Indexing - Substance

Food and Drug Administration
Indexing - Substance

(5IE62321P4)

Substance Information

Mapping	Definition Hash:	97f068f6-1e51-0069-edd1-9614005b5d0d

Moiety (mixture component)

Name		Quantity	Undefined not 0

Moiety Characteristics


```
  -FDASRS-06071412322D

138145  0  0  1  0  0  0  0  0999 V2000
   15.6083   -9.2648    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1243   -9.4249    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.4500   -9.0109    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   15.1251   -9.5083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.1167  -10.0000    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   14.6500  -10.2375    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   15.5917  -10.2417    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.0667  -10.0041    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   16.5417  -10.2458    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.0125  -10.0083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.5941  -10.7334    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   17.5000  -10.2958    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   15.6083   -8.7565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1282   -8.6017    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.2378   -8.1046    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.8371   -7.7654    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.3146   -7.9229    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2063   -8.4191    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9124   -9.1982    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.4284   -9.3583    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.7500   -8.9442    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.4292   -9.4417    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9124   -8.6898    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.4323   -8.5350    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.5461   -8.0379    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.1413   -7.6987    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.6230   -7.8562    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.5104   -8.3525    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7541   -9.2065    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2743   -9.3666    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.5959   -8.9566    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   10.8482  -10.6708    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.2750   -9.4542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.2667   -9.9417    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   10.8458  -10.1791    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    8.9542  -10.1750    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.4291   -9.9334    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    9.9041  -10.1750    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.3791   -9.9375    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   11.3208   -9.9417    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.7958  -10.1792    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.7417  -10.1875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2167   -9.9458    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   13.6917  -10.1916    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   14.1583   -9.9458    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9042  -10.6667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
```

```
 11.3268   -9.4500    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 12.7399  -10.6750    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 13.6959  -10.6791    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 14.1626   -9.4584    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 11.3185  -10.9245    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 12.7583   -8.6981    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 13.2740   -8.5433    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 13.3878   -8.0463    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 12.9871   -7.7071    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 12.4647   -7.8646    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 12.3521   -8.3608    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.0583   -9.1440    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.5784   -9.3041    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.9000   -8.8942    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 -4.7643   -9.4000    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
 -1.9268   -9.3917    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.4999  -10.6083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.5083  -10.1166    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
 -1.9250   -9.8833    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
 -5.2417  -10.1334    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 -4.7667   -9.8876    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
 -4.2917  -10.1292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.8208   -9.8834    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 -3.3458  -10.1291    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -2.8708   -9.8874    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -2.3958  -10.1250    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 -1.4500  -10.1167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.9750   -9.8792    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 -0.0333   -9.8749    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  0.4417  -10.1125    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  0.9167   -9.8708    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  1.3875  -10.1125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.2899  -10.6167    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 -2.8666   -9.3958    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 -1.4482  -10.6083    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 -0.0309   -9.3875    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  0.9208   -9.3834    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1.3917  -10.6000    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1.8404   -9.8659    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  2.3149  -10.5958    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  5.1523  -10.6042    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.5792   -9.3876    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.5750   -9.8792    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  5.1541  -10.1125    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
  2.3125  -10.1124    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  2.7875   -9.8667    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  3.2625  -10.1125    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  3.7334   -9.8709    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  4.2084  -10.1126    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.6834   -9.8708    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  5.6291   -9.8833    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.1041  -10.1208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  7.0500  -10.1251    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.5250   -9.8833    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  8.0000  -10.1250    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
  8.4666   -9.8834    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  2.7893   -9.3792    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  3.7375   -9.3792    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.2124   -9.1375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.2083  -10.6042    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  5.6310   -9.3875    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  7.0482  -10.6125    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  8.0000  -10.6166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  8.4709   -9.3958    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 -4.3153   -9.1589    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -5.2151   -9.1620    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.0244  -10.8579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.0154  -11.3660    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  0.4463  -10.5950    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  2.7638  -10.8369    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1.8641  -10.8338    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  3.2856   -9.1308    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.6802  -10.8587    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  5.6268  -10.8620    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.0624   -8.6357    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.5823   -8.4808    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.6919   -7.9837    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  7.2912   -7.6445    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.7688   -7.8020    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE	6.6604 -8.2983 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.4566 -10.8552 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.4607 -11.3469 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.9089 -10.6105 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.3208 -11.4329 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.7948 -10.6698 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.1523 -10.9178 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.1566 -11.4094 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.6047 -10.6729 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.7096 -9.8770 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.7125 -9.3625 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -3.8647 -9.4011 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -4.2917 -9.6292 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 17 18 2 0 0 0 0 18 13 1 0 0 0 0 23 19 1 0 0 0 0 10 12 1 0 0 0 0 5 4 1 1 0 0 0 6 5 1 0 0 0 0 19 20 2 0 0 0 0 20 21 1 0 0 0 0 21 24 1 0 0 0 0 5 7 1 0 0 0 0 22 19 1 0 0 0 0 7 8 1 0 0 0 0 8 9 1 0 0 0 0 73 81 2 0 0 0 0 75 82 2 0 0 0 0 77 83 1 1 0 0 0 78 84 2 0 0 0 0 64 63 1 1 0 0 0 65 62 1 1 0 0 0 67 61 1 0 0 0 0 66 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 69 70 1 0 0 0 0 70 71 1 0 0 0 0 71 72 1 0 0 0 0 72 65 1 0 0 0 0 65 73 1 0 0 0 0 73 74 1 0 0 0 0 74 64 1 0 0 0 0 64 75 1 0 0 0 0 75 76 1 0 0 0 0 76 77 1 0 0 0 0 77 78 1 0 0 0 0 68 79 2 0 0 0 0 71 80 2 0 0 0 0 23 24 2 0 0 0 0 78 85 1 0 0 0 0 40 47 2 0 0 0 0 42 48 2 0 0 0 0 44 49 1 1 0 0 0 45 50 2 0 0 0 0 45 6 1 0 0 0 0 34 33 1 1 0 0 0 35 32 1 1 0 0 0 36 37 1 0 0 0 0 37 38 1 0 0 0 0 38 39 1 0 0 0 0 39 35 1 0 0 0 0 35 40 1 0 0 0 0 40 41 1 0 0 0 0 41 34 1 0 0 0 0 34 42 1 0 0 0 0 42 43 1 0 0 0 0 43 44 1 0 0 0 0 44 45 1 0 0 0 0 37 22 1 1 0 0 0 38 46 2 0 0 0 0 9 10 1 0 0 0 0 32 51 1 0 0 0 0 33 29 1 0 0 0 0 24 25 1 0 0 0 0 4 1 1 0 0 0 0 97107 2 0 0 0 0 99108 2 0 0 0 0 101109 1 1 0 0 0

