Molecule 1

SMILES: [13C-]#[O+]

Molecular Formula: CO

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.647 ± 1.578

Molecule 2

SMILES: [13CH3]O

Molecular Formula: CH$_4$O

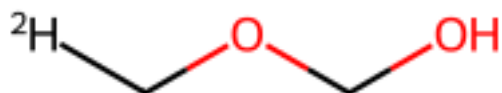Predicted Column Density ($\log_{10}$ cm^{-2}): 16.803 ± 1.596

Molecule 3

SMILES: [H]OC([H])([H])OC([H])([H])[2H]

Molecular Formula: C$_2$H$_6$O$_2$

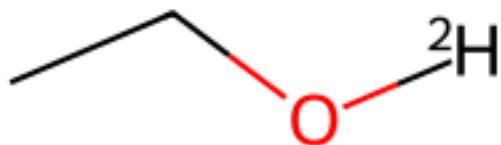Predicted Column Density ($\log_{10}$ cm^{-2}): 16.283 ± 1.259

Molecule 4

SMILES: [H]C([H])([H])C([H])([H])O[2H]

Molecular Formula: C_2H_6O

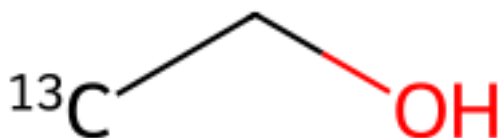Predicted Column Density ($\log_{10}$ cm^{-2}): 16.280 ± 1.214

Molecule 5

SMILES: [13CH3]CO

Molecular Formula: C_2H_6O

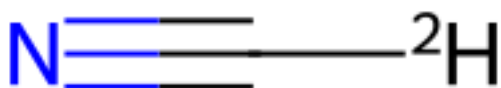Predicted Column Density ($\log_{10}$ cm^{-2}): 16.080 ± 1.687

Molecule 6

SMILES: [2H]C#N

Molecular Formula: CHN

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.060 ± 1.181
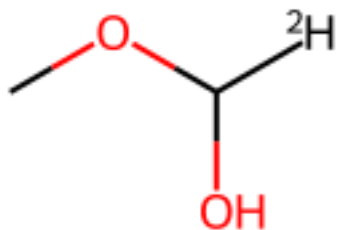
Molecule 7

SMILES: [H]OC([H])([2H])OC([H])([H])[H]

Molecular Formula: $C_2H_6O_2$

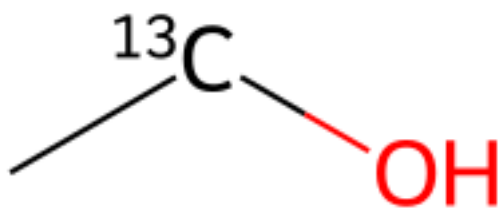Predicted Column Density ($\log_{10}$ cm^{-2}): 16.037 ± 1.647

Molecule 8

SMILES: C[13CH2]O

Molecular Formula: C_2H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.024 ± 1.642

Molecule 9

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

Molecular Formula: C_2H_4O
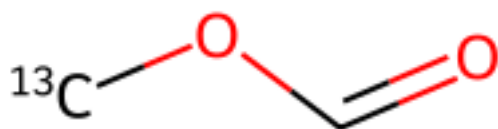
Predicted Column Density ($\log_{10}$ cm^{-2}): 15.913 ± 2.090

Molecule 10

SMILES: [13CH3]OC=O

Molecular Formula: $C_2H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.803 ± 1.708
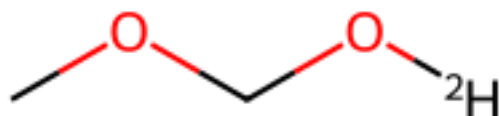
Molecule 11

SMILES: [H]C([H])([H])OC([H])([H])O[2H]

Molecular Formula: $C_2H_6O_2$

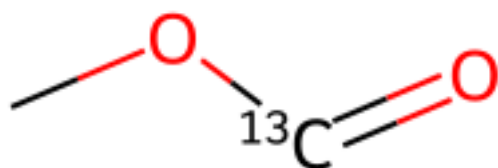Predicted Column Density ($\log_{10}$ cm^{-2}): 15.788 ± 1.464

Molecule 12

SMILES: CO[13CH]=O

Molecular Formula: $C_2H_4O_2$
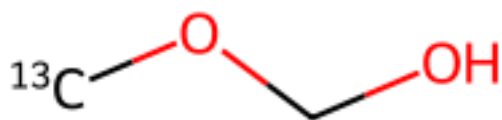
Predicted Column Density ($\log_{10}$ cm^{-2}): 15.685 ± 1.339

