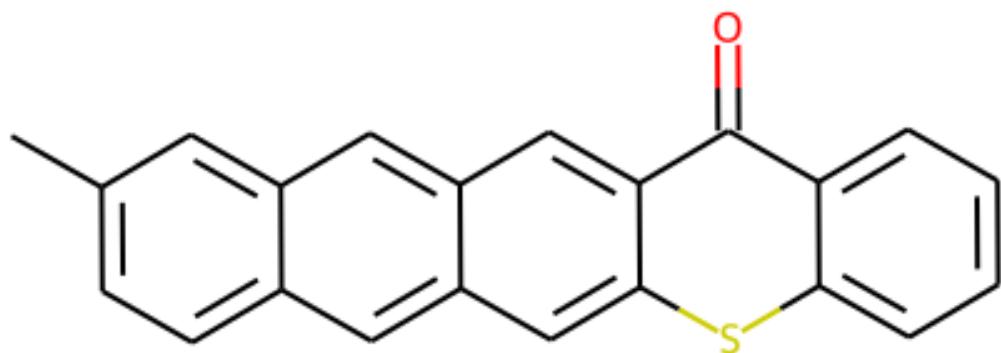
prob: 0.71



No.556

SMILES: Cc1ccc2cc3cc4sc5ccccc5c(=O)c4cc3cc2c1

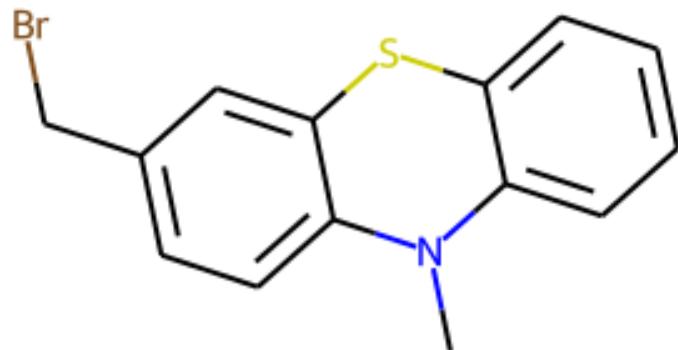
prob: 0.71



No.557

SMILES: CN1c2ccccc2Sc2cc(CBr)ccc1

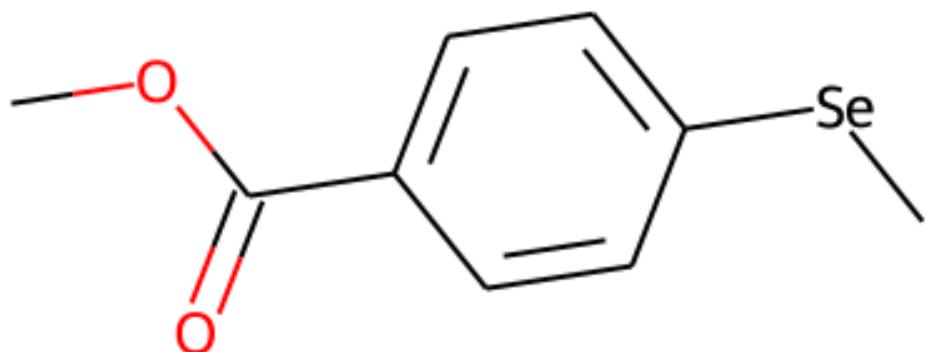
prob: 0.71



No.558

SMILES: COC(=O)c1ccc([Se]C)cc1

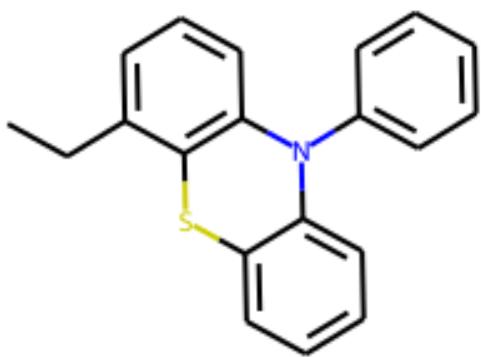
prob: 0.71



No.559

SMILES: CCc1ccccc2c1Sc1ccccc1N2c1ccccc1

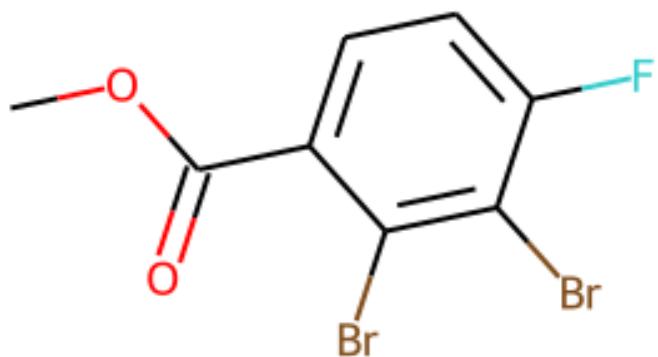
prob: 0.71



No. 560

SMILES: COC(=O)c1ccc(F)c(Br)c1Br

prob: 0.71

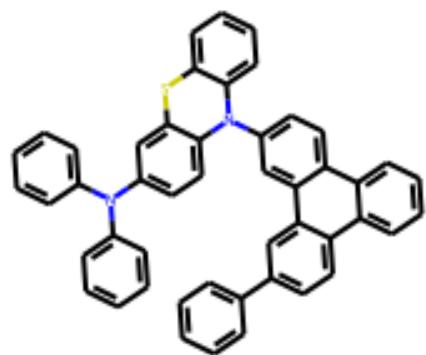


No. 561

SMILES:

c1ccc(-c2ccc3c4cccc4c4ccc(N5c6ccccc6S)c6cc(N(c7cccc7)c7cccc7)ccc65)cc4c3c2)cc1

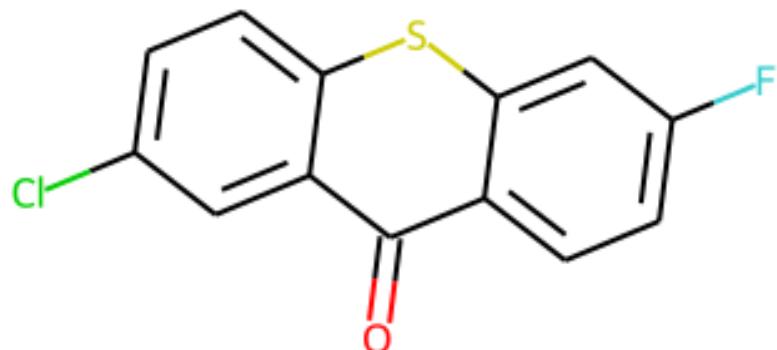
prob: 0.71



No.562

SMILES: O=c1c2ccc(F)cc2sc2ccc(Cl)cc12

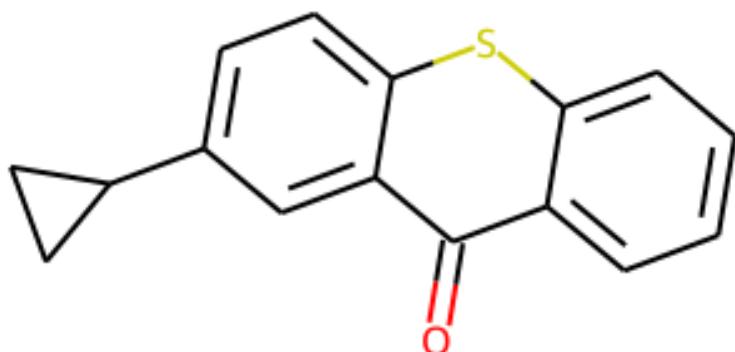
prob: 0.71



No.563

SMILES: O=c1c2cccc2sc2ccc(C3CC3)cc12

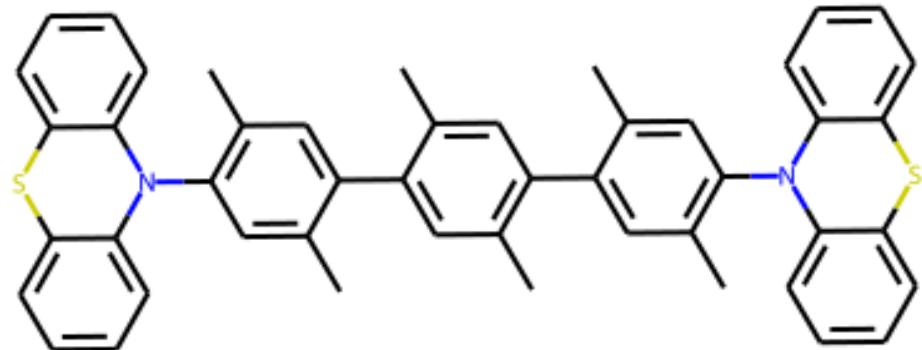
prob: 0.71



No.564

SMILES: Cc1cc(-c2cc(C)c(N3c4cccc4Sc4cccc43)cc2C)c(C)cc1-c1cc(C)c(N2c3cccc3Sc3cccc32)cc1C

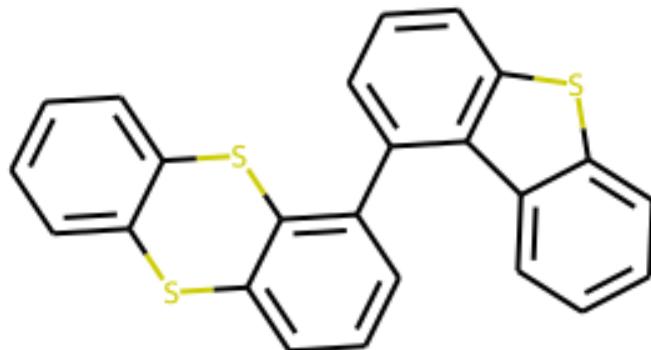
prob: 0.71



No.565

SMILES: c1ccc2c(c1)Sc1cccc(-c3cccc4sc5cccc5c34)c1S2

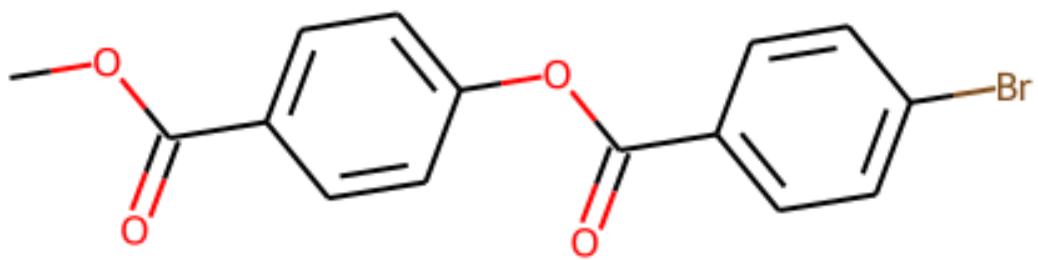
prob: 0.71



No.566

SMILES: COC(=O)c1ccc(OCC(=O)c2ccc(Br)cc2)cc1

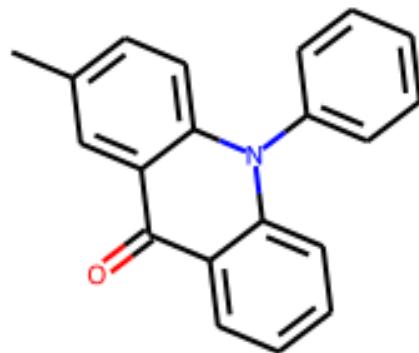
prob: 0.71



No.567

SMILES: Cc1ccc2c(c1)c(=O)c1ccccc1n2-c1ccccc1

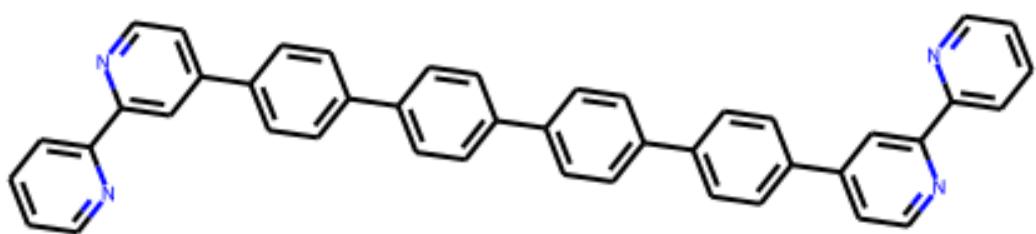
prob: 0.71



No.568

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccc(-c5ccc(-c6ccc(-c7ccnc(-c8cccn8)c7)cc6)cc5)cc4)cc3)ccn2)nc1

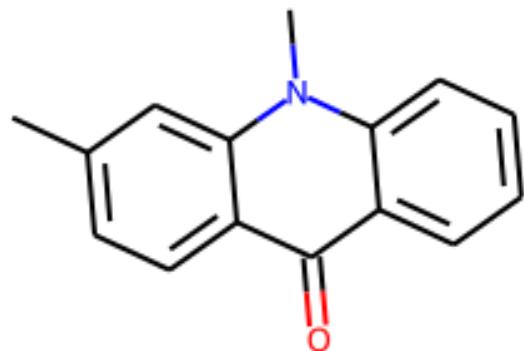
prob: 0.71



No.569

SMILES: Cc1ccc2c(=O)c3ccccc3n(C)c2c1

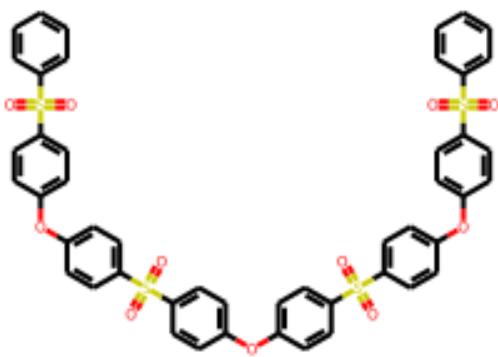
prob: 0.71



No.570

SMILES: O=S(=O)(c1ccccc1)c1ccc(Oc2ccc(S(=O)(=O)c3ccc(Oc4ccc(S(=O)(=O)c5ccc(Oc6cc
c(S(=O)(=O)c7ccccc7)cc6)cc5)cc4)cc3)cc2)cc1