```
102110  2  0  0  0  0
102 36  1  0  0  0  0
 89 88  1  1  0  0  0
 90 87  1  1  0  0  0
 91 86  1  1  0  0  0
 85 91  1  0  0  0  0
 91 92  1  0  0  0  0
 92 93  1  0  0  0  0
 93 94  1  0  0  0  0
 94 95  1  0  0  0  0
 95 96  1  0  0  0  0
 96 90  1  0  0  0  0
 90 97  1  0  0  0  0
 97 98  1  0  0  0  0
 98 89  1  0  0  0  0
 89 99  1  0  0  0  0
 99100  1  0  0  0  0
100101  1  0  0  0  0
101102  1  0  0  0  0
 92103  2  0  0  0  0
 94104  1  1  0  0  0
104105  1  0  0  0  0
 95106  2  0  0  0  0
 52 53  2  0  0  0  0
 61111  1  0  0  0  0
 25 26  2  0  0  0  0
 61112  1  1  0  0  0
 53 54  1  0  0  0  0
 63113  1  0  0  0  0
  3 14  1  0  0  0  0
113114  1  0  0  0  0
 54 55  2  0  0  0  0
113115  1  0  0  0  0
 26 27  1  0  0  0  0
 86116  1  0  0  0  0
 55 56  1  0  0  0  0
 86117  1  0  0  0  0
 13  1  1  0  0  0  0
104118  1  0  0  0  0
 56 57  2  0  0  0  0
 87119  1  0  0  0  0
 57 52  1  0  0  0  0
 87120  1  0  0  0  0
 88 58  1  0  0  0  0
121 58  1  0  0  0  0
 27 28  2  0  0  0  0
121122  2  0  0  0  0
 28 23  1  0  0  0  0
122123  1  0  0  0  0
 52 29  1  0  0  0  0
123124  2  0  0  0  0
 58 59  2  0  0  0  0
124125  1  0  0  0  0
 59 60  1  0  0  0  0
125126  2  0  0  0  0
126121  1  0  0  0  0
 60122  1  0  0  0  0
109127  1  0  0  0  0
 13 14  2  0  0  0  0
127128  1  0  0  0  0
127129  1  0  0  0  0
 14 15  1  0  0  0  0
 51130  1  0  0  0  0
 29 30  2  0  0  0  0
 51131  1  0  0  0  0
 30 31  1  0  0  0  0
 49132  1  0  0  0  0
 31 53  1  0  0  0  0
132133  1  0  0  0  0
  1  2  2  0  0  0  0
132134  1  0  0  0  0
 15 16  2  0  0  0  0
 66135  1  0  0  0  0
  2  3  1  0  0  0  0
135136  2  0  0  0  0
 16 17  1  0  0  0  0
111137  1  0  0  0  0
  7 11  2  0  0  0  0
 67138  1  6  0  0  0
```

	M END
Chemical Structures, InChI	InChI=1S/C100H142N20O17/c1-19-59(16)86(107-51-122)97(134)106-50-82(123)108-60(17)87(124)110-74(38-52(2)3)90(127)109-61(18)88(125)118-84(57(12)13)99(136)120-85(58(14)15)100(137)119-83(56(10)11)98(135)117-81(45-65-49-105-73-35-27-23-31-69(65)73)96(133)113-77(41-55(8)9)93(130)116-80(44-64-48-104-72-34-26-22-30-68(64)72)95(132)112-76(40-54(6)7)92(129)115-79(43-63-47-103-71-33-25-21-29-67(63)71)94(131)111-75(39-53(4)5)91(128)114-78(89(126)101-36-37-121)42-62-46-102-70-32-24-20-28-66(62)70/h20-35,46-49,51-61,74-81,83-86,102-105,121H,19,36-45,50H2,1-18H3,(H,101,126)(H,106,134)(H,107,122)(H,108,123)(H,109,127)(H,110,124)(H,111,131)(H,112,132)(H,113,133)(H,114,128)(H,115,129)(H,116,130)(H,117,135)(H,118,125)(H,119,137)(H,120,136)/t59-,60-,61-,74+,75+,76+,77+,78-,79-,80-,81-,83+,84+,85-,86-/m0/s1
Chemical Structure, InChI Key	YKMZGZLYVAUETK-LQJUTOEZSA-N

Moiety (mixture component)

Name		**Quantity**	Undefined not 0

Moiety Characteristics