Molecule 13

SMILES: [13CH3]OCO

Molecular Formula: $C_2H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.532 ± 1.846
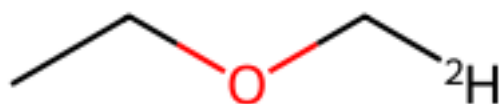

Molecule 14

SMILES: [H]C([H])([2H])OC([H])([H])C([H])([H])[H]

Molecular Formula: C_3H_8O

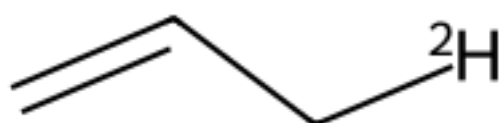Predicted Column Density ($\log_{10}$ cm^{-2}): 15.500 ± 1.364

Molecule 15

SMILES: [H]C([H])=C([H])C([H])([H])[2H]

Molecular Formula: C_3H_6

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.498 ± 1.523

Molecule 16

SMILES: [H]C([2H])=C([H])C([H])([H])[H]

Molecular Formula: C_3H_6

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.498 ± 1.523

Molecule 17
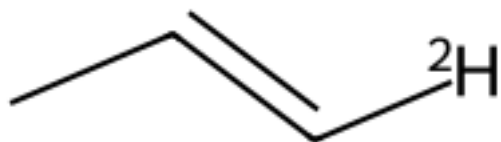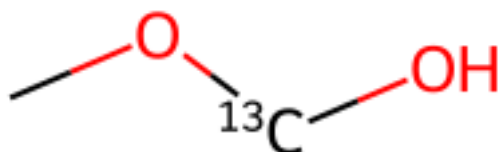
SMILES: CO[13CH2]O

Molecular Formula: $C_2H_6O_2$

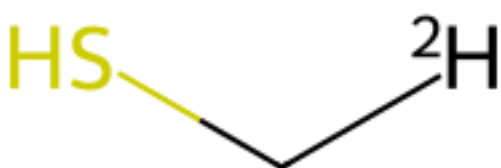Predicted Column Density ($\log_{10}$ cm^{-2}): 15.477 ± 2.118

Molecule 18

SMILES: [H]SC([H])([H])[2H]

Molecular Formula: CH_4S

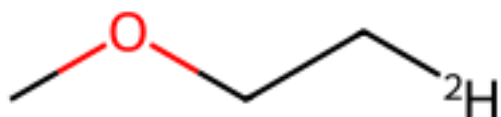Predicted Column Density ($\log_{10}$ cm^{-2}): 15.454 ± 1.194

Molecule 19

SMILES: [H]C([H])([H])OC([H])([H])C([H])([H])[2H]

Molecular Formula: C_3H_8O

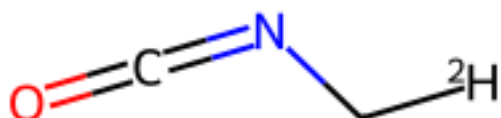Predicted Column Density ($\log_{10}$ cm^{-2}): 15.278 ± 1.429

Molecule 20

SMILES: [H]C([H])([2H])N=C=O

Molecular Formula: C_2H_3NO

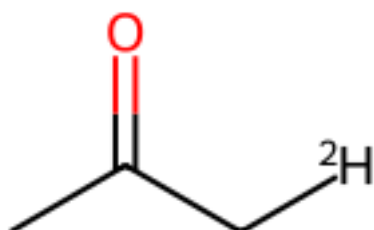Predicted Column Density ($\log_{10}$ cm^{-2}): 15.194 ± 1.229

Molecule 21

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

Molecular Formula: C_3H_6O

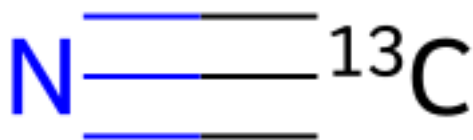Predicted Column Density ($\log_{10}$ cm^{-2}): 15.098 ± 1.239

Molecule 22

SMILES: [13CH]#N

Molecular Formula: CHN

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.047 ± 1.538

Molecule 23
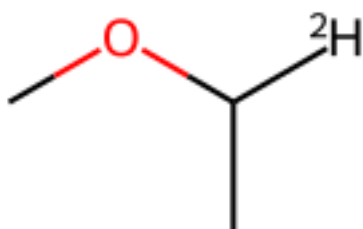
SMILES: [H]C([H])([H])OC([H])([2H])C([H])([H])[H]

