```
 1 C:\Users\Minh\anaconda3\envs\my-rdkit-env\python.exe D:\Minh\Books\
   Research\Accelerated-Paper\Github\scripts\prepare_dataset.py
 2 Start indexing over 519758 rows.
 3 Index: [(0, 'Br/C1=C\\CCCCCC1'),
 4  (8, 'Br/C=C/C1CCCCC1'),
 5  (16, 'Br/C=C/Cc1ccccc1'),
 6  (25, 'Br/C=C/[C@@H]1CC=CCC1'),
 7  (35, 'Br/C=C/[C@H]1CC=CCC1'),
 8  (45, 'Br/C=C/c1ccccn1'),
 9  (53, 'Br/C=C/c1cccnc1'),
10  (60, 'Br/C=C\\c1ccccc1'),
11  (67, 'Br/C=C\\c1ccccn1'),
12  (75, 'BrC(Br)(Br)Br')]
13 Start filtering over 519758 rows with 63229 partitions.
14 Completed 1000 partitions under 3.54 seconds with progress 1.58%.
15 Completed 2000 partitions under 4.06 seconds with progress 3.16%.
16 Completed 3000 partitions under 4.54 seconds with progress 4.74%.
17 Expected: ([H], C1=CC2C=C[C]1C2) --> Result: ([H], C1=C[C@H]2C=C[C@]1C2)
18 Identical validation failed on [946496, 'C1=C[C@H]2C=C[C@@H]1C2', 10, '[H
   ]', 'C1=CC2C=C[C]1C2', 107.81357630802847, 99.269413764, 114.5091218315581
   , 'train'] at row 25386 in Excel.
19 Expected: ([H], [CH]1C2C=CC1C=C2) --> Result: ([H], C1=C[C@H]2C=C[C@@H]1[
   CH]2)
20 Identical validation failed on [946500, 'C1=C[C@H]2C=C[C@@H]1C2', 14, '[H
   ]', '[CH]1C2C=CC1C=C2', 103.27103865701162, 94.603884349, 110.
   49056581595802, 'train'] at row 25387 in Excel.
21 Expected: ([H], [C]1=C/C=C\/C=C\C/1) --> Result: ([H], [C]1=C\C=C/C/C=C\C
   /1)
22 Identical validation failed on [96734, 'C1=C\\C/C=C\\C\\C=C/1', 9, '[H
   ]', '[C]1=C/C=C\\C/C=C\\C/1', 105.32111056004346, 96.634503473, 112.
   14011287818788, 'train'] at row 25534 in Excel.
23 Expected: ([H], [C]1=C/C=N\C=C\C=N/C/1) --> Result: ([H], [C]1=C\C=N/C=C\C
   =N/C/1)
24 Identical validation failed on [193107, 'C1=C\\C/N=C\\C=C\\N=C/1', 10, '[H
   ]', '[C]1=C/C=N\\C=C\\C=N/C/1', 103.3193568500323, 94.655967596, 110.
   31762443058798, 'train'] at row 25538 in Excel.
25 Expected: ([H], [C]1=C/N=C\C=C/C/N=C/1) --> Result: ([H], [C]1=C/N=C/C=C\C
   \N=C/1)
26 Identical validation failed on [193111, 'C1=C\\C/N=C\\C=C\\N=C/1', 14, '[H
   ]', '[C]1=C/N=C\\C=C/C/N=C/1', 106.28496438403552, 97.488543222, 113.
   082205106039658, 'train'] at row 25541 in Excel.
27 Expected: ([H], [C]1=C/C=N\C/C=C/C=N/1) --> Result: ([H], [C]1=C/C=N\C/C=C
   \C=N/1)
28 Identical validation failed on [193112, 'C1=C\\C/N=C\\C=C\\N=C/1', 15, '[H
   ]', '[C]1=C/C=N\\C/C=C/C=N/1', 83.15498264404171, 74.767069841, 90.
   27831687533438, 'train'] at row 25542 in Excel.
29 Expected: ([H], [C]1=N\C=C\C=N\C\C=C/1) --> Result: ([H], [C]1=N/C=C/C=N\C
   \C=C/1)
30 Identical validation failed on [193113, 'C1=C\\C/N=C\\C=C\\N=C/1', 16, '[H
   ]', '[C]1=N\\C=C\\C=N\\C\\C=C/1', 94.7833519230391, 85.91853228, 102.
   25402525911878, 'train'] at row 25543 in Excel.
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31 Expected: ([H], [C]1=C/C=C\C/C=C\C=C/1) --> Result: ([H], [C]1=C\C=C/C=C
  \C=C/1)
32 Identical validation failed on [150568, 'C1=C\\C=C/C/C=C\\C=C/1', 9, '[H
  ]', '[C]1=C/C=C\\C/C=C\\C=C/1', 87.74646599704201, 79.590731524, 95.
  11194200067312, 'train'] at row 25544 in Excel.
33 Expected: ([H], [C]1=C/C=C\C=C/C\C=C/1) --> Result: ([H], [C]1=C\C=C/C=C/C
  \C=C/1)
34 Identical validation failed on [150569, 'C1=C\\C=C/C/C=C\\C=C/1', 10, '[H
  ]', '[C]1=C/C=C\\C=C/C/C\\C=C/1', 95.24394352901766, 87.059971151, 102.
  47551385162978, 'train'] at row 25545 in Excel.
35 Expected: ([H], [C]1=C/C=C\C=C\C=C/C/1) --> Result: ([H], [C]1=C\C=C/C=C\C
  =C/C/1)
36 Identical validation failed on [150571, 'C1=C\\C=C/C/C=C\\C=C/1', 12, '[H
  ]', '[C]1=C/C=C\\C=C\\C=C/C/1', 103.23464313503216, 94.649692506, 110.
  2902525030682, 'train'] at row 25547 in Excel.
37 Expected: ([H], [C]1=C/C=C\C=C\C=C/1) --> Result: ([H], [C]1=C\C=C/C=C\C=C
  /1)
38 Identical validation failed on [165278, 'C1=C\\C=C/C=C\\C=C/1', 8, '[H
  ]', '[C]1=C/C=C\\C=C\\C=C/1', 96.21469995202796, 87.634769395, 103.
  4919216234497, 'train'] at row 25548 in Excel.
39 Expected: ([H], [C]1=C/C=N\C/C=C\N=C/1) --> Result: ([H], [C]1=C\C=N/C/C=C
  \N=C/1)
40 Identical validation failed on [19820, 'C1=C\\C=N/C/C=C\\N=C/1', 9, '[H
  ]', '[C]1=C/C=N\\C/C=C\\N=C/1', 91.72424554802228, 83.719740744, 99.
  0227070894696, 'train'] at row 25549 in Excel.
41 Expected: ([H], [C]1=C/C=N\C=C/C\N=C/1) --> Result: ([H], [C]1=C\C=N/C=C/C
  \N=C/1)
42 Identical validation failed on [19821, 'C1=C\\C=N/C/C=C\\N=C/1', 10, '[H
  ]', '[C]1=C/C=N\\C=C/C/C\\N=C/1', 100.1836943770304, 91.98654431, 107.
  44312337002998, 'train'] at row 25550 in Excel.
43 Expected: ([H], [C]1=N\C/C=C\N=C\C=C/1) --> Result: ([H], [C]1=N/C/C=C\N=C
  \C=C/1)
44 Identical validation failed on [19822, 'C1=C\\C=N/C/C=C\\N=C/1', 11, '[H
  ]', '[C]1=N\\C/C=C\\N=C\\C=C/1', 78.05584451000334, 69.957840865, 85.
  20362865251298, 'train'] at row 25551 in Excel.
45 Expected: ([H], [C]1=C/N=C\C=C\C=N/C/1) --> Result: ([H], [C]1=C\N=C/C=C\C
  =N/C/1)
46 Identical validation failed on [19825, 'C1=C\\C=N/C/C=C\\N=C/1', 14, '[H
  ]', '[C]1=C/N=C\\C=C\\C=N/C/1', 106.18958301602665, 97.858146023, 113.