```
  -FDASRS-06071412322D

135141  0  0  1  0  0  0  0  0999 V2000
   15.6083   -3.7065    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1284   -3.8666    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.4458   -3.4525    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   15.1292   -3.9500    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.1208   -4.4417    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   14.6541   -4.6792    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   15.5958   -4.6834    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.0708   -4.4458    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   16.5458   -4.6875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.0166   -4.4458    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.5940   -5.1750    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   17.5041   -4.7416    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   15.6082   -3.1981    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1281   -3.0433    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.2419   -2.5463    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.8412   -2.2071    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.3188   -2.3646    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2062   -2.8608    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9124   -3.6398    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.4334   -3.8833    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7583   -3.6482    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2743   -3.8083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.6000   -3.3983    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   10.8482   -5.1083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.2751   -3.8959    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.2667   -4.3834    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   10.8500   -4.6167    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    8.9542   -4.6208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.4292   -4.3751    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    9.9042   -4.6167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.3792   -4.3750    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   11.3250   -4.3875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.8000   -4.6250    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.7417   -4.6292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2167   -4.3875    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   13.6917   -4.6292    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   14.1625   -4.3875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9084   -5.1084    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   11.3268   -3.8917    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   12.7441   -5.1167    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   13.6958   -5.1208    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.1667   -3.9000    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   11.3226   -5.3662    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7583   -3.1398    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2782   -2.9850    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.3920   -2.4879    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.9871   -2.1487    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.4688   -2.3062    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