Molecular Formula: C_3H_8O

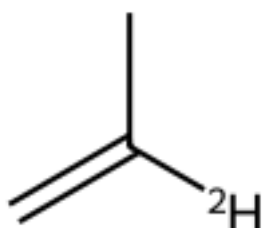Predicted Column Density ($\log_{10}$ cm^{-2}): 15.032 ± 1.486

Molecule 24

SMILES: [H]C([H])=C([2H])C([H])([H])[H]

Molecular Formula: C_3H_6
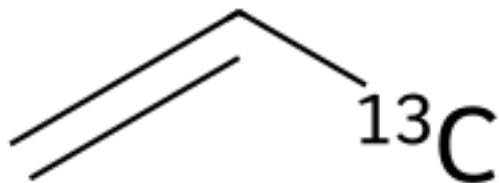
Predicted Column Density ($\log_{10}$ cm^{-2}): 15.031 ± 1.898

Molecule 25

SMILES: C=C[13CH3]

Molecular Formula: C_3H_6

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.025 ± 2.073

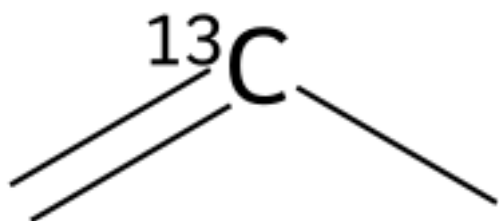## Molecule 26

SMILES: C=[13CH]C

Molecular Formula: C_3H_6

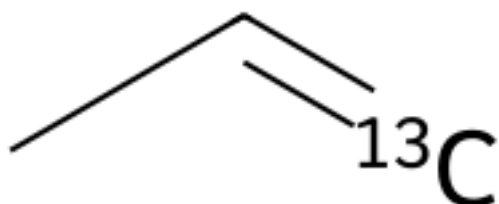Predicted Column Density ($\log_{10}$ cm^{-2}): 14.962 ± 1.690

Molecule 27

SMILES: CC=[13CH2]

Molecular Formula: C_3H_6

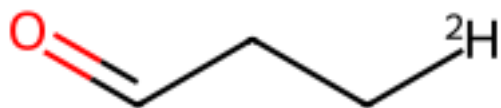Predicted Column Density ($\log_{10}$ cm^{-2}): 14.962 ± 1.690

Molecule 28

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

Molecular Formula: C_3H_6O

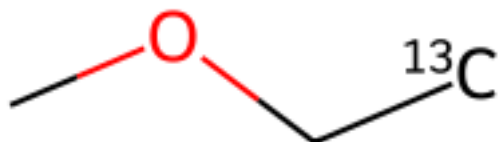Predicted Column Density ($\log_{10}$ cm^{-2}): 14.864 ± 2.169

Molecule 29

SMILES: COC[13CH3]

Molecular Formula: C_3H_8O

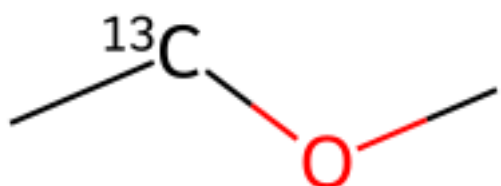Predicted Column Density ($\log_{10}$ cm^{-2}): 14.805 ± 2.026

Molecule 30

SMILES: C[13CH2]OC

Molecular Formula: C_3H_8O

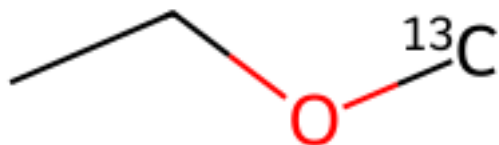Predicted Column Density ($\log_{10}$ cm^{-2}): 14.749 ± 1.983

Molecule 31

SMILES: CCO[13CH3]

Molecular Formula: C_3H_8O

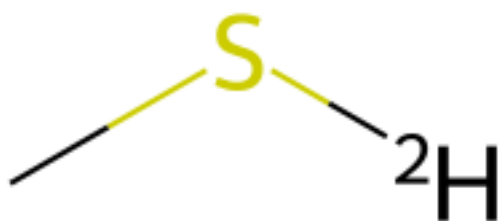Predicted Column Density ($\log_{10}$ cm^{-2}): 14.749 ± 1.983

Molecule 32

SMILES: [H]C([H])([H])S[2H]

Molecular Formula: CH_4S

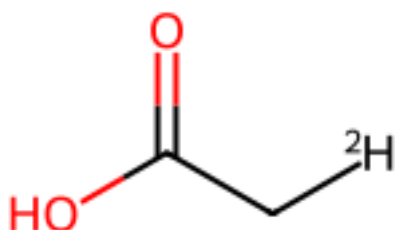Predicted Column Density ($\log_{10}$ cm^{-2}): 14.668 ± 1.529

