Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Insight into structural properties of polyethylene glycol monolaurate in water alcohols from molecular dynamics studies

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Table S.1
Include file for topology (itp file) of PEGML and the calculated atomic charges by using AM1-BCC. Atomic numbering is given in Figure S.1.

```
[ moleculetype ]
; Name      nrexcl
  PEGML       3

[ atoms ]
;  nr  type    resnr residue  atom cgnr     charge    mass
    1 opls_490  1     ML      C1     1    -0.0141079
    2 opls_182  1     ML      C2     2    -0.0213862
    3 opls_180  1     ML      O1     2    -0.2826303
    4 opls_465  1     ML      C3     3     0.3040785
    5 opls_136  1     ML      C4     4    -0.1545249
    6 opls_136  1     ML      C5     5    -0.1549852
    7 opls_136  1     ML      C6     6    -0.1592751
    8 opls_136  1     ML      C7     7    -0.1567743
    9 opls_136  1     ML      C8     8    -0.1579672
   10 opls_136  1     ML      C9     9    -0.1574738
   11 opls_136  1     ML      C10   10    -0.1576485
   12 opls_136  1     ML      C11   11    -0.1576251
   13 opls_136  1     ML      C12   12    -0.1579151
   14 opls_136  1     ML      C13   13    -0.1586728
   15 opls_135  1     ML      C14   14    -0.2105497
   16 opls_466  1     ML      O2     3    -0.3536118
   17 opls_467  1     ML      O3     3    -0.2813521
   18 opls_182  1     ML      C15   15    -0.0205762
   19 opls_182  1     ML      C16   16    -0.0207722
   20 opls_180  1     ML      O4    16    -0.2866073
   21 opls_182  1     ML      C17   17    -0.0207861
   22 opls_182  1     ML      C18   18    -0.0203461
   23 opls_180  1     ML      O5    18    -0.2861399
   24 opls_182  1     ML      C19   19    -0.0204555
   25 opls_182  1     ML      C20   20    -0.0203821
   26 opls_180  1     ML      O6    20    -0.2877822
   27 opls_182  1     ML      C21   21    -0.0207379
   28 opls_157  1     ML      C22   22    -0.0229443
   29 opls_154  1     ML      O7    22    -0.3297824
   30 opls_469  1     ML      H1     1     0.1055632
   31 opls_469  1     ML      H2     1     0.1053012
   32 opls_185  1     ML      H3     2     0.0803985
   33 opls_185  1     ML      H4     2     0.0805453
   34 opls_140  1     ML      H5     4     0.1200091
   35 opls_140  1     ML      H6     4     0.1199183
   36 opls_140  1     ML      H7     5     0.0953492
   37 opls_140  1     ML      H8     5     0.0948379
   38 opls_140  1     ML      H9     6     0.0801070
   39 opls_140  1     ML      H10    6     0.0800527
   40 opls_140  1     ML      H11    7     0.0812427
   41 opls_140  1     ML      H12    7     0.0812498
   42 opls_140  1     ML      H13    8     0.0793930
   43 opls_140  1     ML      H14    8     0.0793732
   44 opls_140  1     ML      H15    9     0.0793988
   45 opls_140  1     ML      H16    9     0.0794083
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  56  opls_140  1     ML      H27   14     0.0718732
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  58  opls_185  1     ML      H29   15     0.0816882
  59  opls_185  1     ML      H30   16     0.0829934
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  62  opls_185  1     ML      H33   17     0.0823872
  63  opls_185  1     ML      H34   18     0.0814915
  64  opls_185  1     ML      H35   18     0.0815223