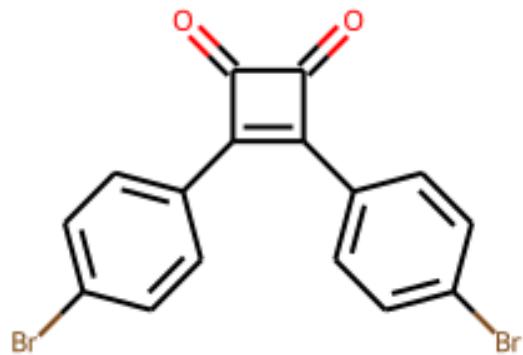
prob: 0.71



No.571

SMILES: O=c1c(-c2ccc(Br)cc2)c(-c2ccc(Br)cc2)c1=O

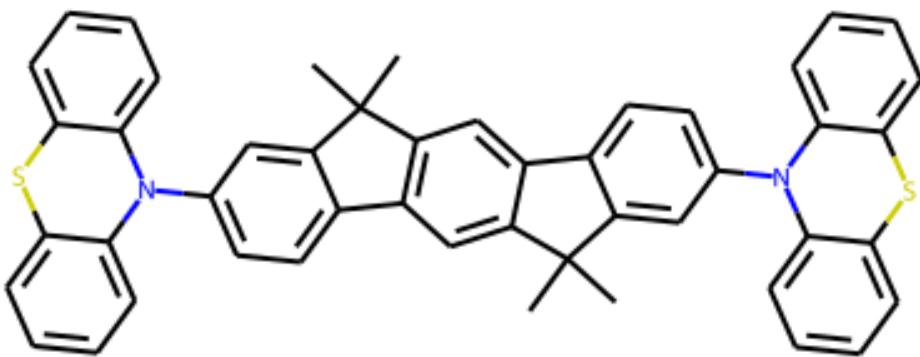
prob: 0.71



No.572

SMILES: CC1(C)c2cc(N3c4cccc4Sc4cccc43)ccc2-c2cc3c(cc21)-c1ccc(N2c4cccc4Sc4ccc42)cc1C3(C)C

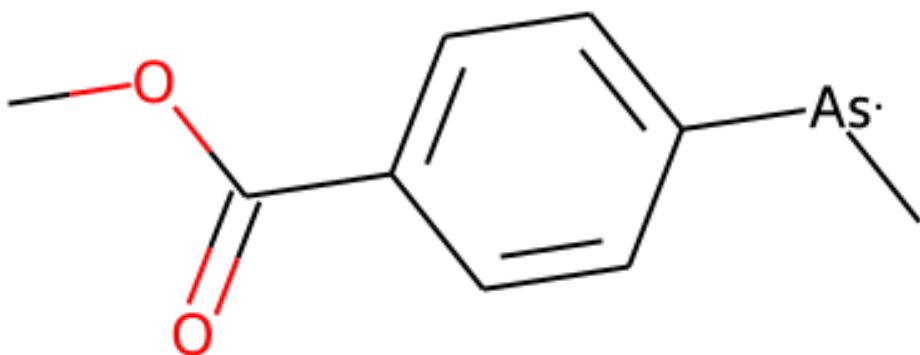
prob: 0.71



No.573

SMILES: COC(=O)c1ccc([As]C)cc1

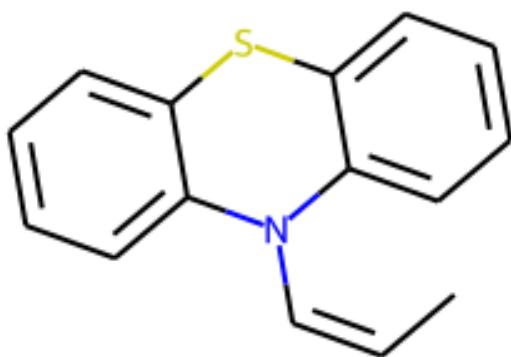
prob: 0.71



No.574

SMILES: C/C=C\N1c2ccccc2Sc2ccccc21

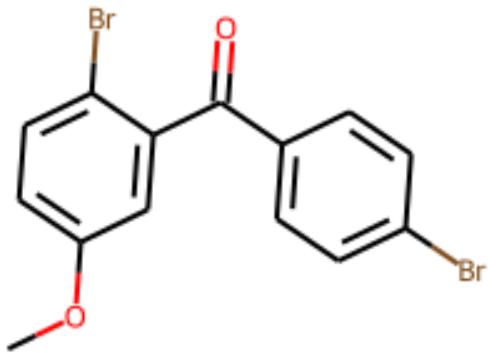
prob: 0.71



No.575

SMILES: C0c1ccc(Br)c(C(=O)c2ccc(Br)cc2)c1

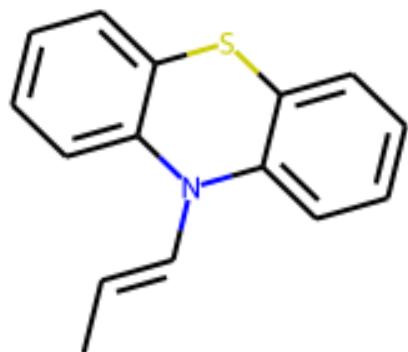
prob: 0.71



No.576

SMILES: CC=CN1c2cccc2Sc2cccc21

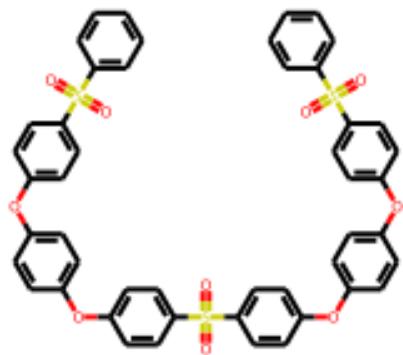
prob: 0.71



No.577

SMILES: O=S(=O)(c1ccccc1)c1ccc(Oc2ccc(Oc3ccc(S(=O)(=O)c4ccc(Oc5ccc(Oc6ccc(S(=O)(=O)c7cccc7)cc6)cc5)cc4)cc3)cc2)cc1