12.3563	-2.8025	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.0624	-3.5856	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.5826	-3.7457	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.9000	-3.3359	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
-4.7643	-3.8417	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
-1.9227	-3.8334	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.5000	-5.0500	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.5042	-4.5583	0.0000	C	0	0	1	0	0	0	0	0	0	0	0	0	0	
-1.9209	-4.3250	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
-5.2375	-4.5750	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
-4.7625	-4.3292	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
-4.2875	-4.5709	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-3.8167	-4.3291	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
-3.3458	-4.5708	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-2.8708	-4.3291	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-2.3958	-4.5667	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
-1.4459	-4.5583	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.9709	-4.3208	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.0292	-4.3166	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
0.4458	-4.5542	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
0.9208	-4.3125	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
1.3916	-4.5542	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-4.2899	-5.0584	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
-2.8667	-3.8375	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
-1.4440	-5.0500	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.0310	-3.8250	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
0.9209	-3.8251	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
1.3917	-5.0458	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
1.8404	-4.3076	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
2.3148	-5.0374	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
5.1565	-5.0499	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
6.5792	-3.8292	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
6.5750	-4.3208	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
5.1542	-4.5583	0.0000	C	0	0	1	0	0	0	0	0	0	0	0	0	0	
2.3166	-4.5541	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
2.7916	-4.3084	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
3.2625	-4.5542	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
3.7375	-4.3125	0.0000	C	0	0	2	0	0	0	0	0	0	0	0	0	0	
4.2125	-4.5542	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
4.6875	-4.3166	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
5.6292	-4.3208	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
6.1042	-4.5583	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.0500	-4.5667	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.5250	-4.3249	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0	0	
8.0000	-4.5708	0.0000	C	0	0	1	0	0	0	0	0	0	0	0	0	0	
8.4667	-4.3291	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
2.7893	-3.8209	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
3.7375	-3.8209	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
4.2166	-3.5792	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
4.2125	-5.0458	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
5.6310	-3.8292	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.0482	-5.0542	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
8.0001	-5.0542	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
8.4709	-3.8375	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	
-4.3154	-3.6005	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-5.2150	-3.6036	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.0202	-5.2995	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-0.0112	-5.8077	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
0.4464	-5.0366	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
2.7638	-5.2786	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
1.8642	-5.2755	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
3.2898	-3.5725	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
4.6803	-5.3004	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
5.6268	-5.3036	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.0624	-3.0774	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.5823	-2.9225	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.6961	-2.4254	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
7.2913	-2.0862	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
6.7730	-2.2437	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
6.6604	-2.7399	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
8.4607	-5.2969	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
8.4649	-5.7885	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
8.9131	-5.0522	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
11.3208	-5.8745	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
11.7947	-5.1115	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
14.1565	-5.3594	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
14.1608	-5.8511	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
14.6047	-5.1146	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	
-5.7055	-4.3187	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	