  65  opls_185  1     ML      H36   19     0.0814240
  66  opls_185  1     ML      H37   19     0.0814311
  67  opls_185  1     ML      H38   20     0.0819437
  68  opls_185  1     ML      H39   20     0.0819366
  69  opls_185  1     ML      H40   21     0.0823078
  70  opls_185  1     ML      H41   21     0.0822967
  71  opls_140  1     ML      H42   22     0.0749899
  72  opls_140  1     ML      H43   22     0.0750044
  73  opls_155  1     ML      H44   22     0.2042815

[ bonds ]
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  1    30   1
  1    31   1
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  2    32   1
  2    33   1
  3    18   1
  4     5   1
  4    16   1
  4    17   1
  5     6   1
  5    34   1
  5    35   1
  6     7   1
  6    36   1
  6    37   1
  7     8   1
  7    38   1
  7    39   1
  8     9   1
  8    40   1
  8    41   1
  9    10   1
  9    42   1
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```
  9    43   1
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  10   44   1
  10   45   1
  11   12   1
  11   46   1
  11   47   1
  12   13   1
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  12   49   1
  13   14   1
  13   50   1
  13   51   1
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  25   67   1
  25   68   1
  26   27   1
  27   28   1
  27   69   1
  27   70   1
  28   29   1
  28   71   1
  28   72   1
  29   73   1

[ angles ]
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    1    2   33   1
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    2    1   30   1
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 3   18   58   1
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 5    6   37   1
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 6    5   35   1
 6    7    8   1
 6    7   38   1
 6    7   39   1
 7    6   36   1
 7    6   37   1
 7    8    9   1
 7    8   40   1
 7    8   41   1
 8    7   38   1
 8    7   39   1
 8    9   10   1
 8    9   42   1
 8    9   43   1
 9    8   40   1
 9    8   41   1
 9   10   11   1
 9   10   44   1
 9   10   45   1
10    9   42   1
10    9   43   1
10   11   12   1
10   11   46   1
10   11   47   1
11   10   44   1
11   10   45   1
11   12   13   1
11   12   48   1
11   12   49   1
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12   11   47   1
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13   12   48   1
13   12   49   1
13   14   15   1
13   14   52   1
13   14   53   1
14   13   50   1
14   13   51   1
14   15   54   1
14   15   55   1
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14   15   56   1
15   14   52   1
15   14   53   1
16    4   17   1
17    1   30   1
17     1  31   1
18   19   20   1
18   19   59   1
18   19   60   1
19   18   57   1
19   18   58   1
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20   19   59   1
20   19   60   1
20   21   22   1
20   21   61   1
20   21   62   1
21   22   23   1
21   22   63   1
21   22   64   1
22   21   61   1
22   21   62   1
22   23   24   1
23   22   63   1
23   22   64   1
23   24   25   1
23   24   65   1
23   24   66   1
24   25   26   1
24   25   67   1
24   25   68   1
25   24   65   1
25   24   66   1
25   26   27   1
26   25   67   1
26   25   68   1
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26   27   70   1
27   28   29   1
27   28   71   1
27   28   72   1