  31420353497384, 'train'] at row 25553 in Excel.
47 Expected: ([H], [C]1=C/C=N\C=N/C\C=C/1) --> Result: ([H], [C]1=C\C=N/C=N/C
  \C=C/1)
48 Identical validation failed on [288078, 'C1=C\\C=N/C=N\\C\\C=C/1', 9, '[H
  ]', '[C]1=C/C=N\\C=N/C\\C=C/1', 102.32475508504656, 93.551551756, 109.
  49419941556732, 'train'] at row 25555 in Excel.
49 Expected: ([H], [C]1=C/C=C\C/N=C\N=C/1) --> Result: ([H], [C]1=C\C=C/C/N=C
  \N=C/1)
50 Identical validation failed on [288079, 'C1=C\\C=N/C=N\\C\\C=C/1', 10, '[H
  ]', '[C]1=C/C=C\\C/N=C\\N=C/1', 98.22461127901852, 89.860543818, 105.
  35850259426566, 'train'] at row 25556 in Excel.
51 Expected: ([H], [C]1=N\C=N\C/C=C/C=C/1) --> Result: ([H], [C]1=N\C=N/C/C=C

51 \C=C/1)
52 Identical validation failed on [288080, 'C1=C\\C=N/C=N\\C\\C=C/1', 11, '[
   H]', '[C]1=N\\C=N\\C/C=C/C=C/1', 88.89668999402721, 80.2584011, 95.
   97930391672809, 'train'] at row 25557 in Excel.
53 Expected: ([H], [C]1=N\C/C=C\C=C/C=N/1) --> Result: ([H], [C]1=N\C/C=C/C=
   C\C=N/1)
54 Identical validation failed on [288081, 'C1=C\\C=N/C=N\\C\\C=C/1', 12, '[
   H]', '[C]1=N\\C/C=C\\C=C/C=N/1', 76.76756853304565, 67.698180956, 83.
   75411691683655, 'train'] at row 25558 in Excel.
55 Expected: ([H], [C]1=C/C=C\C=N\C=N/C/1) --> Result: ([H], [C]1=C\C=C/C=N\
   C=N/C/1)
56 Identical validation failed on [288084, 'C1=C\\C=N/C=N\\C\\C=C/1', 15, '[
   H]', '[C]1=C/C=C\\C=N\\C=N/C/1', 103.5157671670358, 94.894421016, 110.
   53490306753976, 'train'] at row 25560 in Excel.
57 Expected: ([H], [C]1=C/C=N/C=C/CO\C=C/1) --> Result: ([H], [C]1=C\C=N\C=C
   /CO\C=C/1)
58 Identical validation failed on [19039, 'C1=C\\C=N\\C=C/CO\\C=C/1', 10, '[
   H]', '[C]1=C/C=N/C=C/CO\\C=C/1', 92.14781412302295, 83.92305366, 98.
   95631667370276, 'train'] at row 25562 in Excel.
59 Expected: ([H], [C]1=N/C=C/CO/C=C/C=C/1) --> Result: ([H], [C]1=N/C=C\CO/
   C=C\C=C/1)
60 Identical validation failed on [19041, 'C1=C\\C=N\\C=C/CO\\C=C/1', 12, '[
   H]', '[C]1=N/C=C/CO/C=C/C=C/1', 79.94652912700957, 71.128772659, 86.
   78991405713063, 'train'] at row 25563 in Excel.
61 Expected: ([H], [C]1=C/N=C/C=C\C=C/OC/1) --> Result: ([H], [C]1=C\N=C\C=C
   \C=C/OC/1)
62 Identical validation failed on [19043, 'C1=C\\C=N\\C=C/CO\\C=C/1', 14, '[
   H]', '[C]1=C/N=C/C=C\\C=C/OC/1', 110.12469195500763, 101.291247762, 116.
   96661264274726, 'train'] at row 25565 in Excel.
63 Expected: ([H], [C]1=C/C=C\C=N\C=C/CO/1) --> Result: ([H], [C]1=C\C=C/C=N
   \C=C/CO/1)
64 Identical validation failed on [19046, 'C1=C\\C=N\\C=C/CO\\C=C/1', 17, '[
   H]', '[C]1=C/C=C\\C=N\\C=C/CO/1', 103.50886456801756, 95.016157762, 109.
   86744595621646, 'train'] at row 25567 in Excel.
65 Expected: ([H], [C]1=C/C=C\CCCC/1) --> Result: ([H], [C]1=C\C=C/CCCC/1)
66 Identical validation failed on [897735, 'C1=C\\CCCC\\C=C/1', 9, '[H]', '[
   C]1=C/C=C\\CCCC/1', 105.85261068302134, 97.160983524, 112.7779170679875
   , 'train'] at row 25576 in Excel.
67 Expected: ([H], [C]1=C/N=C\C=C\N=C/1) --> Result: ([H], [C]1=C\N=C/C=C\N=
   C/1)
68 Identical validation failed on [18298, 'C1=C\\N=C/C=C\\N=C/1', 8, '[H
   ]', '[C]1=C/N=C\\C=C\\N=C/1', 107.09507850302334, 98.43106174, 113.
   85275028818587, 'train'] at row 25579 in Excel.
69 Expected: ([H], [C]1=C/C=N\C=C\C=N/1) --> Result: ([H], [C]1=C\C=N/C=C\C=
   N/1)
70 Identical validation failed on [18299, 'C1=C\\N=C/C=C\\N=C/1', 9, '[H
   ]', '[C]1=C/C=N\\C=C\\C=N/1', 92.70755215103657, 83.832692364, 100.
   22106413338469, 'train'] at row 25580 in Excel.
71 Expected: ([H], [C]1=N/C=C\C=N\C=C/1) --> Result: ([H], [C]1=N\C=C/C=N\C=
   C/1)
72 Identical validation failed on [18300, 'C1=C\\N=C/C=C\\N=C/1', 10, '[H

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 72 ]', '[C]1=N/C=C\\C=N\\C=C/1', 92.71570976801596, 83.845242544, 100.
    22121850053593, 'train'] at row 25581 in Excel.
 73 Expected: ([H], [C]1=C/N=C\C=N\C=C/C/1) --> Result: ([H], [C]1=C\N=C/C=N\
    C=C/C/1)
 74 Identical validation failed on [279113, 'C1=C\\N=C/C=N\\C=C/C/1', 9, '[H
    ]', '[C]1=C/N=C\\C=N\\C=C/C/1', 104.72497701001475, 96.202777281, 111.
    6532276575142, 'train'] at row 25582 in Excel.
 75 Expected: ([H], [C]1=N\C=C/C/C=C/N=C/1) --> Result: ([H], [C]1=N\C=C\C/C=
    C\N=C/1)
 76 Identical validation failed on [279115, 'C1=C\\N=C/C=N\\C=C/C/1', 11, '[H
    ]', '[C]1=N\\C=C/C/C=C/N=C/1', 82.71384381701405, 74.541166601, 89.
    28730626122154, 'train'] at row 25584 in Excel.
 77 Expected: ([H], [C]1=N\C=N\C=N/C=N/1) --> Result: ([H], [C]1=N\C=N/C=N\C=
    N/1)
 78 Identical validation failed on [18404, 'C1=N\\C=N/C=N\\C=N/1', 8, '[H
    ]', '[C]1=N\\C=N\\C=N/C=N/1', 102.0624563229954, 93.440482663, 108.
    92475162615222, 'train'] at row 26152 in Excel.