Molecule 33

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

Molecular Formula: $C_2H_4O_2$

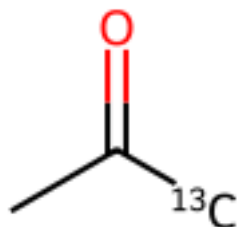Predicted Column Density ($\log_{10}$ cm^{-2}): 14.646 ± 3.392

Molecule 34

SMILES: CC([13CH3])=O

Molecular Formula: C_3H_6O

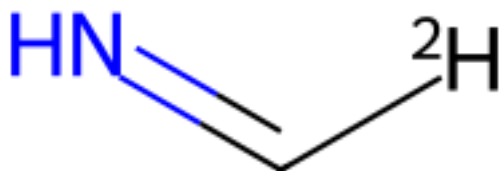Predicted Column Density ($\log_{10}$ cm^{-2}): 14.625 ± 1.873

Molecule 35

SMILES: [H]N=C([H])[2H]

Molecular Formula: CH_3N

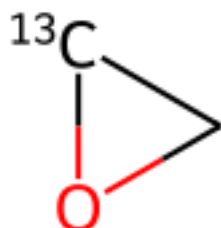Predicted Column Density ($\log_{10}$ cm^{-2}): 14.607 ± 2.638

Molecule 36

SMILES: C1[13CH2]O1

Molecular Formula: C_2H_4O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.599 ± 1.799

Molecule 37

SMILES: [13CH3]S

Molecular Formula: CH_4S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.513 ± 1.935

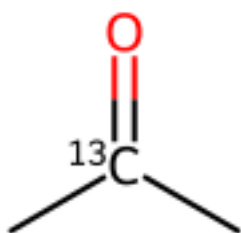## Molecule 38

SMILES: C[13C](C)=O

Molecular Formula: C_3H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.507 ± 1.270
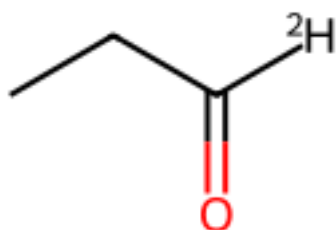

Molecule 39

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

Molecular Formula: C_3H_6O

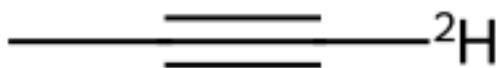Predicted Column Density ($\log_{10}$ cm^{-2}): 14.483 ± 2.146

Molecule 40

SMILES: [H]C([H])([H])C#C[2H]

Molecular Formula: C_3H_4

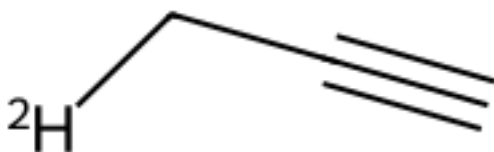Predicted Column Density ($\log_{10}$ cm^{-2}): 14.477 ± 5.290

Molecule 41

SMILES: [H]C#CC([H])([H])[2H]

Molecular Formula: C_3H_4

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.477 ± 5.290
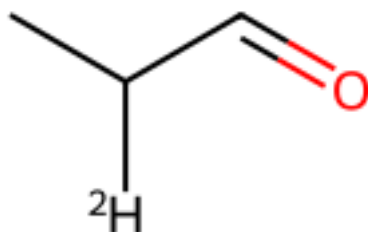

Molecule 42

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

Molecular Formula: C_3H_6O

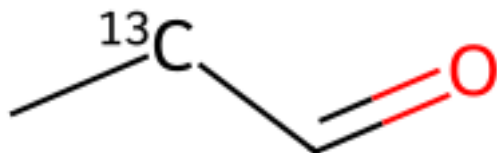Predicted Column Density ($\log_{10}$ cm^{-2}): 14.396 ± 2.409

Molecule 43

SMILES: C[13CH2]C=O

Molecular Formula: C_3H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.390 ± 2.586

Molecule 44
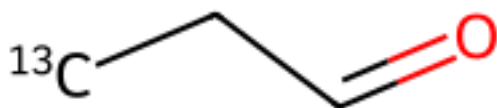
SMILES: [13CH3]CC=O

Molecular Formula: C_3H_6O
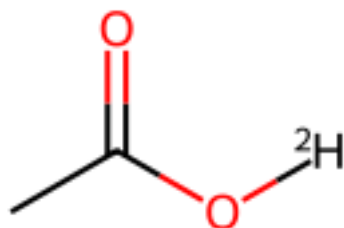
Predicted Column Density ($\log_{10}$ cm^{-2}): 14.390 ± 2.586