28   27   69   1
28   27   70   1
28   29   73   1
29   28   71   1
29   28   72   1
30    1   31   1
32    2   33   1
34    5   35   1
36    6   37   1
38    7   39   1
40    8   41   1
42    9   43   1
44   10   45   1
46   11   47   1
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  50   13   51   1
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  54   15   56   1
  55   15   56   1
  57   18   58   1
  59   19   60   1
  61   21   62   1
  63   22   64   1
  65   24   66   1
  67   25   68   1
  69   27   70   1
  71   28   72   1

[ dihedrals ]
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  30    1    2   32    3
  31    1    2   32    3
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  31    1   17    4    3
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   2    3   18   58    3
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  35    5    4   17    3
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   4    5    6   36    3
  34    5    6   36    3
  35    5    6   36    3
   4    5    6   37    3
  34    5    6   37    3
  35    5    6   37    3
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  36    6    7   38    3
  37    6    7   38    3
   5    6    7   39    3
  36    6    7   39    3
  37    6    7   39    3
```

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6     7    8   40    3
38    7    8   40    3
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38    7    8   41    3
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41    8    9   10    3
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41    8    9   42    3
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40    8    9   43    3
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42    9   10   11    3
43    9   10   11    3
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42    9   10   44    3
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45   10   11   46    3
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44   10   11   47    3
45   10   11   47    3
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46   11   12   13    3
47   11   12   13    3
10   11   12   48    3
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46   11   12   49    3
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11   12   13   51    3
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50   13   14   15    3
51   13   14   15    3
12   13   14   52    3
50   13   14   52    3
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50   13   14   53    3
51   13   14   53    3
13   14   15   54    3
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53   14   15   54    3
13   14   15   55    3
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 3   18   19   60    3
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18   19   20   21    3
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60   19   20   21    3
19   20   21   22    3
19   20   21   61    3
19   20   21   62    3
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61   21   22   23    3
62   21   22   23    3
20   21   22   63    3
61   21   22   63    3
62   21   22   63    3
20   21   22   64    3
61   21   22   64    3
62   21   22   64    3
21   22   23   24    3
63   22   23   24    3
64   22   23   24    3
22   23   24   25    3
22   23   24   65    3
22   23   24   66    3
23   24   25   26    3