 79 Completed 4000 partitions under 2.98 seconds with progress 6.33%.
 80 Completed 5000 partitions under 4.26 seconds with progress 7.91%.
 81 Completed 6000 partitions under 4.62 seconds with progress 9.49%.
 82 Completed 7000 partitions under 3.28 seconds with progress 11.07%.
 83 Completed 8000 partitions under 4.98 seconds with progress 12.65%.
 84 Completed 9000 partitions under 6.06 seconds with progress 14.23%.
 85 Completed 10000 partitions under 5.35 seconds with progress 15.82%.
 86 Completed 11000 partitions under 3.91 seconds with progress 17.40%.
 87 Completed 12000 partitions under 4.55 seconds with progress 18.98%.
 88 Completed 13000 partitions under 4.29 seconds with progress 20.56%.
 89 Completed 14000 partitions under 3.69 seconds with progress 22.14%.
 90 Completed 15000 partitions under 4.81 seconds with progress 23.72%.
 91 Expected: ([H], CC(C)SC[C@]1C[C@@H](O)C1) --> Result: ([H], CC(C)SC[C@]1C
    [C@H](O)C1)
 92 Identical validation failed on [1293369, 'CC(C)SC[C@H]1C[C@@H](O)C1', 19
    , '[H]', 'CC(C)SC[C@]1C[C@@H](O)C1', 96.81146101098372, 87.434594024, 104
    .18545673942504, 'train'] at row 125808 in Excel.
 93 Expected: ([H], CC(C)SC[C@H]1C[C@](O)C1) --> Result: ([H], CC(C)SC[C@H]1C
    [C@@](O)C1)
 94 Identical validation failed on [1293372, 'CC(C)SC[C@H]1C[C@@H](O)C1', 22
    , '[H]', 'CC(C)SC[C@H]1C[C@](O)C1', 93.83204827901538, 85.484923561, 100.
    77297242834794, 'train'] at row 125810 in Excel.
 95 Completed 16000 partitions under 5.82 seconds with progress 25.30%.
 96 Completed 17000 partitions under 4.61 seconds with progress 26.89%.
 97 Expected: (C/C1=C\C=[C]\C=C/C=C/1, [CH3]) --> Result: (CC1=C/C=[C]/C=C\C=
    C\1, [CH3])
 98 Identical validation failed on [254774, 'CC1=C/C=C(C)\\C=C\\C=C/1', 0, 'C
    /C1=C\\C=[C]\\C=C/C=C/1', '[CH3]', 90.57715909602912, 77.246985409, 96.
    624445760345, 'train'] at row 141540 in Excel.
 99 Expected: ([H], [CH2]1=C/C=C(C)\C=C/C=C\1) --> Result: ([H], [CH2]1=C\C
    =C(C)/C=C/C=C\1)
100 Identical validation failed on [254776, 'CC1=C/C=C(C)\\C=C\\C=C/1', 10
    , '[H]', '[CH2]1=C/C=C(C)\\C=C/C=C\\1', 86.2630347210063, 77.440258181,
    93.40856410840884, 'train'] at row 141541 in Excel.
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101 Expected: ([H], C/C1=[C]\C=C(C)\C=C/C=C/1) --> Result: ([H], CC1=C/[C]=C(
    C)/C=C\C=C\1)
102 Identical validation failed on [254779, 'CC1=C/C=C(C)\\C=C\\C=C/1', 13
    , '[H]', 'C/C1=[C]\\C=C(C)\\C=C/C=C/1', 101.3276432839958, 92.226252748,
    108.28179935537176, 'train'] at row 141542 in Excel.
103 Expected: ([H], [CH2]C1=C/C=C(C)/C=C/C=C/1) --> Result: ([H], [CH2]C1=C/C
    =C(C)/C=C\C=C\1)
104 Identical validation failed on [254781, 'CC1=C/C=C(C)\\C=C\\C=C/1', 15
    , '[H]', '[CH2]C1=C/C=C(C)/C=C/C=C/1', 86.28437002702378, 77.467868577,
    93.40375864709728, 'train'] at row 141543 in Excel.
105 Expected: ([H], C/C1=C\C=C(C)\C=C/C=[C]/1) --> Result: ([H], CC1=C/C=C(C
    )/C=C\C=[C]\1)
106 Identical validation failed on [254784, 'CC1=C/C=C(C)\\C=C\\C=C/1', 18
    , '[H]', 'C/C1=C\\C=C(C)\\C=C/C=[C]/1', 102.55379587000331, 93.653835723
    , 109.55062060131677, 'train'] at row 141544 in Excel.
107 Expected: ([H], C/C1=C\C=C(C)\C=C/[C]=C/1) --> Result: ([H], CC1=C/C=C(C
    )/C=C\[C]=C\1)
108 Identical validation failed on [254785, 'CC1=C/C=C(C)\\C=C\\C=C/1', 19
    , '[H]', 'C/C1=C\\C=C(C)\\C=C/[C]=C/1', 101.50962089400004, 92.521809487
    , 108.7094446213991, 'train'] at row 141545 in Excel.
109 Completed 18000 partitions under 3.54 seconds with progress 28.47%.
110 Completed 19000 partitions under 3.93 seconds with progress 30.05%.
111 Completed 20000 partitions under 4.92 seconds with progress 31.63%.
112 Completed 21000 partitions under 5.14 seconds with progress 33.21%.
113 Completed 22000 partitions under 7.55 seconds with progress 34.79%.
114 Completed 23000 partitions under 6.56 seconds with progress 36.38%.
115 Completed 24000 partitions under 7.04 seconds with progress 37.96%.
116 Completed 25000 partitions under 5.46 seconds with progress 39.54%.
117 Completed 26000 partitions under 5.35 seconds with progress 41.12%.
118 Completed 27000 partitions under 5.66 seconds with progress 42.70%.
119 Expected: ([H], CCSC[C@]1C[C@@H](O)C1) --> Result: ([H], CCSC[C@]1C[C@H](
    O)C1)
120 Identical validation failed on [1003065, 'CCSC[C@H]1C[C@@H](O)C1', 16, '[
    H]', 'CCSC[C@]1C[C@@H](O)C1', 94.80719726505023, 86.42053948, 102.
    22075600528004, 'train'] at row 237498 in Excel.
121 Expected: ([H], CCSC[C@H]1C[C@](O)C1) --> Result: ([H], CCSC[C@H]1C[C@@](
    O)C1)
122 Identical validation failed on [1003068, 'CCSC[C@H]1C[C@@H](O)C1', 19, '[
    H]', 'CCSC[C@H]1C[C@](O)C1', 93.9123694310266, 85.047549788, 100.
    93298211542468, 'train'] at row 237500 in Excel.
123 Expected: ([H], CCSC[C@]1C[C@@H](OC)C1) --> Result: ([H], CCSC[C@]1C[C@H
    ](OC)C1)
124 Identical validation failed on [1406669, 'CCSC[C@H]1C[C@@H](OC)C1', 17
    , '[H]', 'CCSC[C@]1C[C@@H](OC)C1', 94.72813113103584, 86.664640481, 102.
    06051100251656, 'train'] at row 237512 in Excel.
125 Expected: ([H], CCSC[C@H]1C[C@](OC)C1) --> Result: ([H], CCSC[C@H]1C[C
    @@](OC)C1)
126 Identical validation failed on [1406672, 'CCSC[C@H]1C[C@@H](OC)C1', 20
    , '[H]', 'CCSC[C@H]1C[C@](OC)C1', 94.4796375670212, 85.464843273, 101.
    35914897100731, 'train'] at row 237514 in Excel.
127 Completed 28000 partitions under 6.70 seconds with progress 44.28%.
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128 Completed 29000 partitions under 6.90 seconds with progress 45.87%.
129 Completed 30000 partitions under 6.60 seconds with progress 47.45%.
130 Completed 31000 partitions under 5.09 seconds with progress 49.03%.
131 Completed 32000 partitions under 4.26 seconds with progress 50.61%.
132 Completed 33000 partitions under 4.19 seconds with progress 52.19%.
133 Expected: ([H], CNC(=S)N[C@]1C[C@@H](O)C1) --> Result: ([H], CNC(=S)N[C@]
    1C[C@H](O)C1)
134 Identical validation failed on [1504379, 'CNC(=S)N[C@H]1C[C@@H](O)C1', 15
    , '[H]', 'CNC(=S)N[C@]1C[C@@H](O)C1', 96.24231034806525, 87.934718697,
    103.0614757863994, 'train'] at row 294128 in Excel.