Molecule 45

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

Molecular Formula: $C_2H_4O_2$

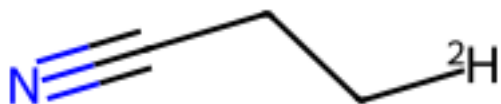Predicted Column Density ($\log_{10}$ cm^{-2}): 14.372 ± 3.395

Molecule 46

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

Molecular Formula: C_3H_5N

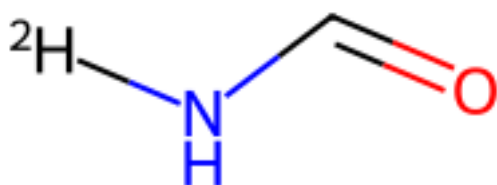Predicted Column Density ($\log_{10}$ cm^{-2}): 14.302 ± 1.358

Molecule 47

SMILES: [H]C(=O)N([H])[2H]

Molecular Formula: CH_3NO

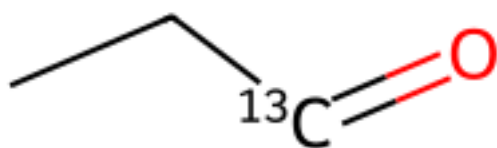Predicted Column Density ($\log_{10}$ cm^{-2}): 14.286 ± 1.383

Molecule 48

SMILES: CC[13CH]=O

Molecular Formula: C_3H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.272 ± 2.127
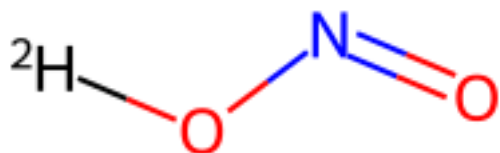
Molecule 49

SMILES: [2H]ON=O

Molecular Formula: HNO_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.270 ± 1.799

Molecule 50

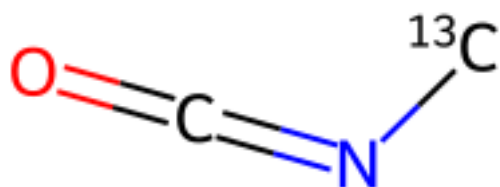SMILES: [13CH3]N=C=O

Molecular Formula: C_2H_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.254 ± 1.915

Molecule 51

SMILES: [13CH3]C(=O)O

Molecular Formula: $C_2H_4O_2$
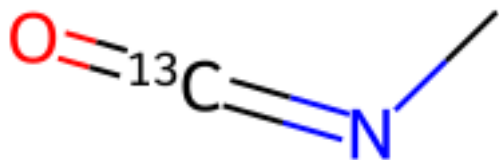
Predicted Column Density ($\log_{10}$ cm^{-2}): 14.173 ± 3.737
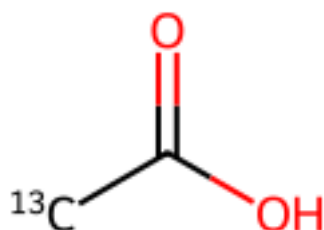
Molecule 52

SMILES: CN=[13C]=O

Molecular Formula: C_2H_3NO

Predicted Column Density (log_{10} cm^{-2}): 14.126 ± 1.433

Molecule 53

SMILES: C#C[13CH3]

Molecular Formula: C_3H_4

Predicted Column Density (log_{10} cm^{-2}): 14.004 ± 5.416
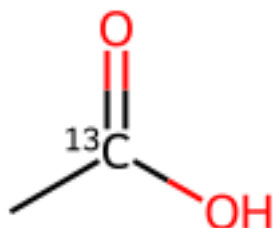

Molecule 54

SMILES: C[13C](=O)O

Molecular Formula: $C_2H_4O_2$

Predicted Column Density (log_{10} cm^{-2}): 13.999 ± 3.403

Molecule 55

SMILES: [13C-]#[S+]

Molecular Formula: CS

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.938 ± 1.589

Molecule 56
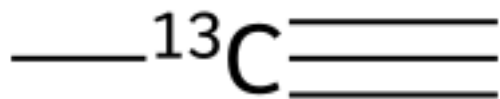
SMILES: C#[13C]C

Molecular Formula: C_3H_4

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.932 ± 5.342
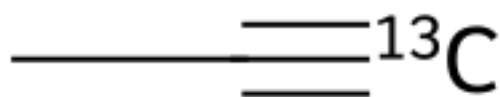
Molecule 57

SMILES: CC#[13CH]