65   24   25   26    3
23   24   25   67    3
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66   24   25   67    3
23   24   25   68    3
65   24   25   68    3
66   24   25   68    3
67   25   26   27    3
68   25   26   27    3
25   26   27   28    3
25   26   27   69    3
25   26   27   70    3
26   27   28   29    3
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   70   27   28   29    3
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   69   27   28   71    3
   70   27   28   71    3
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   72   28   29   73    3

[ dihedrals ]
#define improper_O_C_X_Y

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   38   36   1
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   39   36   1
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    9    6   1
```

```
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42   40   1
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43   40   1
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14   49   1
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50   48   1
50   49   1
51   11   1
51   48   1
51   49   1
15   12   1
15   50   1
15   51   1
```

```
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53   51   1
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54   52   1
54   53   1
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55   53   1
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56   52   1
56   53   1
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20   58   1
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59   57   1
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60   57   1
60   58   1
21   18   1
21   59   1
21   60   1
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62   19   1
23   20   1
23   61   1
23   62   1
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63   61   1
63   62   1
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64   61   1
64   62   1
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24   63   1
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67   23   1
67   65   1
67   66   1
68   23   1
68   65   1
68   66   1
27   24   1
27   67   1
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```
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28   25   1
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70   25   1
29   26   1
29   69   1
29   70   1
71   26   1
71   69   1
71   70   1
72   26   1
72   69   1
72   70   1
73   27   1
73   71   1
73   72   1
```

Table S.2
The calculated atomic charges of PEGML by using RESP.

```
[ moleculetype ]
; Name      nrexcl
  PEGML       3

[ atoms ]
; nr  type   resnr residue  atom  cgnr   charge    mass
   1  opls_490  1  ML  C1    1    0.3691043962    12.011
   2  opls_182  1  ML  C2    2    0.4689230369    12.011
   3  opls_180  1  ML  O1    2   -0.8364129330    15.9994
   4  opls_465  1  ML  C3    3    1.2539006151    12.011
   5  opls_136  1  ML  C4    4   -0.6718680437    12.011
   6  opls_136  1  ML  C5    5    0.3319010221    12.011
   7  opls_136  1  ML  C6    6    0.0442016085    12.011
   8  opls_136  1  ML  C7    7   -0.1018270467    12.011
   9  opls_136  1  ML  C8    8    0.1084576434    12.011
  10  opls_136  1  ML  C9    9    0.0747121790    12.011
  11  opls_136  1  ML  C10  10    0.0550785378    12.011