135 Expected: ([H], CNC(=S)N[C@H]1C[C@](O)C1) --> Result: ([H], CNC(=S)N[C@H]
    1C[C@@](O)C1)
136 Identical validation failed on [1504382, 'CNC(=S)N[C@H]1C[C@@H](O)C1', 18
    , '[H]', 'CNC(=S)N[C@H]1C[C@](O)C1', 94.55431113804669, 86.060349314, 101
    .56094069443598, 'train'] at row 294130 in Excel.
137 Expected: ([H], CNC(=S)N[C@]1C[C@H](O)C1) --> Result: ([H], CNC(=S)N[C@]
    1C[C@@H](O)C1)
138 Identical validation failed on [1499106, 'CNC(=S)N[C@H]1C[C@H](O)C1', 15
    , '[H]', 'CNC(=S)N[C@]1C[C@H](O)C1', 95.50122221901016, 87.513660158, 102
    .24438484362284, 'train'] at row 294153 in Excel.
139 Expected: ([H], CNC(=S)N[C@H]1C[C@@](O)C1) --> Result: ([H], CNC(=S)N[C@H
    ]1C[C@](O)C1)
140 Identical validation failed on [1499109, 'CNC(=S)N[C@H]1C[C@H](O)C1', 18
    , '[H]', 'CNC(=S)N[C@H]1C[C@@](O)C1', 93.56221940898324, 84.97099369, 100
    .54504371454674, 'train'] at row 294155 in Excel.
141 Completed 34000 partitions under 4.63 seconds with progress 53.77%.
142 Completed 35000 partitions under 5.75 seconds with progress 55.35%.
143 Completed 36000 partitions under 4.04 seconds with progress 56.94%.
144 Expected: ([F], COC(=O)[C@]1C[C@@H](N)C1) --> Result: ([F], COC(=O)[C@]1C
    [C@H](N)C1)
145 Identical validation failed on [1681458, 'COC(=O)[C@@]1(F)C[C@@H](N)C1',
    4, '[F]', 'COC(=O)[C@]1C[C@@H](N)C1', 105.83755046702368, 94.838572715,
    108.49633973965936, 'train'] at row 314388 in Excel.
146 Expected: ([H], COC(=O)[C@]1(F)C[C@@](N)C1) --> Result: ([H], COC(=O)[C@]
    1(F)C[C@](N)C1)
147 Identical validation failed on [1681465, 'COC(=O)[C@@]1(F)C[C@@H](N)C1',
    15, '[H]', 'COC(=O)[C@]1(F)C[C@@](N)C1', 90.86644074501216, 81.355286832
    , 98.07227181247896, 'train'] at row 314392 in Excel.
148 Expected: ([F], COC(=O)[C@]1C[C@H](N)C1) --> Result: ([F], COC(=O)[C@]1C[
    C@@H](N)C1)
149 Identical validation failed on [1681473, 'COC(=O)[C@@]1(F)C[C@H](N)C1', 4
    , '[F]', 'COC(=O)[C@]1C[C@H](N)C1', 106.79261916503792, 97.175416231, 109
    .42685663692826, 'train'] at row 314398 in Excel.
150 Expected: ([H], COC(=O)[C@]1(F)C[C@](N)C1) --> Result: ([H], COC(=O)[C@]1
    (F)C[C@@](N)C1)
151 Identical validation failed on [1681480, 'COC(=O)[C@@]1(F)C[C@H](N)C1',
    15, '[H]', 'COC(=O)[C@]1(F)C[C@](N)C1', 92.19236726201748, 83.840849981,
    99.36521449114352, 'train'] at row 314401 in Excel.
152 Expected: ([O]/C1=C/C=C\C=C\C=C/1, [CH3]) --> Result: ([O]C1=C\C=C/C=C/C=
    C\1, [CH3])
153 Identical validation failed on [151422, 'COC1=C/C=C\\C=C\\C=C/1', 0, '[O
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153  ]/C1=C/C=C\\C=C\\C=C/1', '[CH3]', 58.47003360197881, 43.727964665, 64.
     15988136563892, 'train'] at row 319634 in Excel.
154  Expected: ([C]1=C/C=C/C=C/C=C/1, C[O]) --> Result: (C[O], [C]1=C/C=C\C=C\
     C=C/1)
155  Identical validation failed on [151423, 'COC1=C/C=C\\C=C\\C=C/1', 1, '[C]
     1=C/C=C/C=C/C=C/1', 'C[O]', 88.94187064198448, 75.141692714, 94.
     70053647727435, 'train'] at row 319635 in Excel.
156  Expected: ([C]1=C/C=C/C=C/C=C/1, C[O]) --> Result: (C[O], [C]1=C/C=C\C=C\
     C=C/1)
157  Chiral validation failed on [151423, 'COC1=C/C=C\\C=C\\C=C/1', 1, '[C]1=C
     /C=C/C=C/C=C/1', 'C[O]', 88.94187064198448, 75.141692714, 94.
     70053647727435, 'train'] at row 319635 in Excel.
158  Expected: ([H], [CH2]OC1=C/C=C\C=C/C=C\1) --> Result: ([H], [CH2]OC1=C\C=
     C/C=C/C=C\1)
159  Identical validation failed on [151424, 'COC1=C/C=C\\C=C\\C=C/1', 10, '[H
     ]', '[CH2]OC1=C/C=C\\C=C/C=C\\1', 96.6884692470089, 88.144306703, 104.
     15754515447902, 'train'] at row 319636 in Excel.
160  Expected: ([H], CO/C1=[C]\C=C\C=C/C=C/1) --> Result: ([H], COC1=[C]\C=C/C
     =C/C=C\1)
161  Identical validation failed on [151427, 'COC1=C/C=C\\C=C\\C=C/1', 13, '[H
     ]', 'CO/C1=[C]\\C=C\\C=C/C=C/1', 102.21431350100436, 93.137395816, 109.
     17787230246222, 'train'] at row 319637 in Excel.
162  Expected: ([H], CO/C1=C\[C]=C\C=C/C=C/1) --> Result: ([H], COC1=C\[C]=C/C
     =C/C=C\1)
163  Identical validation failed on [151428, 'COC1=C/C=C\\C=C\\C=C/1', 14, '[H
     ]', 'CO/C1=C\\[C]=C\\C=C/C=C/1', 100.78422049001236, 92.103260984, 107.
     73201329469184, 'train'] at row 319638 in Excel.
164  Expected: ([H], CO/C1=C\C=[C]\C=C/C=C/1) --> Result: ([H], COC1=C\C=[C]/C
     =C/C=C\1)
165  Identical validation failed on [151429, 'COC1=C/C=C\\C=C\\C=C/1', 15, '[H
     ]', 'CO/C1=C\\C=[C]\\C=C/C=C/1', 99.95590860999911, 90.732153819, 107.
     68375411405012, 'train'] at row 319639 in Excel.
166  Expected: ([H], CO/C1=C\C=C\[C]=C/C=C/1) --> Result: ([H], COC1=C\C=C/[C
     ]=C/C=C\1)
167  Identical validation failed on [151430, 'COC1=C/C=C\\C=C\\C=C/1', 16, '[H
     ]', 'CO/C1=C\\C=C\\[C]=C/C=C/1', 100.24519025901782, 90.885893524, 107.
     6290165340378, 'train'] at row 319640 in Excel.
168  Expected: ([H], CO/C1=C\C=C\C=[C]/C=C/1) --> Result: ([H], COC1=C\C=C/C=[
     C]/C=C\1)
169  Identical validation failed on [151431, 'COC1=C/C=C\\C=C\\C=C/1', 17, '[H
     ]', 'CO/C1=C\\C=C\\C=[C]/C=C/1', 102.19988079400513, 93.232777184, 109.