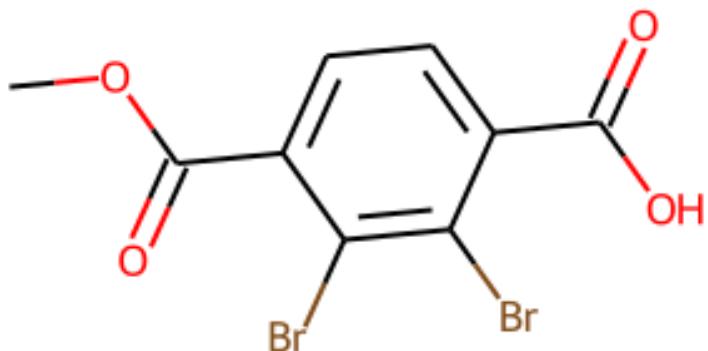
prob: 0.71



No. 578

SMILES: COC(=O)c1ccc(C(=O)O)c(Br)c1Br

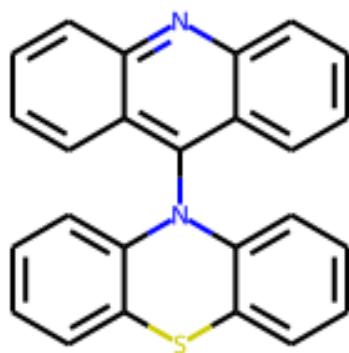
prob: 0.71



No. 579

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1c2ccccc2nc2ccccc12

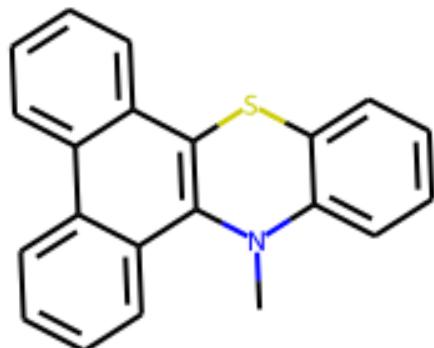
prob: 0.71



No.580

SMILES: CN1c2ccccc2Sc2c1c1ccccc1c1ccccc21

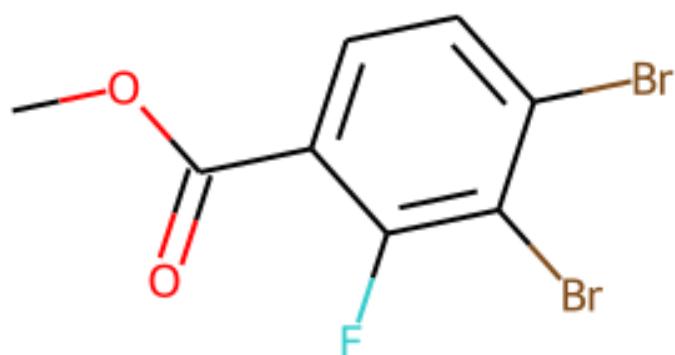
prob: 0.71



No.581

SMILES: COC(=O)c1ccc(Br)c(Br)c1F

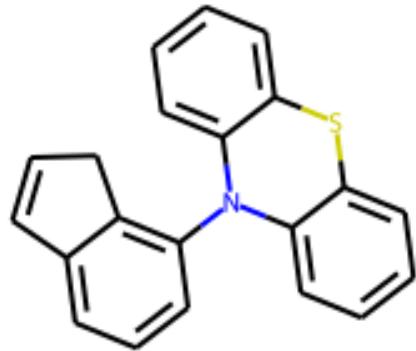
prob: 0.71



No.582

SMILES: C1=Cc2ccccc(N3c4ccccc4Sc4ccccc43)c2C1

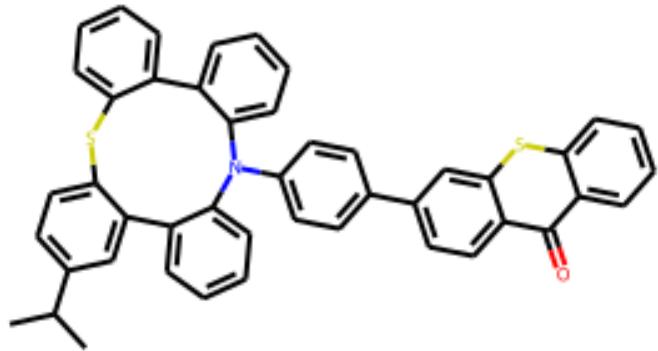
prob: 0.71



No. 583

SMILES: CC(C)c1ccc2c(c1)-c1ccccc1N(c1ccc(-c3ccc4c(=O)c5ccccc5sc4c3)cc1)c1ccccc1-c1ccccc1S2

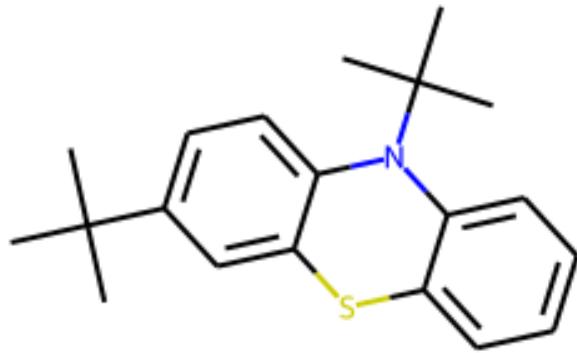
prob: 0.71



No. 584

SMILES: CC(C)(C)c1ccc2c(c1)Sc1ccccc1N2C(C)(C)C

prob: 0.71

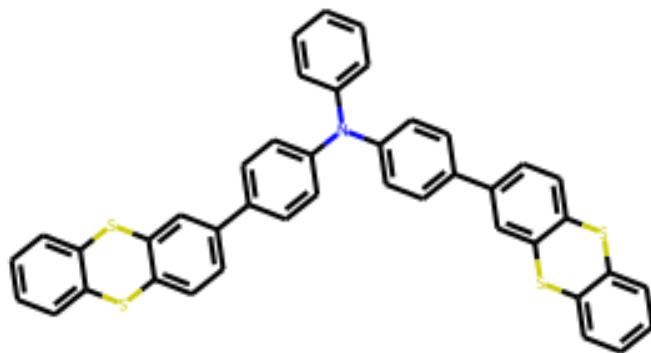


No.585

SMILES:

c1ccc(N(c2ccc(-c3ccc4c(c3)Sc3ccccc3S4)cc2)c2ccc(-c3ccc4c(c3)Sc3ccccc3S4)cc2)cc1

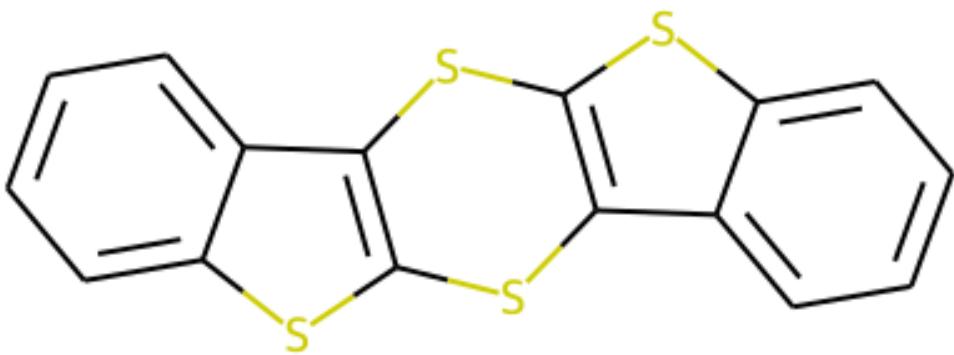
prob: 0.71



No.586

SMILES: c1ccc2c3c(sc2c1)Sc1c(sc2ccccc12)S3

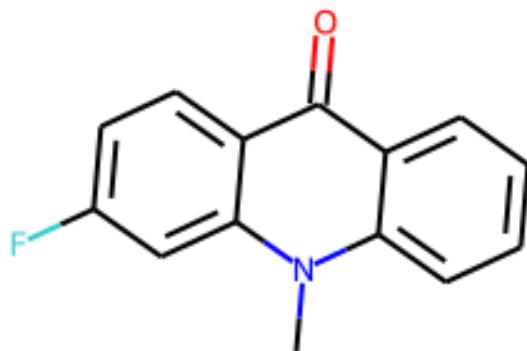
prob: 0.71



No. 587

SMILES: Cn1c2ccccc2c(=O)c2ccc(F)cc21

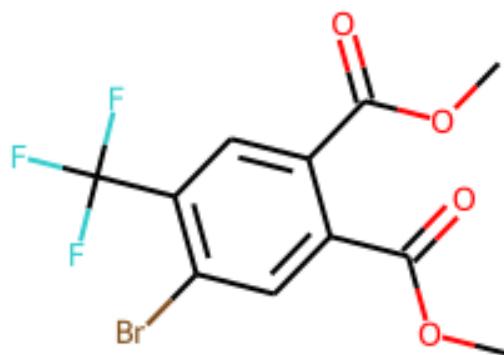
prob: 0.71



No. 588

SMILES: COC(=O)c1cc(Br)c(C(F)(F)F)cc1C(=O)OC

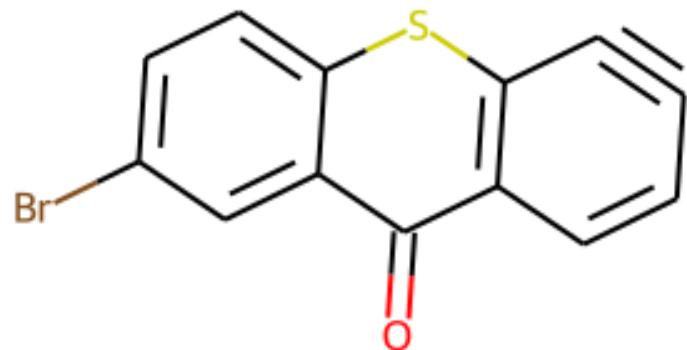
prob: 0.71



No.589

SMILES: O=c1c2ccc#cc2sc2ccc(Br)cc12

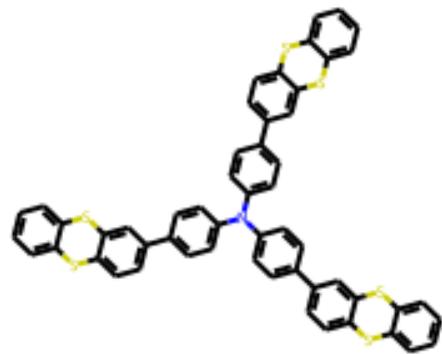
prob: 0.71



No.590

SMILES: c1ccc2c(c1)Sc1ccc(-c3ccc(N(c4ccc(-c5ccc6c(c5)Sc5cccc5S6)cc4)c4ccc(-c5cc
c6c(c5)Sc5cccc5S6)cc4)cc3)cc1S2

