```
9444
  -OEChem-04052211553D

 29 30  0     1  0  0  0  0  0999 V2000
   -1.3610   -0.5442    1.0197 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2258    2.3520   -1.0905 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3947    1.5578    0.3599 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3334   -3.0676    0.2750 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.5399    2.2986    0.7076 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.7200    0.1982    0.2563 N   0  0  0  0  0  0  0  0  0  0  0  0
    3.0456    0.6838    0.1553 N   0  0  0  0  0  0  0  0  0  0  0  0
    2.2632   -1.4889   -0.3176 N   0  0  0  0  0  0  0  0  0  0  0  0
    4.5620   -0.9798   -0.4099 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3576    0.9761   -0.7980 C   0  0  2  0  0  0  0  0  0  0  0  0
   -2.7891    0.5875   -0.4940 C   0  0  1  0  0  0  0  0  0  0  0  0
   -2.6084   -0.6947    0.3070 C   0  0  1  0  0  0  0  0  0  0  0  0
   -0.6446    0.5801    0.4835 C   0  0  1  0  0  0  0  0  0  0  0  0
   -2.5096   -1.9398   -0.5642 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7608    1.1291    0.3911 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0581   -1.0888   -0.1008 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.2744   -0.5592   -0.1803 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9913    0.4013   -1.6572 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4182    0.4863   -1.3821 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6756    1.3881    1.2239 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3902   -0.8285    1.0633 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6715   -1.8970   -1.2643 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4332   -2.0773   -1.1359 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2769    2.5400   -1.1881 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9111    1.5850    1.2023 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2319   -1.7989   -0.1987 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2847   -3.8492   -0.3014 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.7632   -1.9389   -0.6709 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.3464   -0.3428   -0.3243 H   0  0  0  0  0  0  0  0  0  0  0  0
  1 12  1  0  0  0  0
  1 13  1  0  0  0  0
  2 10  1  0  0  0  0
  2 24  1  0  0  0  0
  3 11  1  0  0  0  0
  3 25  1  0  0  0  0
  4 14  1  0  0  0  0
  4 27  1  0  0  0  0
  5 15  2  0  0  0  0
  6 13  1  0  0  0  0
  6 15  1  0  0  0  0
  6 16  1  0  0  0  0
  7 15  1  0  0  0  0
  7 17  2  0  0  0  0
  8 16  2  0  0  0  0
  8 17  1  0  0  0  0
  9 17  1  0  0  0  0
```

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  9 28  1  0  0  0  0
  9 29  1  0  0  0  0
 10 11  1  0  0  0  0
 10 13  1  0  0  0  0
 10 18  1  0  0  0  0
 11 12  1  0  0  0  0
 11 19  1  0  0  0  0
 12 14  1  0  0  0  0
 12 21  1  0  0  0  0
 13 20  1  0  0  0  0
 14 22  1  0  0  0  0
 14 23  1  0  0  0  0
 16 26  1  0  0  0  0
M  END
> <PUBCHEM_COMPOUND_CID>
9444

> <PUBCHEM_CONFORMER_RMSD>
0.6

> <PUBCHEM_CONFORMER_DIVERSEORDER>
1
12
13
7
5
14
10
2
6
11
4
9
8
3

> <PUBCHEM_MMFF94_PARTIAL_CHARGES>
23
1 -0.56
10 0.28
11 0.28
12 0.28
13 0.58
14 0.28
15 0.84
16 0.45
17 0.71
2 -0.68
24 0.4
25 0.4
```

```
26 0.06
27 0.4
28 0.4
29 0.4
3 -0.68
4 -0.68
5 -0.57
6 -0.42
7 -0.66
8 -0.66
9 -0.85

> <PUBCHEM_EFFECTIVE_ROTOR_COUNT>
3

> <PUBCHEM_PHARMACOPHORE_FEATURES>
12
1 1 acceptor
1 2 acceptor
1 2 donor
1 3 acceptor
1 3 donor
1 4 acceptor
1 4 donor
1 5 acceptor
1 7 donor
1 9 donor
5 1 10 11 12 13 rings
6 6 7 8 15 16 17 rings

> <PUBCHEM_HEAVY_ATOM_COUNT>
17

> <PUBCHEM_ATOM_DEF_STEREO_COUNT>
4

> <PUBCHEM_ATOM_UDEF_STEREO_COUNT>
0

> <PUBCHEM_BOND_DEF_STEREO_COUNT>
0

> <PUBCHEM_BOND_UDEF_STEREO_COUNT>
0

> <PUBCHEM_ISOTOPIC_ATOM_COUNT>
0

> <PUBCHEM_COMPONENT_COUNT>
1
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> <PUBCHEM_CACTVS_TAUTO_COUNT>
3

> <PUBCHEM_CONFORMER_ID>
000024E400000001

> <PUBCHEM_MMFF94_ENERGY>
50.9521

> <PUBCHEM_FEATURE_SELFOVERLAP>
60.962

> <PUBCHEM_SHAPE_FINGERPRINT>
10608611 8 18411694409049253760
11132069 177 18412541020444494778
12138202 97 18115012001220561597
12500047 106 18337105674893126407
12932764 1 17967523554309708816
12969540 114 17969481746681867365
13024252 1 16008756779798805865
14115302 16 18337121076640867588
14965852 173 18412545426753782225
15219456 202 18411978091654822960
15375462 6 18194680603708808396
15775835 57 18261114006691984659
16945 1 18263910082036207721
200 152 17703782604885574207
20201158 50 18340205189608376350
21501502 16 18409730707041059616
221490 88 18268153230900097050
22802520 49 18409727395758327137
23388829 49 17762053646393732453
23402539 116 17385722483089480382
23559900 14 18270389607048294688
25 1 18194116309536170397
2748010 2 18265888245114462605
2871803 45 18264760133526972055
5493415 88 18342737442455005866
6333449 129 18335699421259755389
69090 78 18410569549046287917
74978 22 18341892987106739929
81228 2 18115583893723206425
8809292 202 18409731750839594346
93112 12 18412260640293982853
9709674 26 18341890856908754887

> <PUBCHEM_SHAPE_MULTIPOLES>
300.58
6.14

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2.47
0.84
3.95
0.5
0.04
1.55
0.49
-1.36
0.1
-0.24
-0.17
0.57

> <PUBCHEM_SHAPE_SELFOVERLAP>
635.496

> <PUBCHEM_SHAPE_VOLUME>
168.2

> <PUBCHEM_COORDINATE_TYPE>
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5
10

$$$$
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