     46316158245249, 'train'] at row 319641 in Excel.
170  Expected: ([H], CO/C1=C\C=C\C=C/[C]=C/1) --> Result: ([H], COC1=C\C=C/C=C
     /[C]=C\1)
171  Identical validation failed on [151432, 'COC1=C/C=C\\C=C\\C=C/1', 18, '[H
     ]', 'CO/C1=C\\C=C\\C=C/[C]=C/1', 96.2849809599932, 87.642299503, 103.
     48747446965164, 'train'] at row 319642 in Excel.
172  Expected: ([H], CO/C1=C\C=C\C=C/C=[C]/1) --> Result: ([H], COC1=C\C=C/C=C
     /C=[C]\1)
173  Identical validation failed on [151433, 'COC1=C/C=C\\C=C\\C=C/1', 19, '[H
     ]', 'CO/C1=C\\C=C\\C=C/C=[C]/1', 99.34847989799891, 90.354393401, 106.
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173 58730133815976, 'train'] at row 319643 in Excel.
174 Completed 37000 partitions under 4.13 seconds with progress 58.52%.
175 Completed 38000 partitions under 5.19 seconds with progress 60.10%.
176 Completed 39000 partitions under 5.38 seconds with progress 61.68%.
177 Completed 40000 partitions under 4.98 seconds with progress 63.26%.
178 Expected: ([H], CS(=O)(=O)N[C@H]1C[C@](N)C1) --> Result: ([H], CS(=O)(=O)
    N[C@H]1C[C@@](N)C1)
179 Identical validation failed on [1658282, 'CS(=O)(=O)N[C@H]1C[C@@H](N)C1
    ', 17, '[H]', 'CS(=O)(=O)N[C@H]1C[C@](N)C1', 92.00662459798706, 82.
    688743457, 99.27569598880174, 'train'] at row 350348 in Excel.
180 Expected: ([H], CS(=O)(=O)N[C@]1C[C@@H](O)C1) --> Result: ([H], CS(=O)(=O
)N[C@]1C[C@H](O)C1)
181 Identical validation failed on [1509591, 'CS(=O)(=O)N[C@H]1C[C@@H](O)C1
    ', 14, '[H]', 'CS(=O)(=O)N[C@]1C[C@@H](O)C1', 96.38412738199256, 86.
    89744632, 103.68273382782276, 'train'] at row 350357 in Excel.
182 Expected: ([H], CS(=O)(=O)N[C@H]1C[C@](O)C1) --> Result: ([H], CS(=O)(=O)
    N[C@H]1C[C@@](O)C1)
183 Identical validation failed on [1509594, 'CS(=O)(=O)N[C@H]1C[C@@H](O)C1
    ', 17, '[H]', 'CS(=O)(=O)N[C@H]1C[C@](O)C1', 94.54552601199752, 86.
    099882381, 101.57575554613386, 'train'] at row 350359 in Excel.
184 Expected: ([H], CS(=O)(=O)N[C@H]1C[C@@](N)C1) --> Result: ([H], CS(=O)(=O
)N[C@H]1C[C@](N)C1)
185 Identical validation failed on [1507089, 'CS(=O)(=O)N[C@H]1C[C@H](N)C1',
    17, '[H]', 'CS(=O)(=O)N[C@H]1C[C@@](N)C1', 93.53460901305294, 85.
    048804806, 100.37934126902228, 'train'] at row 350370 in Excel.
186 Expected: ([H], CS(=O)(=O)N[C@]1C[C@H](O)C1) --> Result: ([H], CS(=O)(=O)
    N[C@]1C[C@@H](O)C1)
187 Identical validation failed on [1522302, 'CS(=O)(=O)N[C@H]1C[C@H](O)C1',
    14, '[H]', 'CS(=O)(=O)N[C@]1C[C@H](O)C1', 93.5107636710418, 85.808718205
    , 100.59092526481112, 'train'] at row 350379 in Excel.
188 Expected: ([H], CS(=O)(=O)N[C@H]1C[C@@](O)C1) --> Result: ([H], CS(=O)(=O
)N[C@H]1C[C@](O)C1)
189 Identical validation failed on [1522305, 'CS(=O)(=O)N[C@H]1C[C@H](O)C1',
    17, '[H]', 'CS(=O)(=O)N[C@H]1C[C@@](O)C1', 93.64379557906264, 85.
    017429356, 100.5994367923063, 'train'] at row 350381 in Excel.
190 Expected: ([H], CS(=O)(=O)[C@]1C[C@@H](N)C1) --> Result: ([H], CS(=O)(=O
)[C@]1C[C@H](N)C1)
191 Identical validation failed on [1055523, 'CS(=O)(=O)[C@H]1C[C@@H](N)C1',
    12, '[H]', 'CS(=O)(=O)[C@]1C[C@@H](N)C1', 98.05204630406185, 87.385648322
    , 105.28887925407612, 'train'] at row 350908 in Excel.
192 Expected: ([H], CS(=O)(=O)[C@H]1C[C@](N)C1) --> Result: ([H], CS(=O)(=O)[
    C@H]1C[C@@](N)C1)
193 Identical validation failed on [1055526, 'CS(=O)(=O)[C@H]1C[C@@H](N)C1',
    15, '[H]', 'CS(=O)(=O)[C@H]1C[C@](N)C1', 90.2000261870539, 81.018942008,
    97.4535394934001, 'train'] at row 350910 in Excel.
194 Expected: ([H], CS(=O)(=O)[C@]1C[C@H](N)C1) --> Result: ([H], CS(=O)(=O)[
    C@]1C[C@@H](N)C1)
195 Identical validation failed on [1054972, 'CS(=O)(=O)[C@H]1C[C@H](N)C1',
    12, '[H]', 'CS(=O)(=O)[C@]1C[C@H](N)C1', 99.66097938006602, 90.41777181,
    106.75827673883052, 'train'] at row 350981 in Excel.
196 Expected: ([H], CS(=O)(=O)[C@H]1C[C@@](N)C1) --> Result: ([H], CS(=O)(=O

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196 )[C@H]1C[C@](N)C1)
197 Identical validation failed on [1054975, 'CS(=O)(=O)[C@H]1C[C@H](N)C1',
    15, '[H]', 'CS(=O)(=O)[C@H]1C[C@@](N)C1', 92.31661404406049, 82.5801844,
    99.8523356550757, 'train'] at row 350983 in Excel.
198 Expected: ([H], CSCCO[C@]1C[C@@H](O)C1) --> Result: ([H], CSCCO[C@]1C[C@H
    ](O)C1)
199 Identical validation failed on [1725379, 'CSCCO[C@]1C[C@@H](O)C1', 17
    , '[H]', 'CSCCO[C@]1C[C@@H](O)C1', 95.75724589107716, 87.071266313, 102.
    70331769107725, 'train'] at row 355049 in Excel.
200 Expected: ([H], CSCCO[C@]1C[C@H](O)C1) --> Result: ([H], CSCCO[C@]1C[C@@H
    ](O)C1)
201 Identical validation failed on [1725302, 'CSCCO[C@]1C[C@H](O)C1', 17, '[
    H]', 'CSCCO[C@]1C[C@H](O)C1', 94.44951713502589, 85.473628399, 101.
    31236506330296, 'train'] at row 355061 in Excel.
202 Expected: ([H], CSCCO[C@H]1C[C@@](O)C1) --> Result: ([H], CSCCO[C@H]1C[C
    @](O)C1)
203 Identical validation failed on [1725305, 'CSCCO[C@H]1C[C@H](O)C1', 20, '[
    H]', 'CSCCO[C@H]1C[C@@](O)C1', 93.39530201497662, 84.315246785, 100.
    40269274863812, 'train'] at row 355063 in Excel.