  12  opls_136  1  ML  C11  11    0.0342192661    12.011
  13  opls_136  1  ML  C12  12    0.0147417429    12.011
  14  opls_136  1  ML  C13  13    0.1658651316    12.011
  15  opls_135  1  ML  C14  14   -0.2370784739    12.011
  16  opls_466  1  ML  O2    3   -0.7500293071    15.9994
  17  opls_467  1  ML  O3    3   -0.7930093275    15.9994
  18  opls_182  1  ML  C15  15    0.4998390010    12.011
  19  opls_182  1  ML  C16  16    0.5710990373    12.011
  20  opls_180  1  ML  O4   16   -0.8779960864    15.9994
  21  opls_182  1  ML  C17  17    0.5050389716    12.011
  22  opls_182  1  ML  C18  18    0.5744649402    12.011
  23  opls_180  1  ML  O5   18   -0.8796376655    15.9994
  24  opls_182  1  ML  C19  19    0.4919900476    12.011
  25  opls_182  1  ML  C20  20    0.5817423126    12.011
  26  opls_180  1  ML  O6   20   -0.8407686412    15.9994
  27  opls_182  1  ML  C21  21    0.3934631471    12.011
  28  opls_157  1  ML  C22  22    0.4218024291    12.011
  29  opls_154  1  ML  O7   22   -0.8769199458    15.9994
  30  opls_469  1  ML  H1    1    0.0253328963    1.008
  31  opls_469  1  ML  H2    1    0.0253328963    1.008
  32  opls_185  1  ML  H3    2   -0.0206468332    1.008
  33  opls_185  1  ML  H4    2   -0.0206468332    1.008
  34  opls_140  1  ML  H5    4    0.1504141913    1.008
  35  opls_140  1  ML  H6    4    0.1504141913    1.008
  36  opls_140  1  ML  H7    5   -0.0556463752    1.008
  37  opls_140  1  ML  H8    5   -0.0556463752    1.008
  38  opls_140  1  ML  H9    6   -0.0007769637    1.008
  39  opls_140  1  ML  H10   6   -0.0007769637    1.008
  40  opls_140  1  ML  H11   7    0.0060006861    1.008
  41  opls_140  1  ML  H12   7    0.0060006861    1.008
  42  opls_140  1  ML  H13   8   -0.0377254766    1.008
  43  opls_140  1  ML  H14   8   -0.0377254766    1.008
  44  opls_140  1  ML  H15   9   -0.0266833354    1.008
```

45	opls_140	1	ML	H16	9	-0.0266833354	1.008
46	opls_140	1	ML	H17	10	-0.0276335919	1.008
47	opls_140	1	ML	H18	10	-0.0276335919	1.008
48	opls_140	1	ML	H19	11	-0.0271704691	1.008
49	opls_140	1	ML	H20	11	-0.0271704691	1.008
50	opls_140	1	ML	H21	12	-0.0135801452	1.008
51	opls_140	1	ML	H22	12	-0.0135801452	1.008
52	opls_140	1	ML	H23	13	-0.0319989990	1.008
53	opls_140	1	ML	H24	13	-0.0319989990	1.008
54	opls_140	1	ML	H25	14	0.0532157898	1.008
55	opls_140	1	ML	H26	14	0.0532157898	1.008
56	opls_140	1	ML	H27	14	0.0532157898	1.008
57	opls_185	1	ML	H28	15	-0.0430744089	1.008
58	opls_185	1	ML	H29	15	-0.0430744089	1.008
59	opls_185	1	ML	H30	16	-0.0560840798	1.008
60	opls_185	1	ML	H31	16	-0.0560840798	1.008
61	opls_185	1	ML	H32	17	-0.0427736303	1.008
62	opls_185	1	ML	H33	17	-0.0427736303	1.008
63	opls_185	1	ML	H34	18	-0.0551028934	1.008
64	opls_185	1	ML	H35	18	-0.0551028934	1.008
65	opls_185	1	ML	H36	19	-0.0431525860	1.008
66	opls_185	1	ML	H37	19	-0.0431525860	1.008
67	opls_185	1	ML	H38	20	-0.0544585624	1.008
68	opls_185	1	ML	H39	20	-0.0544585624	1.008
69	opls_185	1	ML	H40	21	-0.0242281794	1.008
70	opls_185	1	ML	H41	21	-0.0242281794	1.008
71	opls_140	1	ML	H42	22	0.0063324461	1.008
72	opls_140	1	ML	H43	22	0.0063324461	1.008
73	opls_155	1	ML	H44	22	0.4906676549	1.008

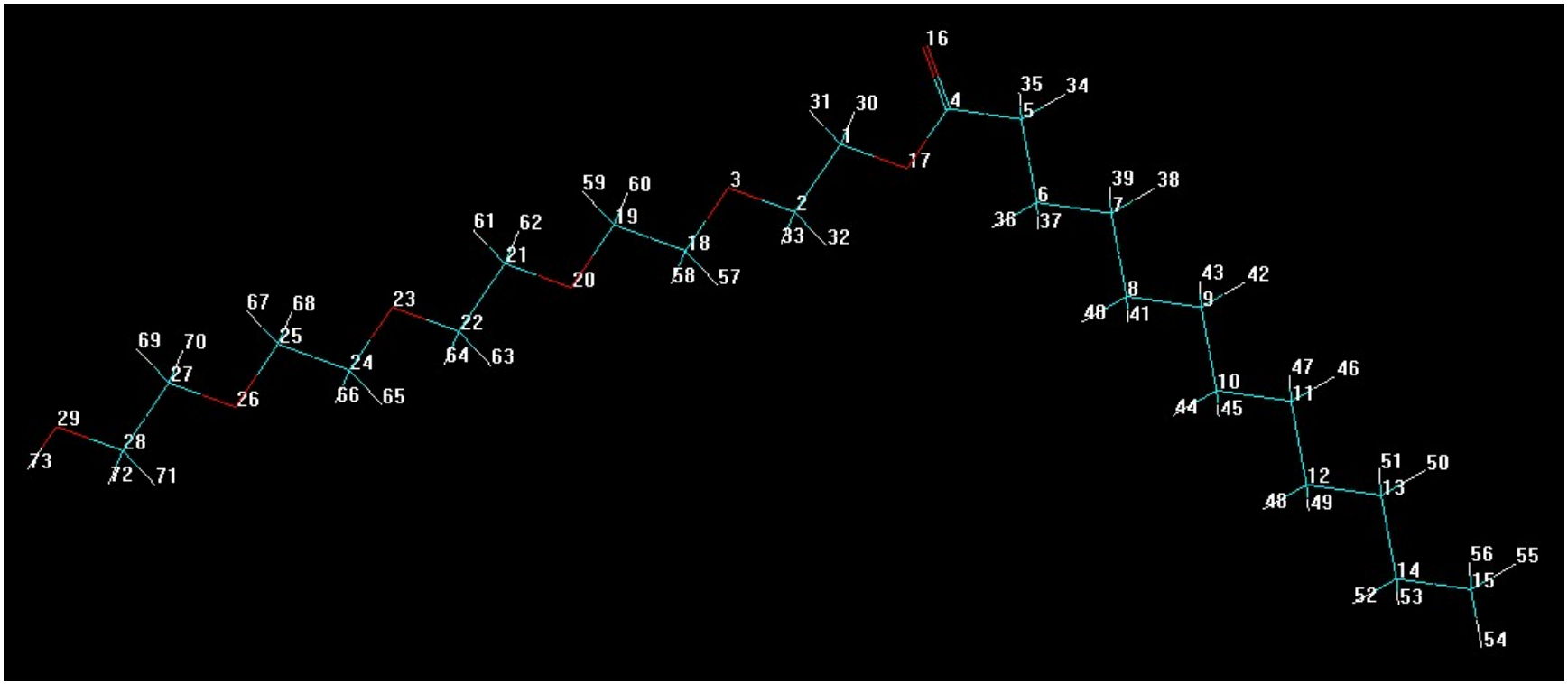

Fig. A.1 PEGML molecule with its atomic numbering. The hydrogen atoms, including the polar hydrogen, were depicted by white color, carbon atoms by blue, and oxygen atoms by red.