Molecular Formula: C_3H_4

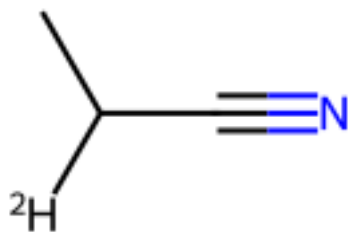Predicted Column Density ($\log_{10}$ cm^{-2}): 13.932 ± 5.342

Molecule 58

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

Molecular Formula: C_3H_5N

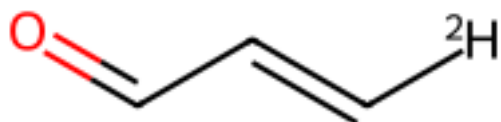Predicted Column Density ($\log_{10}$ cm^{-2}): 13.835 ± 1.731

Molecule 59

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

Molecular Formula: C_3H_4O

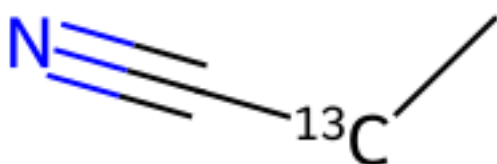Predicted Column Density ($\log_{10}$ cm^{-2}): 13.831 ± 1.444

Molecule 60

SMILES: C[13CH2]C#N

Molecular Formula: C_3H_5N
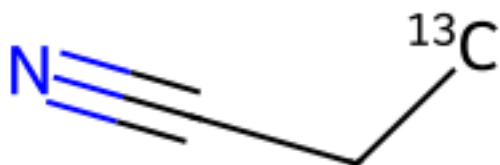
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.829 ± 1.920

Molecule 61

SMILES: [13CH3]CC#N

Molecular Formula: C_3H_5N
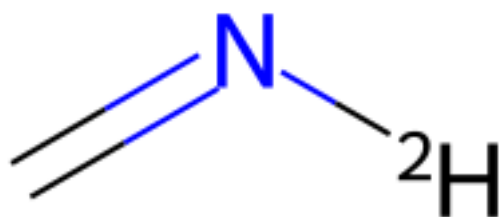
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.829 ± 1.920

Molecule 62

SMILES: [H]C([H])=N[2H]

Molecular Formula: CH_3N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.822 ± 2.723

Molecule 63

SMILES: [H]N([H])C(=O)C([H])([H])[2H]

Molecular Formula: C_2H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.820 ± 1.387

Molecule 64

SMILES: CC[13C]#N

Molecular Formula: C_3H_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.756 ± 1.652

Molecule 65

SMILES: [H]C([2H])=C([H])C#N

Molecular Formula: C_3H_3N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.689 ± 3.957

Molecule 66

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

Molecular Formula: $C_3H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.617 ± 1.467

Molecule 67

SMILES: [13CH2]=N

Molecular Formula: CH_3N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.604 ± 2.817

Molecule 68

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

Molecular Formula: $C_3H_4O_2$
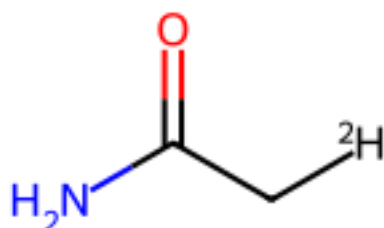
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.589 ± 1.548

Molecule 69

SMILES: [H]N([2H])C(=O)C([H])([H])[H]

Molecular Formula: C_2H_5NO

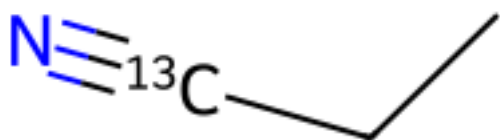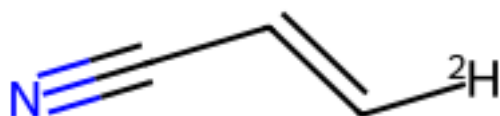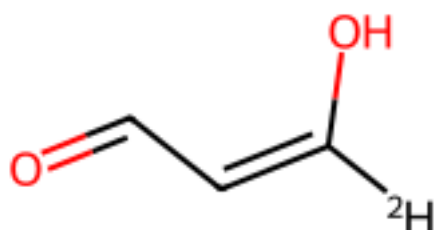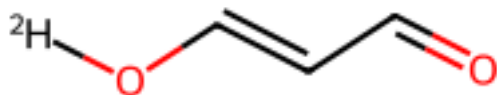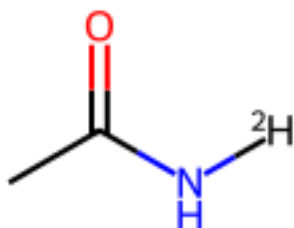Predicted Column Density ($\log_{10}$ cm^{-2}): 13.502 ± 1.601