204 Completed 41000 partitions under 5.27 seconds with progress 64.84%.
205 Expected: ([H], CSC[C@]1CC[C@H](N)CC1) --> Result: ([H], CSC[C@]1CC[C@@H
    ](N)CC1)
206 Identical validation failed on [1222940, 'CSC[C@H]1CC[C@H](N)CC1', 15, '[
    H]', 'CSC[C@]1CC[C@H](N)CC1', 94.18533584605083, 85.309221041, 101.
    25219953345268, 'train'] at row 358207 in Excel.
207 Expected: ([H], CSC[C@H]1CC[C@@](N)CC1) --> Result: ([H], CSC[C@H]1CC[C
    @](N)CC1)
208 Identical validation failed on [1222945, 'CSC[C@H]1CC[C@H](N)CC1', 20, '[
    H]', 'CSC[C@H]1CC[C@@](N)CC1', 90.67003042800869, 82.494215667, 97.
    43084564296528, 'train'] at row 358210 in Excel.
209 Expected: ([H], CS[C@]1C[C@H](NC(C)=O)C1) --> Result: ([H], CS[C@]1C[C@@H
    ](NC(C)=O)C1)
210 Identical validation failed on [1303711, 'CS[C@H]1C[C@H](NC(C)=O)C1', 13
    , '[H]', 'CS[C@]1C[C@H](NC(C)=O)C1', 91.14505474102214, 81.973383197, 98.
    00867757533524, 'train'] at row 360552 in Excel.
211 Expected: ([H], CS[C@H]1C[C@@](NC(C)=O)C1) --> Result: ([H], CS[C@H]1C[C
    @](NC(C)=O)C1)
212 Identical validation failed on [1303714, 'CS[C@H]1C[C@H](NC(C)=O)C1', 16
    , '[H]', 'CS[C@H]1C[C@@](NC(C)=O)C1', 90.42153686406536, 82.118337776, 97
    .3951441654348, 'train'] at row 360554 in Excel.
213 Expected: ([H], CS[C@]1C[C@H](NC(C)C)C1) --> Result: ([H], CS[C@]1C[C@@H
    ](NC(C)C)C1)
214 Identical validation failed on [1303849, 'CS[C@H]1C[C@H](NC(C)C)C1', 13
    , '[H]', 'CS[C@]1C[C@H](NC(C)C)C1', 91.67843739103093, 82.622227503, 98.
    66318165301531, 'train'] at row 360562 in Excel.
215 Expected: ([H], CS[C@H]1C[C@@](NC(C)C)C1) --> Result: ([H], CS[C@H]1C[C
    @](NC(C)C)C1)
216 Identical validation failed on [1303852, 'CS[C@H]1C[C@H](NC(C)C)C1', 16
    , '[H]', 'CS[C@H]1C[C@@](NC(C)C)C1', 90.70956349505155, 81.859176559, 98.
    05855635592158, 'train'] at row 360564 in Excel.
217 Expected: ([H], CS[C@]1C[C@H](NC(N)=O)C1) --> Result: ([H], CS[C@]1C[C@@H
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217 ](NC(N)=O)C1)
218 Identical validation failed on [1735587, 'CS[C@H]1C[C@H](NC(N)=O)C1', 13
    , '[H]', 'CS[C@]1C[C@H](NC(N)=O)C1', 91.33581747696854, 82.635405192, 98.
    22112000312232, 'train'] at row 360573 in Excel.
219 Expected: ([H], CS[C@H]1C[C@@](NC(N)=O)C1) --> Result: ([H], CS[C@H]1C[C
    @](NC(N)=O)C1)
220 Identical validation failed on [1735590, 'CS[C@H]1C[C@H](NC(N)=O)C1', 16
    , '[H]', 'CS[C@H]1C[C@@](NC(N)=O)C1', 92.88890225197105, 84.383645266, 99
    .9992655515218, 'train'] at row 360575 in Excel.
221 Completed 42000 partitions under 5.58 seconds with progress 66.43%.
222 Completed 43000 partitions under 5.69 seconds with progress 68.01%.
223 Completed 44000 partitions under 5.26 seconds with progress 69.59%.
224 Completed 45000 partitions under 6.00 seconds with progress 71.17%.
225 Completed 46000 partitions under 5.81 seconds with progress 72.75%.
226 Completed 47000 partitions under 4.10 seconds with progress 74.33%.
227 Completed 48000 partitions under 4.52 seconds with progress 75.91%.
228 Completed 49000 partitions under 4.19 seconds with progress 77.50%.
229 Completed 50000 partitions under 3.74 seconds with progress 79.08%.
230 Completed 51000 partitions under 3.95 seconds with progress 80.66%.
231 Completed 52000 partitions under 2.94 seconds with progress 82.24%.
232 Completed 53000 partitions under 3.56 seconds with progress 83.82%.
233 Completed 54000 partitions under 4.21 seconds with progress 85.40%.
234 Completed 55000 partitions under 4.77 seconds with progress 86.99%.
235 Expected: ([H], NS(=O)(=O)N[C@]1C[C@@H](O)C1) --> Result: ([H], NS(=O)(=O
    )N[C@]1C[C@H](O)C1)
236 Identical validation failed on [1624118, 'NS(=O)(=O)N[C@H]1C[C@@H](O)C1
    ', 13, '[H]', 'NS(=O)(=O)N[C@]1C[C@@H](O)C1', 97.18733890203347, 87.
    15472501, 104.58914560754336, 'train'] at row 466034 in Excel.
237 Expected: ([H], NS(=O)(=O)N[C@H]1C[C@](O)C1) --> Result: ([H], NS(=O)(=O)
    N[C@H]1C[C@@](O)C1)
238 Identical validation failed on [1624121, 'NS(=O)(=O)N[C@H]1C[C@@H](O)C1
    ', 16, '[H]', 'NS(=O)(=O)N[C@]1C[C@](O)C1', 94.50473792702915, 85.
    980028162, 101.49823061703398, 'train'] at row 466036 in Excel.
239 Expected: ([H], NS(=O)(=O)N[C@]1C[C@H](O)C1) --> Result: ([H], NS(=O)(=O)
    N[C@]1C[C@@H](O)C1)
240 Identical validation failed on [1621494, 'NS(=O)(=O)N[C@H]1C[C@H](O)C1',
    13, '[H]', 'NS(=O)(=O)N[C@]1C[C@H](O)C1', 95.4692192600196, 85.965595455
    , 102.70017261785176, 'train'] at row 466045 in Excel.
241 Expected: ([H], NS(=O)(=O)N[C@H]1C[C@@](O)C1) --> Result: ([H], NS(=O)(=O
    )N[C@H]1C[C@](O)C1)
242 Identical validation failed on [1621497, 'NS(=O)(=O)N[C@H]1C[C@H](O)C1',
    16, '[H]', 'NS(=O)(=O)N[C@H]1C[C@@](O)C1', 93.37208418203524, 84.
    684849586, 100.35505856661524, 'train'] at row 466047 in Excel.
243 Expected: (F[C](F)F, N[C@H]1C[C@](O)C1) --> Result: (F[C](F)F, N[C@H]1C[C
    @@](O)C1)
244 Identical validation failed on [1530363, 'N[C@H]1C[C@@](O)(C(F)(F)F)C1',
    4, 'F[C](F)F', 'N[C@H]1C[C@](O)C1', 97.056817029935, 82.3919317, 100.
    29755286453543, 'train'] at row 470358 in Excel.
245 Expected: ([H], N[C@]1C[C@@](O)(C(F)(F)F)C1) --> Result: ([H], N[C@]1C[C
    @](O)(C(F)(F)F)C1)
246 Identical validation failed on [1530369, 'N[C@H]1C[C@@](O)(C(F)(F)F)C1',
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246 12, '[H]', 'N[C@]1C[C@@](O)(C(F)(F)F)C1', 93.86844380099484, 85.652468464
    , 100.58512018231518, 'train'] at row 470361 in Excel.