Chemical Structure, MOLFILE	-5.7084 -3.8042 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -3.8646 -3.8428 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -4.2917 -4.0750 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 10.3798 -3.9007 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.8582 -3.6581 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.8670 -3.1465 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.3930 -2.8840 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.9188 -3.1301 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 69 75 1 1 0 0 0 70 76 2 0 0 0 0 56 55 1 1 0 0 0 57 54 1 1 0 0 0 59 53 1 0 0 0 0 58 59 1 0 0 0 0 59 60 1 0 0 0 0 60 61 1 0 0 0 0 61 62 1 0 0 0 0 62 63 1 0 0 0 0 63 64 1 0 0 0 0 64 57 1 0 0 0 0 57 65 1 0 0 0 0 65 66 1 0 0 0 0 66 56 1 0 0 0 0 56 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 69 70 1 0 0 0 0 60 71 2 0 0 0 0 63 72 2 0 0 0 0 30 31 1 0 0 0 0 70 77 1 0 0 0 0 31 27 1 0 0 0 0 27 32 1 0 0 0 0 32 33 1 0 0 0 0 33 26 1 0 0 0 0 26 34 1 0 0 0 0 34 35 1 0 0 0 0 35 36 1 0 0 0 0 36 37 1 0 0 0 0 29 20 1 1 0 0 0 30 38 2 0 0 0 0 6 5 1 0 0 0 0 24 43 1 0 0 0 0 25 21 1 0 0 0 0 5 7 1 0 0 0 0 7 8 1 0 0 0 0 44 45 2 0 0 0 0 21 22 2 0 0 0 0 45 46 1 0 0 0 0 22 23 1 0 0 0 0 46 47 2 0 0 0 0 23 45 1 0 0 0 0 47 48 1 0 0 0 0 8 9 1 0 0 0 0 48 49 2 0 0 0 0 49 44 1 0 0 0 0 89 99 2 0 0 0 0 91100 2 0 0 0 0 93101 1 1 0 0 0 94102 2 0 0 0 0 94 28 1 0 0 0 0 81 80 1 1 0 0 0 82 79 1 1 0 0 0 83 78 1 1 0 0 0 77 83 1 0 0 0 0 83 84 1 0 0 0 0 84 85 1 0 0 0 0 85 86 1 0 0 0 0 86 87 1 0 0 0 0 87 88 1 0 0 0 0 88 82 1 0 0 0 0 82 89 1 0 0 0 0 89 90 1 0 0 0 0 90 81 1 0 0 0 0 81 91 1 0 0 0 0 91 92 1 0 0 0 0 92 93 1 0 0 0 0 93 94 1 0 0 0 0 84 95 2 0 0 0 0

	86 96 1 1 0 0 0 96 97 1 0 0 0 0 87 98 2 0 0 0 0 113 50 1 0 0 0 0 53103 1 0 0 0 0 9 10 1 0 0 0 0 53104 1 1 0 0 0 4 1 1 0 0 0 0 55105 1 0 0 0 0 3 14 1 0 0 0 0 105106 1 0 0 0 0 50 51 2 0 0 0 0 105107 1 0 0 0 0 51 52 1 0 0 0 0 78108 1 0 0 0 0 52114 1 0 0 0 0 78109 1 0 0 0 0 13 1 1 0 0 0 0 96110 1 0 0 0 0 13 14 2 0 0 0 0 79111 1 0 0 0 0 79112 1 0 0 0 0 80 50 1 0 0 0 0 14 15 1 0 0 0 0 1 2 2 0 0 0 0 113114 2 0 0 0 0 15 16 2 0 0 0 0 114115 1 0 0 0 0 2 3 1 0 0 0 0 115116 2 0 0 0 0 16 17 1 0 0 0 0 116117 1 0 0 0 0 7 11 2 0 0 0 0 117118 2 0 0 0 0 118113 1 0 0 0 0 17 18 2 0 0 0 0 101119 1 0 0 0 0 18 13 1 0 0 0 0 119120 1 0 0 0 0 10 12 1 0 0 0 0 119121 1 0 0 0 0 5 4 1 1 0 0 0 43122 1 0 0 0 0 20 19 1 0 0 0 0 43123 1 0 0 0 0 44 21 1 0 0 0 0 41124 1 0 0 0 0 32 39 2 0 0 0 0 124125 1 0 0 0 0 34 40 2 0 0 0 0 124126 1 0 0 0 0 36 41 1 1 0 0 0 58127 1 0 0 0 0 37 42 2 0 0 0 0 127128 2 0 0 0 0 37 6 1 0 0 0 0 103129 1 0 0 0 0 26 25 1 1 0 0 0 59130 1 6 0 0 0 27 24 1 1 0 0 0 19131 2 0 0 0 0 28 29 1 0 0 0 0 131132 1 0 0 0 0 29 30 1 0 0 0 0 132133 2 0 0 0 0 65 73 2 0 0 0 0 133134 1 0 0 0 0 67 74 2 0 0 0 0 134135 2 0 0 0 0 135 19 1 0 0 0 0 M END
Chemical Structures, InChI	InChI=1S/C98H141N19O17/c1-19-59(16)84(104-51-119)95(131)103-50-80(120)105-60(17)85(121)107-72(39-52(2)3)88(124)106-61(18)86(122)115-82(57(12)13)97(133)117-83(58(14)15)98(134)116-81(56(10)11)96(132)114-79(46-65-49-102-71-36-28-25-33-68(65)71)94(130)110-73(40-53(4)5)89(125)111-76(43-62-29-21-20-22-30-62)92(128)108-75(42-55(8)9)91(127)113-78(45-64-48-101-70-35-27-24-32-67(64)70)93(129)109-74(41-54(6)7)90(126)112-77(87(123)99-37-38-118)44-63-47-100-69-34-26-23-31-66(63)69/h20-36,47-49,51-61,72-79,81-84,100-102,118H,19,37-46,50H2,1-18H3,(H,99,123)(H,103,131)(H,104,119)(H,105,120)(H,106,124)(H,107,121)(H,108,128)(H,109,12