Molecule 70

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

Molecular Formula: $C_3H_4O_2$

Predicted Column Density (log_{10} cm^{-2}): 13.482 ± 1.498

Molecule 71

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

Molecular Formula: C_3H_4O

Predicted Column Density (log_{10} cm^{-2}): 13.451 ± 1.520

Molecule 72

SMILES: [13CH2]=S

Molecular Formula: CH_2S
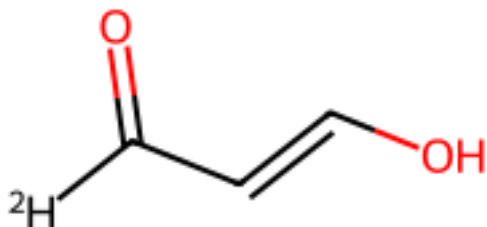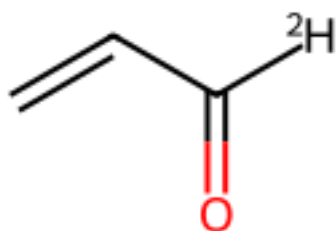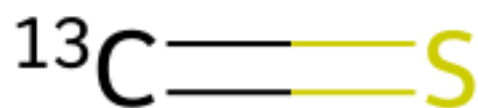
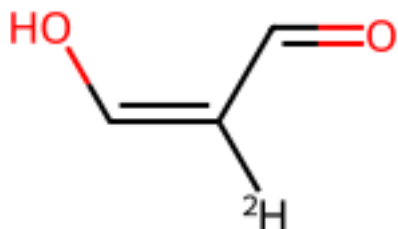Predicted Column Density (log_{10} cm^{-2}): 13.396 ± 1.315

Molecule 73

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

Molecular Formula: $C_3H_4O_2$

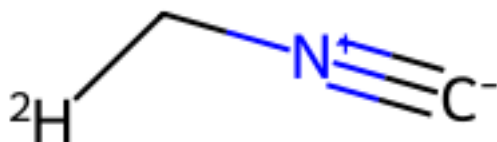Predicted Column Density ($\log_{10}$ cm^{-2}): 13.395 ± 1.805

Molecule 74

SMILES: [H]C([H])([2H])[N+]#[C-]

Molecular Formula: C_2H_3N

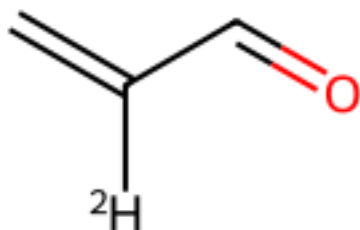Predicted Column Density ($\log_{10}$ cm^{-2}): 13.383 ± 1.474

Molecule 75

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

Molecular Formula: C_3H_4O

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.364 ± 1.830

Molecule 76

SMILES: [13CH3]C(N)=O

Molecular Formula: C_2H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.347 ± 1.980
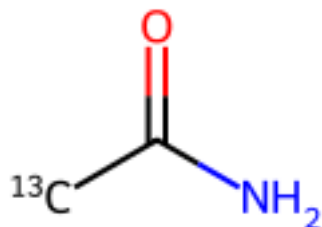
Molecule 77

SMILES: O=C[13CH]=CO

Molecular Formula: $C_3H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.327 ± 1.597
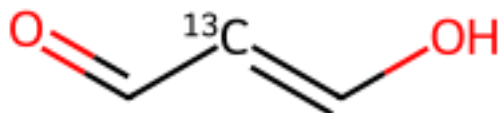

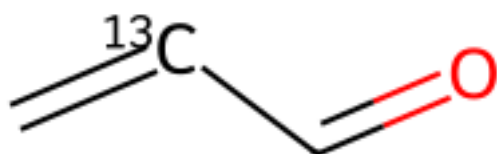## Molecule 78

SMILES: C=[13CH]C=O

Molecular Formula: C_3H_4O

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.295 ± 1.614

Molecule 79
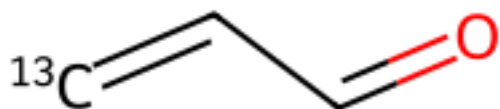
SMILES: [13CH2]=CC=O

Molecular Formula: C_3H_4O

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.295 ± 1.614
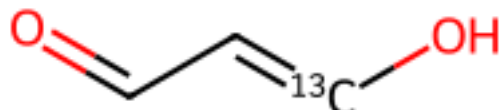

Molecule 80

SMILES: O=CC=[13CH]O

Molecular Formula: $C_3H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.271 ± 1.414