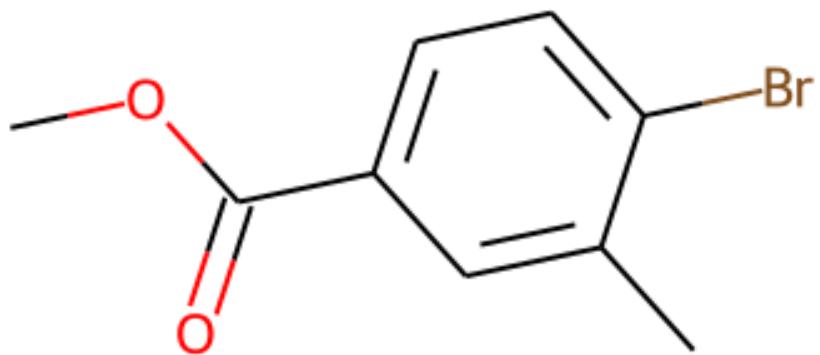
prob: 0.71



No.591

SMILES: COC(=O)c1ccc(Br)c(C)c1

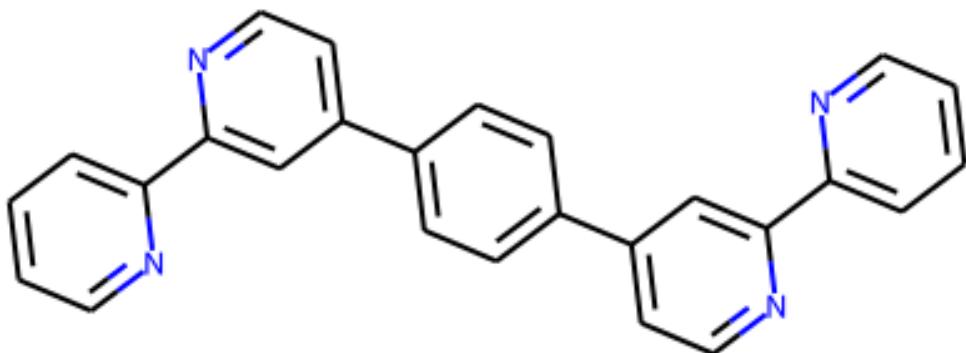
prob: 0.71



No.592

SMILES: c1ccc(-c2cc(-c3ccc(-c4ccnc(-c5ccccc5)c4)cc3)ccn2)nc1

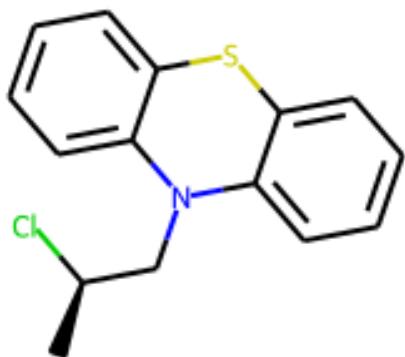
prob: 0.71



No.593

SMILES: C[C@H] (Cl)CN1c2ccccc2Sc2ccccc21

prob: 0.71

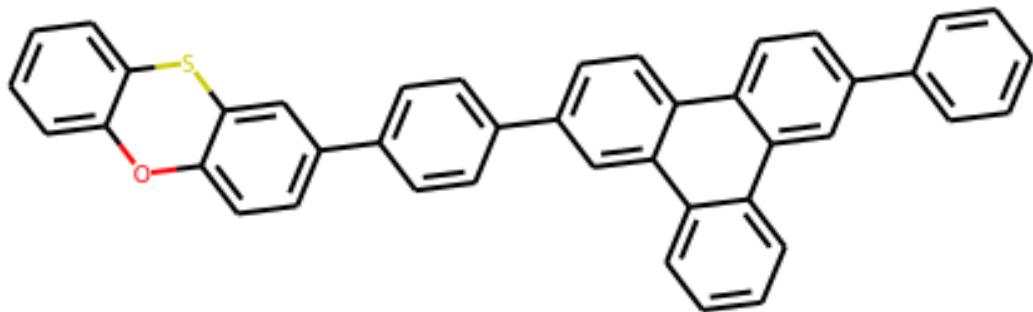


No.594

SMILES:

c1ccc(-c2ccc3c4ccc(-c5ccc(-c6ccc7c(c6)Sc6cccc607)cc5)cc4c4cccc4c3c2)cc1

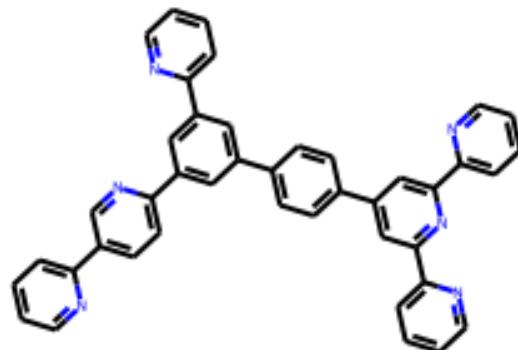
prob: 0.71



No.595

SMILES: c1ccc(-c2ccc(-c3cc(-c4ccc(-c5cc(-c6cccn6)nc(-c6cccn6)c5)cc4)cc(-c4ccccn4)c3)nc2)nc1

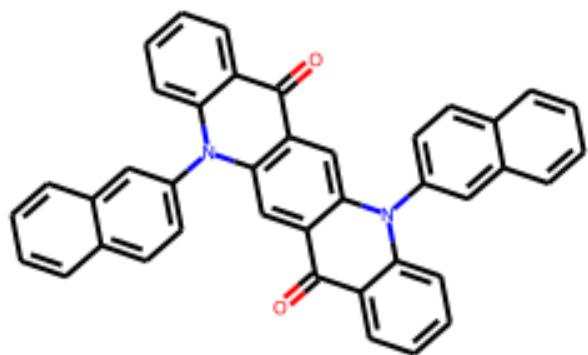
prob: 0.71



No.596

SMILES: O=c1c2ccccc2n(-c2ccc3cccc3c2)c2cc3c(=O)c4cccc4n(-c4ccc5cccc5c4)c3cc12

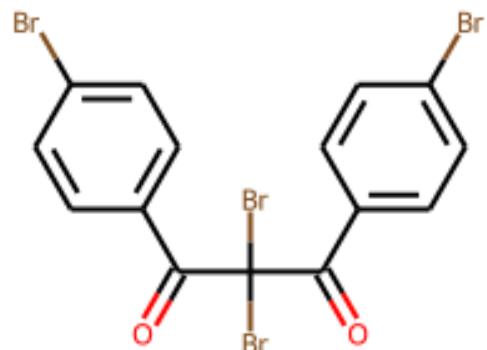
prob: 0.71



No.597

SMILES: O=C(c1ccc(Br)cc1)C(Br)(Br)C(=O)c1ccc(Br)cc1

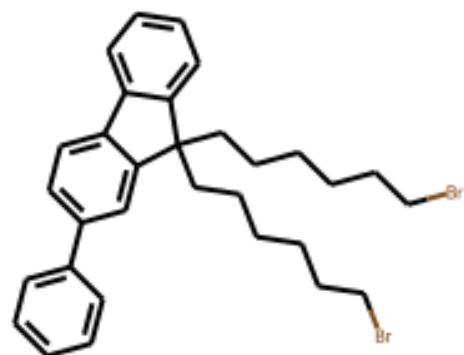
prob: 0.71



No.598

SMILES: BrCCCCCCC1(CCCCCCBr)c2ccccc2-c2ccc(-c3cccc3)cc21

prob: 0.71

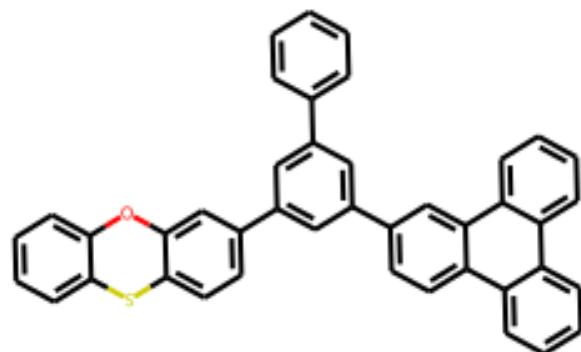


No.599

SMILES:

c1ccc(-c2cc(-c3ccc4c(c3)Oc3cccc3S4)cc(-c3ccc4c5cccc5c5cccc5c4c3)c2)cc1

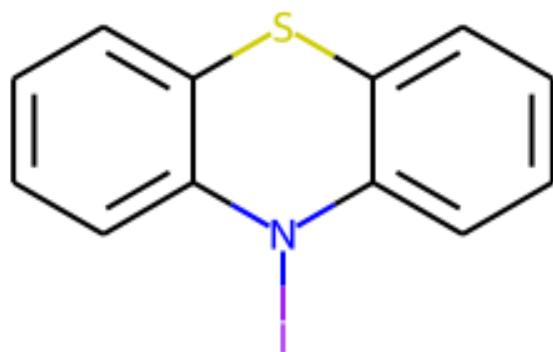
prob: 0.71



No.600

SMILES: IN1c2ccccc2Sc2ccccc21

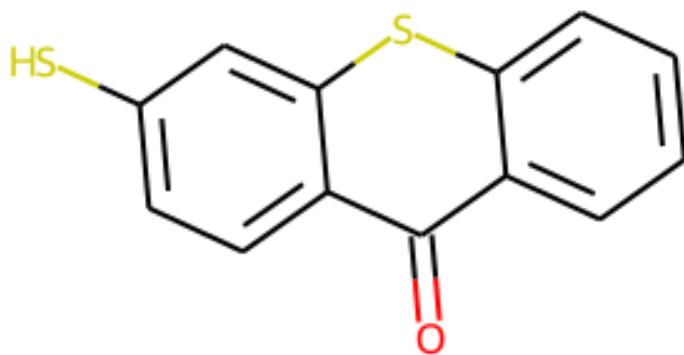
prob: 0.71



No.601

SMILES: O=c1c2ccccc2sc2cc(S)ccc12

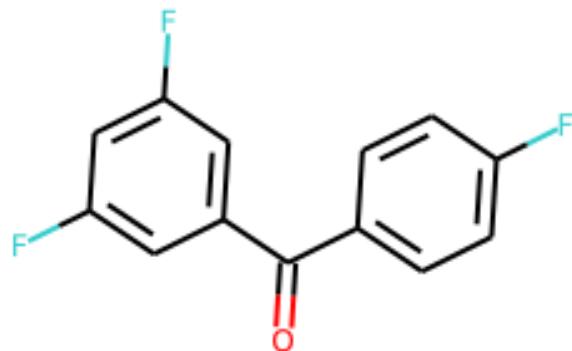
prob: 0.71



No. 602

SMILES: O=C(c1ccc(F)cc1)c1cc(F)cc(F)c1

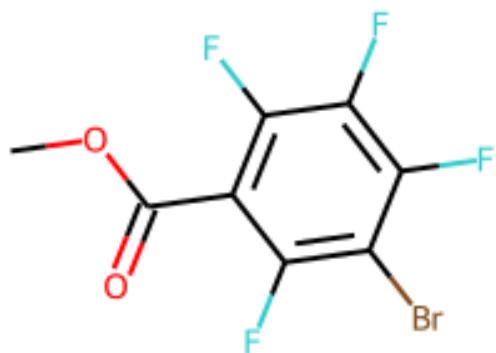
prob: 0.71



No. 603

SMILES: COC(=O)c1c(F)c(F)c(F)c(Br)c1F

prob: 0.71

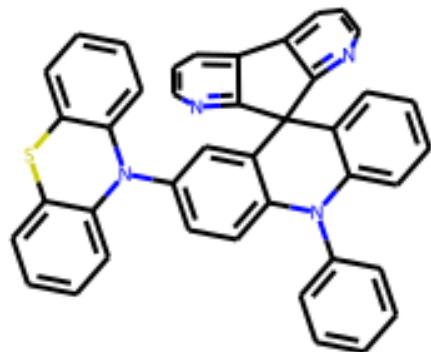


No. 604

SMILES:

c1ccc(N2c3cccc3C3(c4cc(N5c6cccc6Sc6cccc65)ccc42)c2ncccc2-c2cccnc23)cc1

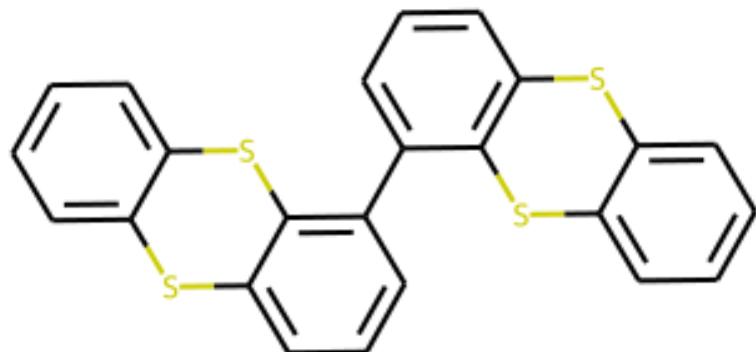
prob: 0.71



No. 605

SMILES: c1ccc2c(c1)Sc1cccc(-c3cccc4c3Sc3cccc3S4)c1S2

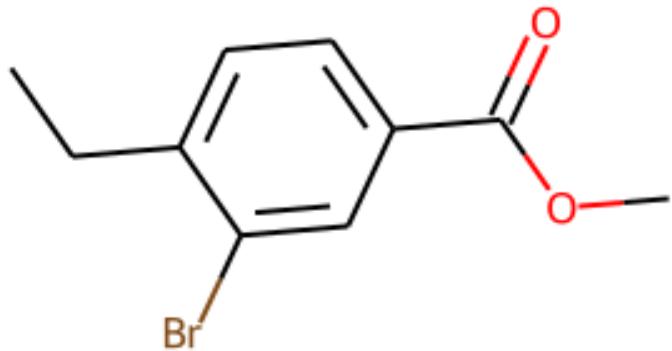
prob: 0.71



No. 606

SMILES: CCc1ccc(C(=O)OC)cc1Br

prob: 0.71

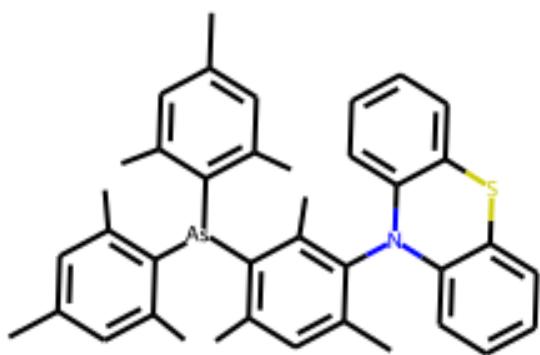


No. 607

SMILES:

Cc1cc(C)c([As](c2cc(C)cc(C)cc2C)c2cc(C)cc(C)c(N3c4cccc4Sc4cccc43)c2C)c(C)c1

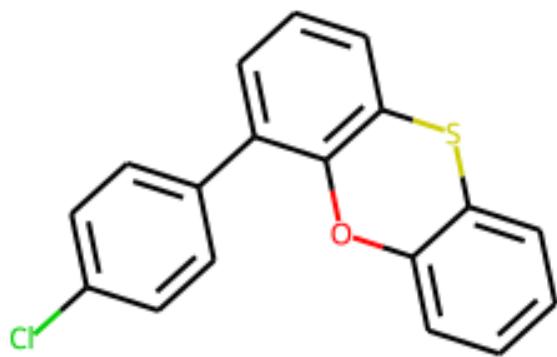
prob: 0.71



No. 608

SMILES: Clc1ccc(-c2cccc3c20c2cccc2S3)cc1

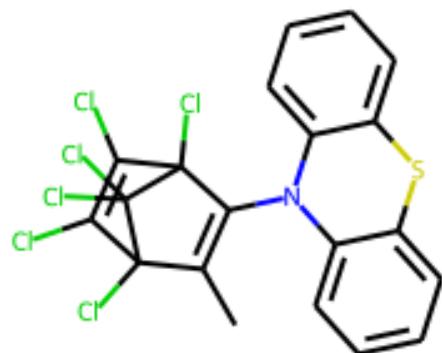
prob: 0.71



No. 609

SMILES: CC1=C(N2c3ccccc3Sc3ccccc32)C2(Cl)C(C1)=C(Cl)C1(C1)C2(Cl)C1

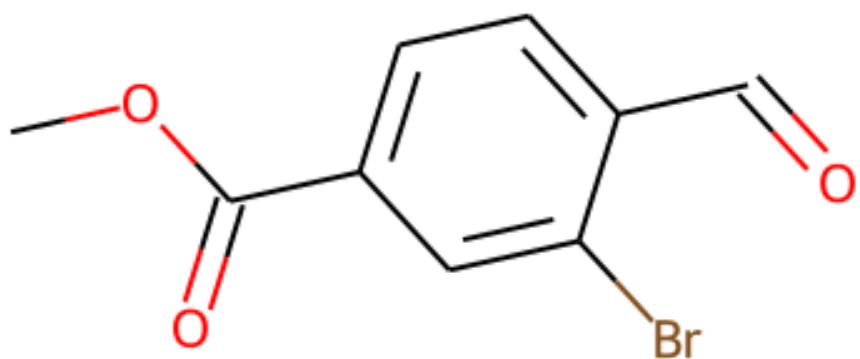
prob: 0.71



No. 610

SMILES: COC(=O)c1ccc(C=O)c(Br)c1

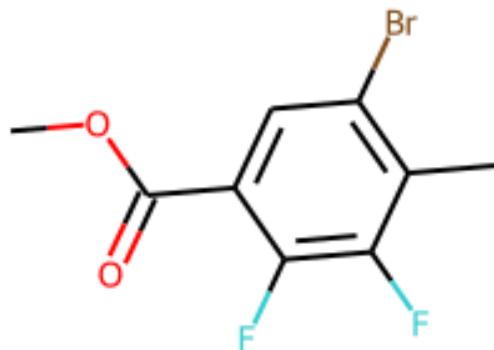
prob: 0.71



No. 611

SMILES: COC(=O)c1cc(Br)c(C)c(F)c1F

prob: 0.71

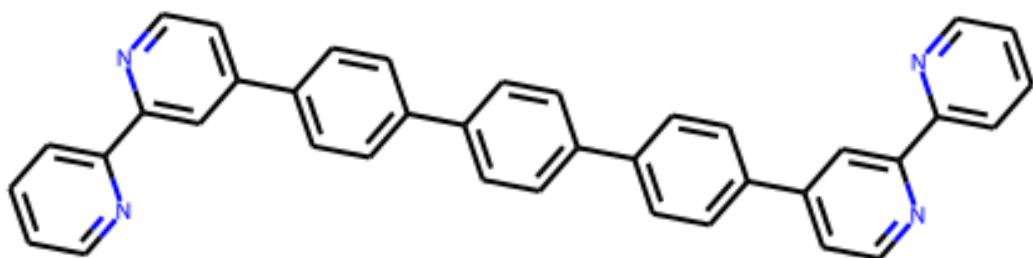


No. 612

SMILES:

c1cccc(-c2cc(-c3ccc(-c4ccc(-c5ccc(-c6ccnc(-c7cccn7)c6)cc5)cc4)cc3)ccn2)nc1

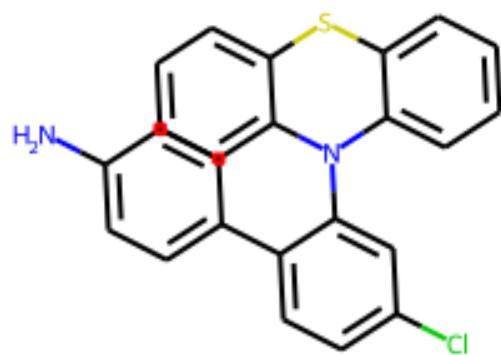
prob: 0.71



No. 613

SMILES: Nc1ccc(-c2ccc(Cl)cc2N2c3cccc3Sc3cccc32)cc1

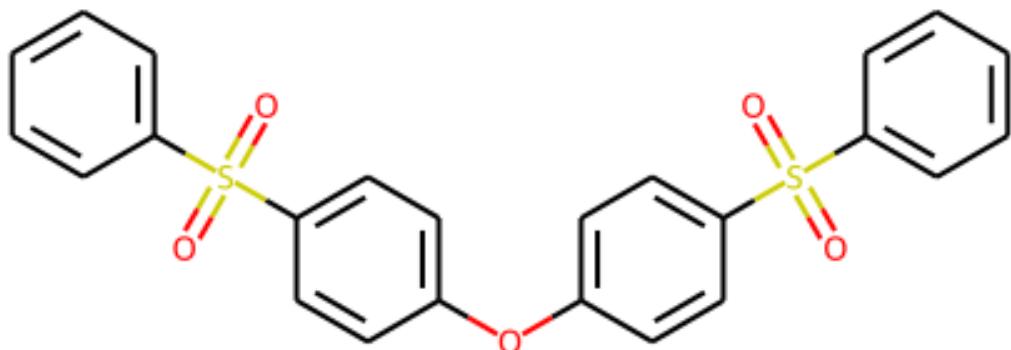
prob: 0.71



No. 614

SMILES: O=S(=O)(c1ccccc1)c1ccc(Oc2ccc(S(=O)(=O)c3ccccc3)cc2)cc1

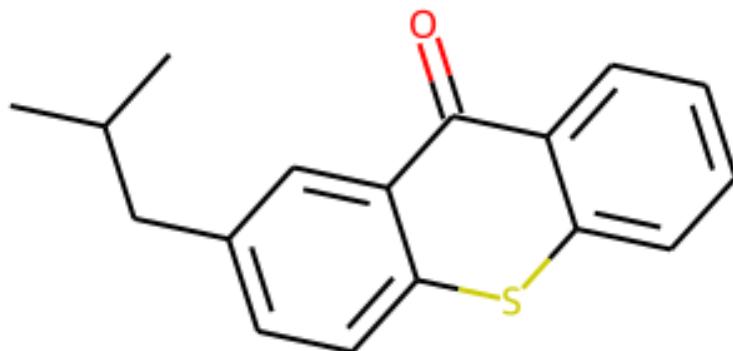
prob: 0.71



No. 615

SMILES: CC(C)Cc1ccc2sc3ccccc3c(=O)c2c1

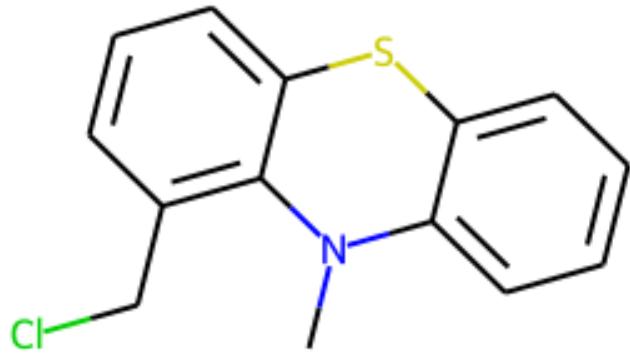
prob: 0.71



No. 616

SMILES: CN1c2ccccc2Sc2cccc(CCl)c21

prob: 0.7075



No. 617

SMILES: c1ccc2c(c1)Sc1ccccc1N2c1cc2scCc2s1

prob: 0.7033333333333335