	9)(H,110,130)(H,111,125)(H,112,126)(H,113,127)(H,114,132)(H,115,122)(H,116,134)(H,117,133)/t59-,60-,61-,72+,73+,74+,75+,76-,77-,78-,79-,81+,82+,83-,84-/m0/s1
Chemical Structure, InChI Key	DIFKDOVAQNEQFQ-APJUGUNFSA-N

Moiety (mixture component)

Name		**Quantity**	Undefined not 0

Moiety Characteristics

```
  -FDASRS-06071412322D

136142  0  0  1  0  0  0  0  0999 V2000
   40.2583   -8.8398    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.3784   -9.2082    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   42.0750   -8.2567    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   39.2250   -9.4125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   39.2083  -10.5500    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   38.1958  -11.1000    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   40.2333  -11.1125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.2583  -10.5541    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   42.2833  -11.1166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   43.2958  -10.5583    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   40.2315  -12.2459    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   44.3541  -11.2375    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   40.2624   -7.6607    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.3823   -7.3017    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.6294   -6.1546    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   40.7579   -5.3654    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   39.6355   -5.7312    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   39.3937   -6.8774    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   27.9666   -8.6857    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   26.9334   -9.2584    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   34.1041   -8.7065    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.2243   -9.0749    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.9208   -8.1233    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   29.9899  -12.0958    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.0709   -9.2792    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.0542  -10.4167    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   29.9917  -10.9583    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   25.9042  -10.9542    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   26.9250  -10.3917    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   27.9500  -10.9542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   28.9750  -10.3958    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   31.0167  -10.4167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   32.0417  -10.9667    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   34.0792  -10.9792    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.1042  -10.4208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   36.1292  -10.9833    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   37.1417  -10.4250    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   27.9584  -12.0917    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   31.0226   -9.2708    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   34.0774  -12.1125    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   36.1375  -12.1166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   37.1500   -9.2917    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   31.0101  -12.6870    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   34.1083   -7.5273    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.2282   -7.1683    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.4753   -6.0213    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   34.6038   -5.2321    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.4813   -5.5979    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.2396   -6.7441    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   21.8124   -8.5607    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   22.9326   -8.9291    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   23.6292   -7.9775    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7101   -9.1625    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    2.4190   -9.1375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5000  -11.9541    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.4833  -10.8166    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    2.4208  -10.2750    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   -4.7333  -10.8584    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -3.7083  -10.2834    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  -2.6833  -10.8500    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.6667  -10.2792    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  -0.6458  -10.8416    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.3792  -10.2791    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.4042  -10.8375    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   3.4458  -10.8167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.4708  -10.2667    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   6.5083  -10.2541    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   7.5333  -10.8125    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   8.5583  -10.2500    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   9.5708  -10.8083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.6857  -11.9750    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   0.3875   -9.1416    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.4518  -11.9625    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   6.5065   -9.1208    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   8.5667   -9.1167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.5792  -11.9417    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  10.5446  -10.2284    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  11.5690  -11.9250    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  17.6982  -11.9500    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  20.7792   -9.1334    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  20.7625  -10.2709    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  17.7000  -10.8125    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