Molecule 81
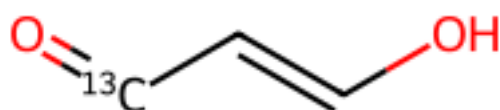
SMILES: O=[13CH]C=CO

Molecular Formula: $C_3H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.271 ± 1.414

Molecule 82
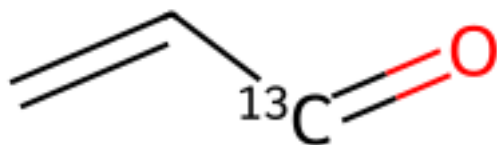
SMILES: C=C[13CH]=O

Molecular Formula: C_3H_4O

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.240 ± 1.456

Molecule 83

SMILES: C[13C](N)=O

Molecular Formula: C_2H_5NO
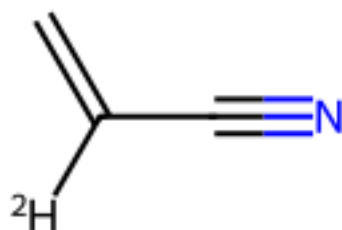
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.229 ± 1.397

Molecule 84

SMILES: [H]C([H])=C([2H])C#N

Molecular Formula: C_3H_3N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.222 ± 4.101

Molecule 85

SMILES: C=[13CH]C#N

Molecular Formula: C_3H_3N

Predicted Column Density (log_{10} cm^{-2}): 13.154 ± 4.016

Molecule 86

SMILES: [13CH2]=CC#N

Molecular Formula: C_3H_3N

Predicted Column Density (log_{10} cm^{-2}): 13.154 ± 4.016
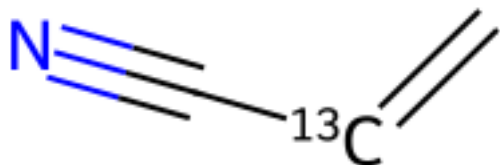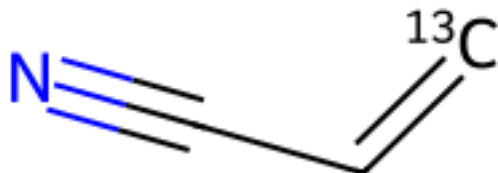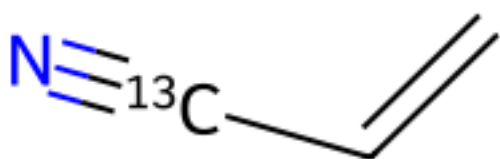
Molecule 87

SMILES: C=C[13C]#N

Molecular Formula: C_3H_3N

Predicted Column Density (log_{10} cm^{-2}): 13.144 ± 4.032

Molecule 88
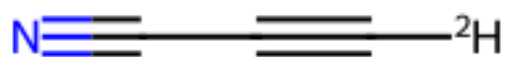
SMILES: [2H]C#CC#N

Molecular Formula: C_3HN

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.144 ± 4.782

$N\equiv\!\!\!\equiv\!\!\!\!-\!\!\!-\!\!\!\equiv\!\!\!\equiv\!\!\!\!-^2H$

Molecule 89

SMILES: C#C[13C]#N

Molecular Formula: C_3HN

Predicted Column Density ($\log_{10}$ cm^{-2}): 12.598 ± 4.811

$N\equiv\!\!\!\equiv^{13}C\!\!\!-\!\!\!-\!\!\!\equiv\!\!\!\equiv$

Molecule 90

SMILES: C#[13C]C#N

Molecular Formula: C_3HN

Predicted Column Density ($\log_{10}$ cm^{-2}): 12.598 ± 4.811

$N\equiv\!\!\!\equiv\!\!\!\!-^{13}C\!\!\!\equiv\!\!\!\equiv$

Molecule 91

SMILES: [13CH]#CC#N

Molecular Formula: C$_3$HN

Predicted Column Density (log$_{10}$ cm^{-2}): 12.598 ± 4.811

$$N\equiv\!\!=\!\!\equiv\!\!=\!\!^{13}C$$

Molecule 92

SMILES: [C-]#[N+][13CH3]

Molecular Formula: C$_2$H$_3$N

Predicted Column Density (log$_{10}$ cm^{-2}): 12.443 ± 2.094

$$^{13}C\!-\!N^+\!\equiv\!C^-$$

Molecule 93

SMILES: C[N+]#[13C-]

Molecular Formula: C$_2$H$_3$N

Predicted Column Density (log$_{10}$ cm^{-2}): 12.370 ± 1.832

$$-\!N^+\!\equiv\!^{13}C^-$$