247 Expected: (F[C](F)F, N[C@H]1C[C@@](O)C1) --> Result: (F[C](F)F, N[C@H]1C[
    C@](O)C1)
248 Identical validation failed on [1530424, 'N[C@H]1C[C@](O)(C(F)(F)F)C1', 4
    , 'F[C](F)F', 'N[C@H]1C[C@@](O)C1', 102.16662281701775, 86.874228487, 105
    .80180527495864, 'train'] at row 470374 in Excel.
249 Expected: ([H], N[C@]1C[C@](O)(C(F)(F)F)C1) --> Result: ([H], N[C@]1C[C
    @@](O)(C(F)(F)F)C1)
250 Identical validation failed on [1530430, 'N[C@H]1C[C@](O)(C(F)(F)F)C1',
    12, '[H]', 'N[C@]1C[C@](O)(C(F)(F)F)C1', 92.6134258010245, 83.005007993,
    99.96518116405682, 'train'] at row 470377 in Excel.
251 Completed 56000 partitions under 4.68 seconds with progress 88.57%.
252 Completed 57000 partitions under 3.88 seconds with progress 90.15%.
253 Expected: ([H], O=C1/[C]=C/C=C/C/C=C/C1) --> Result: ([H], O=C1/[C]=C/C=C
    \C/C=C/C1)
254 Identical validation failed on [412535, 'O=C1/C=C/C=C\\C/C=C/C1', 10, '[H
    ]', 'O=C1/[C]=C/C=C/C/C=C/C1', 104.26752294902828, 95.273436452, 111.
    41448696961687, 'train'] at row 485447 in Excel.
255 Expected: ([H], O=C1/C=[C]/C=C/C/C=C/C1) --> Result: ([H], O=C1/C=[C]/C=C
    \C/C=C/C1)
256 Identical validation failed on [412536, 'O=C1/C=C/C=C\\C/C=C/C1', 11, '[H
    ]', 'O=C1/C=[C]/C=C/C/C=C/C1', 102.97799195403807, 93.587947278, 110.
    44368652684172, 'train'] at row 485448 in Excel.
257 Expected: ([H], O=C1/C=C/C=[C]/C/C=C/C1) --> Result: ([H], O=C1/C=C/C=[C
    ]\C/C=C/C1)
258 Identical validation failed on [412538, 'O=C1/C=C/C=C\\C/C=C/C1', 13, '[H
    ]', 'O=C1/C=C/C=[C]/C/C=C/C1', 109.3635235380389, 100.017404492, 116.
    8243495280296, 'train'] at row 485450 in Excel.
259 Expected: ([H], O=C1/C=C/C=C/C/[C]=C/C1) --> Result: ([H], O=C1/C=C/C=C\C
    /[C]=C/C1)
260 Identical validation failed on [412541, 'O=C1/C=C/C=C\\C/C=C/C1', 16, '[H
    ]', 'O=C1/C=C/C=C/C/[C]=C/C1', 110.93794361902322, 101.813962759, 118.
    26536856151851, 'train'] at row 485452 in Excel.
261 Expected: ([H], O=C1/C=C/C=C/C/C=[C]/C1) --> Result: ([H], O=C1/C=C/C=C\C
    /C=[C]/C1)
262 Identical validation failed on [412542, 'O=C1/C=C/C=C\\C/C=C/C1', 17, '[H
    ]', 'O=C1/C=C/C=C/C/C=[C]/C1', 110.14602726102513, 101.064089504, 117.
    45527496787982, 'train'] at row 485453 in Excel.
263 Expected: ([H], O=C1/[C]=C/C=C\C(=O)CC1) --> Result: ([H], O=C1/[C]=C\C=C
    /C(=O)CC1)
264 Identical validation failed on [337556, 'O=C1/C=C\\C=C/C(=O)CC1', 10, '[H
    ]', 'O=C1/[C]=C/C=C\\C(=O)CC1', 104.22610735502585, 95.560208065, 111.
    45273048465054, 'train'] at row 485463 in Excel.
265 Expected: ([H], O=C1/[C]=C/C=C\CCC1) --> Result: ([H], O=C1/[C]=C\C=C/
    CCC1)
266 Identical validation failed on [159794, 'O=C1/C=C\\C=C/CCC1', 9, '[H]', '
    O=C1/[C]=C/C=C\\CCC1', 109.62582230001873, 100.461680864, 116.
    83707728606734, 'train'] at row 485466 in Excel.
267 Expected: ([H], O=C1/C=C\C=[C]\CCC1) --> Result: ([H], O=C1/C=C\C=[C]/
    CCC1)
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268 Identical validation failed on [159797, 'O=C1/C=C\\C=C/CCC1', 12, '[H
    ]', 'O=C1/C=C\\C=[C]\\CCC1', 106.32951752303003, 97.707543863, 113.
    30619024947404, 'train'] at row 485469 in Excel.
269 Completed 58000 partitions under 3.83 seconds with progress 91.73%.
270 Completed 59000 partitions under 3.08 seconds with progress 93.31%.
271 Expected: ([C]1=C/C=C/C=C/C=C/1, [CH]=O) --> Result: ([C]1=C/C=C\C=C\C=C/
    1, [CH]=O)
272 Identical validation failed on [259420, 'O=CC1=C/C=C\\C=C\\C=C/1', 1, '[C
    ]1=C/C=C/C=C/C=C/1', '[CH]=O', 83.13050979296082, 70.06137985, 88.
    38009736421098, 'train'] at row 491674 in Excel.
273 Expected: ([H], O=[C]/C1=C/C=C\C=C\C=C/1) --> Result: ([H], O=[C]C1=C\C=C
    /C=C/C=C\1)
274 Identical validation failed on [259421, 'O=CC1=C/C=C\\C=C\\C=C/1', 10, '[
    H]', 'O=[C]/C1=C/C=C\\C=C\\C=C/1', 78.24095966499968, 69.564392722, 84.
    52992720257568, 'train'] at row 491675 in Excel.
275 Expected: ([H], O=CC1=[C]/C=C\C=C/C=C\1) --> Result: ([H], O=CC1=[C]\C=C/
    C=C/C=C\1)
276 Identical validation failed on [259422, 'O=CC1=C/C=C\\C=C\\C=C/1', 11, '[
    H]', 'O=CC1=[C]/C=C\\C=C/C=C\\1', 95.32049962700272, 86.747471669, 102.
    45116463323107, 'train'] at row 491676 in Excel.
277 Expected: ([H], O=CC1=C/[C]=C\C=C/C=C\1) --> Result: ([H], O=CC1=C\[C]=C/
    C=C/C=C\1)
278 Identical validation failed on [259423, 'O=CC1=C/C=C\\C=C\\C=C/1', 12, '[
    H]', 'O=CC1=C/[C]=C\\C=C/C=C\\1', 91.10301163802129, 82.839973126, 98.
    12894462924328, 'train'] at row 491677 in Excel.
279 Expected: ([H], O=CC1=C/C=[C]\C=C/C=C\1) --> Result: ([H], O=CC1=C\C=[C]/
    C=C/C=C\1)
280 Identical validation failed on [259424, 'O=CC1=C/C=C\\C=C\\C=C/1', 13, '[
    H]', 'O=CC1=C/C=[C]\\C=C/C=C\\1', 95.8099566470154, 87.471617055, 103.
    1584974095244, 'train'] at row 491678 in Excel.
281 Expected: ([H], O=CC1=C/C=C\[C]=C/C=C\1) --> Result: ([H], O=CC1=C\C=C/[C
    ]=C/C=C\1)
282 Identical validation failed on [259425, 'O=CC1=C/C=C\\C=C\\C=C/1', 14, '[
    H]', 'O=CC1=C/C=C\\[C]=C/C=C\\1', 92.36116718301936, 84.1489569, 99.
    29501760790995, 'train'] at row 491679 in Excel.