  11.5708  -10.8041    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  12.5958  -10.2375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  13.6125  -10.8083    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  14.6333  -10.2459    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  15.6583  -10.8084    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  16.6833  -10.2500    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  18.7250  -10.2708    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  19.7500  -10.8208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  21.7875  -10.8334    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  22.8125  -10.2750    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  23.8375  -10.8375    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
  24.8500  -10.2792    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.5935   -9.1125    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  14.6417   -9.1125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.6708   -8.5500    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.6667  -11.9459    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  18.7310   -9.1250    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  21.7857  -11.9667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  23.8459  -11.9708    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  24.8584   -9.1458    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.7404   -8.6006    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.6817   -8.6037    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.5298  -12.5287    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.5471  -13.7077    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   7.5422  -11.9242    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.5388  -12.4869    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.5975  -12.4838    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  13.6690   -8.5308    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  16.6761  -12.5379    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  18.7185  -12.5412    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  21.8166   -7.3815    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  22.9365   -7.0225    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  23.1836   -5.8754    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  22.3121   -5.0862    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  21.1897   -5.4520    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  20.9479   -6.5983    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  24.8315  -12.5302    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  24.8399  -13.6636    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  25.8089  -11.9563    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  31.0083  -13.8662    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  32.0322  -12.0990    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  37.1232  -12.6761    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  37.1316  -13.8094    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  38.1005  -12.1021    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.7472  -10.2562    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.7542   -9.0750    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  -1.7688   -9.1594    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.6875   -9.6917    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  28.9756   -9.2965    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  30.0082   -8.7248    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  30.0295   -7.5424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  29.0097   -6.9340    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  27.9813   -7.5092    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  31.0500   -6.9500    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 70 76  2  0  0  0  0
```

Chemical Structure, MOLFILE	56 55 1 1 0 0 0 57 54 1 1 0 0 0 59 53 1 0 0 0 0 58 59 1 0 0 0 0 59 60 1 0 0 0 0 60 61 1 0 0 0 0 61 62 1 0 0 0 0 62 63 1 0 0 0 0 63 64 1 0 0 0 0 64 57 1 0 0 0 0 57 65 1 0 0 0 0 65 66 1 0 0 0 0 66 56 1 0 0 0 0 56 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 69 70 1 0 0 0 0 60 71 2 0 0 0 0 63 72 2 0 0 0 0 30 31 1 0 0 0 0 70 77 1 0 0 0 0 31 27 1 0 0 0 0 27 32 1 0 0 0 0 32 33 1 0 0 0 0 33 26 1 0 0 0 0 26 34 1 0 0 0 0 34 35 1 0 0 0 0 35 36 1 0 0 0 0 36 37 1 0 0 0 0 29 20 1 1 0 0 0 30 38 2 0 0 0 0 6 5 1 0 0 0 0 24 43 1 0 0 0 0 25 21 1 0 0 0 0 5 7 1 0 0 0 0 7 8 1 0 0 0 0 44 45 2 0 0 0 0 21 22 2 0 0 0 0 45 46 1 0 0 0 0 22 23 1 0 0 0 0 46 47 2 0 0 0 0 23 45 1 0 0 0 0 47 48 1 0 0 0 0 8 9 1 0 0 0 0 48 49 2 0 0 0 0 49 44 1 0 0 0 0 89 99 2 0 0 0 0 91100 2 0 0 0 0 93101 1 1 0 0 0 94102 2 0 0 0 0 94 28 1 0 0 0 0 81 80 1 1 0 0 0 82 79 1 1 0 0 0 83 78 1 1 0 0 0 77 83 1 0 0 0 0 83 84 1 0 0 0 0 84 85 1 0 0 0 0 85 86 1 0 0 0 0 86 87 1 0 0 0 0 87 88 1 0 0 0 0 88 82 1 0 0 0 0 82 89 1 0 0 0 0 89 90 1 0 0 0 0 90 81 1 0 0 0 0 81 91 1 0 0 0 0 91 92 1 0 0 0 0 92 93 1 0 0 0 0 93 94 1 0 0 0 0 84 95 2 0 0 0 0 86 96 1 1 0 0 0 96 97 1 0 0 0 0 87 98 2 0 0 0 0 113 50 1 0 0 0 0 53103 1 0 0 0 0 9 10 1 0 0 0 0 53104 1 1 0 0 0 4 1 1 0 0 0 0 55105 1 0 0 0 0 3 14 1 0 0 0 0