283 Expected: ([H], O=CC1=C/C=C\C=[C]/C=C\1) --> Result: ([H], O=CC1=C\C=C/C
    =[C]/C=C\1)
284 Identical validation failed on [259426, 'O=CC1=C/C=C\\C=C\\C=C/1', 15, '[
    H]', 'O=CC1=C/C=C\\C=[C]/C=C\\1', 95.19374280900172, 86.921291662, 102.
    45195654916864, 'train'] at row 491680 in Excel.
285 Expected: ([H], O=CC1=C/C=C\C=C/[C]=C\1) --> Result: ([H], O=CC1=C\C=C/C=
    C/[C]=C\1)
286 Identical validation failed on [259427, 'O=CC1=C/C=C\\C=C\\C=C/1', 16, '[
    H]', 'O=CC1=C/C=C\\C=C/[C]=C\\1', 92.56071504501492, 84.189744985, 99.
    58089800103308, 'train'] at row 491681 in Excel.
287 Expected: ([H], O=CC1=C/C=C\C=C/C=[C]\1) --> Result: ([H], O=CC1=C\C=C/C=
    C/C=[C]\1)
288 Identical validation failed on [259428, 'O=CC1=C/C=C\\C=C\\C=C/1', 17, '[
    H]', 'O=CC1=C/C=C\\C=C/C=[C]\\1', 95.33995240598928, 86.787632245, 102.
    44970630310571, 'train'] at row 491682 in Excel.
289 Completed 60000 partitions under 3.42 seconds with progress 94.89%.

290 Expected: ([CH2]C1=C/C=C\C=C/C=C\1, [OH]) --> Result: ([CH2]C1=C\C=C/C=C/
    C=C\1, [OH])
291 Identical validation failed on [348004, 'OCC1=C/C=C\\C=C\\C=C/1', 0, '[
    CH2]C1=C/C=C\\C=C/C=C\\1', '[OH]', 78.76053711700766, 67.718888753, 83.
    0418184204995, 'train'] at row 501874 in Excel.
292 Expected: ([C]1=C/C=C/C=C/C=C/1, [CH2]O) --> Result: ([C]1=C/C=C\C=C\C=C/
    1, [CH2]O)
293 Identical validation failed on [348005, 'OCC1=C/C=C\\C=C\\C=C/1', 1, '[C]
    1=C/C=C/C=C/C=C/1', '[CH2]O', 84.84988445300719, 71.540418563, 89.
    86626564551348, 'train'] at row 501875 in Excel.
294 Expected: ([H], [O]C/C1=C\C=C\C=C/C=C/1) --> Result: ([H], [O]CC1=C\C=C/C
    =C/C=C\1)
295 Identical validation failed on [348006, 'OCC1=C/C=C\\C=C\\C=C/1', 10, '[H
    ]', '[O]C/C1=C\\C=C\\C=C/C=C/1', 103.30053158004417, 95.252728655, 110.
    94255653532382, 'train'] at row 501876 in Excel.
296 Expected: ([H], O[CH]C1=C/C=C\C=C/C=C\1) --> Result: ([H], O[CH]C1=C\C=C/
    C=C/C=C\1)
297 Identical validation failed on [348007, 'OCC1=C/C=C\\C=C\\C=C/1', 11, '[H
    ]', 'O[CH]C1=C/C=C\\C=C/C=C\\1', 75.61797204502318, 67.53251858, 81.
    95266130435249, 'train'] at row 501877 in Excel.
298 Expected: ([H], OCC1=[C]/C=C\C=C/C=C\1) --> Result: ([H], OCC1=[C]\C=C/C=
    C/C=C\1)
299 Identical validation failed on [348009, 'OCC1=C/C=C\\C=C\\C=C/1', 13, '[H
    ]', 'OCC1=[C]/C=C\\C=C/C=C\\1', 96.930060212041, 88.345737092, 103.
    95260020000824, 'train'] at row 501878 in Excel.
300 Expected: ([H], OCC1=C/[C]=C\C=C/C=C\1) --> Result: ([H], OCC1=C\[C]=C/C=
    C/C=C\1)
301 Identical validation failed on [348010, 'OCC1=C/C=C\\C=C\\C=C/1', 14, '[H
    ]', 'OCC1=C/[C]=C\\C=C/C=C\\1', 96.22725013203194, 87.872595306, 103.
    5377077924904, 'train'] at row 501879 in Excel.
302 Expected: ([H], OCC1=C/C=[C]\C=C/C=C\1) --> Result: ([H], OCC1=C\C=[C]/C=
    C/C=C\1)
303 Identical validation failed on [348011, 'OCC1=C/C=C\\C=C\\C=C/1', 15, '[H
    ]', 'OCC1=C/C=[C]\\C=C/C=C\\1', 98.02380839902612, 89.595107511, 105.
    2994897977644, 'train'] at row 501880 in Excel.
304 Expected: ([H], OCC1=C/C=C\[C]=C/C=C\1) --> Result: ([H], OCC1=C\C=C/[C]=
    C/C=C\1)
305 Identical validation failed on [348012, 'OCC1=C/C=C\\C=C\\C=C/1', 16, '[H
    ]', 'OCC1=C/C=C\\[C]=C/C=C\\1', 98.58040888201197, 90.082054495, 105.
    8136798025074, 'train'] at row 501881 in Excel.
306 Expected: ([H], OCC1=C/C=C\C=[C]/C=C\1) --> Result: ([H], OCC1=C\C=C/C=[C
    ]/C=C\1)
307 Identical validation failed on [348013, 'OCC1=C/C=C\\C=C\\C=C/1', 17, '[H
    ]', 'OCC1=C/C=C\\C=[C]/C=C\\1', 97.88136385602904, 89.622717907, 105.
    25686250736052, 'train'] at row 501882 in Excel.
308 Expected: ([H], OCC1=C/C=C\C=C/[C]=C\1) --> Result: ([H], OCC1=C\C=C/C=C
    /[C]=C\1)
309 Identical validation failed on [348014, 'OCC1=C/C=C\\C=C\\C=C/1', 18, '[H
    ]', 'OCC1=C/C=C\\C=C/[C]=C\\1', 96.26803821703596, 87.915893427, 103.
    42152268245616, 'train'] at row 501883 in Excel.
310 Expected: ([H], OCC1=C/C=C\C=C/C=[C]\1) --> Result: ([H], OCC1=C\C=C/C=C/

```
310 C=[C]\1)
311 Identical validation failed on [348015, 'OCC1=C/C=C\\C=C\\C=C/1', 19, '[H
    ]', 'OCC1=C/C=C\\C=C/C=[C]\\1', 96.94261039204498, 88.37836756, 103.
    95197269142751, 'train'] at row 501884 in Excel.
312 Completed 61000 partitions under 3.80 seconds with progress 96.47%.
313 Completed 62000 partitions under 5.15 seconds with progress 98.06%.
314 Completed 63000 partitions under 3.81 seconds with progress 99.64%.
315 Start exporting from ../BDE_data/source_dataset_v2_test.csv to ../
    BDE_data/source_dataset_v2_test_bType.csv.
316       rid          molecule  ...  fragment1_nochiral fragment2_nochiral
317 0  1102691  Br/C1=C\CCCCCC1  ...                [Br]      [C]1=CCCCCCC1
318 1  1102692  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=[C]CCCCCC1
319 2  1102693  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=C[CH]CCCC1
320 3  1102695  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=CC[CH]CCC1
321 4  1102697  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=CCC[CH]CC1
322 5  1102699  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=CCCC[CH]C1
323 6  1102701  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=CCCCC[CH]1
324 7  1102703  Br/C1=C\CCCCCC1  ...                 [H]     BrC1=CCCCCC[CH]1
325 8  1033498  Br/C=C/C1CCCCC1  ...                [Br]      [CH]=CC1CCCCC1
326 9  1033499  Br/C=C/C1CCCCC1  ...       [CH]1CCCCC1          [CH]=CBr
327
328 [10 rows x 16 columns]
329
330 Process finished with exit code 0
331
```