	105106 1 0 0 0 0
	 50 51 2 0 0 0 0
	105107 1 0 0 0 0
	 51 52 1 0 0 0 0
	 78108 1 0 0 0 0
	 52114 1 0 0 0 0
	 78109 1 0 0 0 0
	 13 1 1 0 0 0 0
	 96110 1 0 0 0 0
	 13 14 2 0 0 0 0
	 79111 1 0 0 0 0
	 79112 1 0 0 0 0
	 80 50 1 0 0 0 0
	 14 15 1 0 0 0 0
	  1 2 2 0 0 0 0
	113114 2 0 0 0 0
	 15 16 2 0 0 0 0
	114115 1 0 0 0 0
	  2 3 1 0 0 0 0
	115116 2 0 0 0 0
	 16 17 1 0 0 0 0
	116117 1 0 0 0 0
	  7 11 2 0 0 0 0
	117118 2 0 0 0 0
	118113 1 0 0 0 0
	 17 18 2 0 0 0 0
	101119 1 0 0 0 0
	 18 13 1 0 0 0 0
	119120 1 0 0 0 0
	 10 12 1 0 0 0 0
	119121 1 0 0 0 0
	  5 4 1 1 0 0 0
	 43122 1 0 0 0 0
	 20 19 1 0 0 0 0
	 43123 1 0 0 0 0
	 44 21 1 0 0 0 0
	 41124 1 0 0 0 0
	 32 39 2 0 0 0 0
	124125 1 0 0 0 0
	 34 40 2 0 0 0 0
	124126 1 0 0 0 0
	 36 41 1 1 0 0 0
	 58127 1 0 0 0 0
	 37 42 2 0 0 0 0
	127128 2 0 0 0 0
	 37 6 1 0 0 0 0
	103129 1 0 0 0 0
	 26 25 1 1 0 0 0
	 59130 1 6 0 0 0
	 27 24 1 1 0 0 0
	 19131 2 0 0 0 0
	 28 29 1 0 0 0 0
	131132 1 0 0 0 0
	 29 30 1 0 0 0 0
	132133 2 0 0 0 0
	 65 73 2 0 0 0 0
	133134 1 0 0 0 0
	 67 74 2 0 0 0 0
	134135 2 0 0 0 0
	135 19 1 0 0 0 0
	 69 75 1 1 0 0 0
	133136 1 0 0 0 0
	M END

Chemical Structures, InChI	InChI=1S/C98H141N19O18/c1-19-58(16)84(104-50-119)95(132)103-49-80(121)105-59(17)85(122)107-72(38-51(2)3)88(125)106-60(18)86(123)115-82(56(12)13)97(134)117-83(57(14)15)98(135)116-81(55(10)11)96(133)114-79(45-64-48-102-71-31-25-22-28-68(64)71)94(131)110-73(39-52(4)5)89(126)111-76(42-61-32-34-65(120)35-33-61)92(129)108-75(41-54(8)9)91(128)113-78(44-63-47-101-70-30-24-21-27-67(63)70)93(130)109-74(40-53(6)7)90(127)112-77(87(124)99-36-37-118)43-62-46-100-69-29-23-20-26-66(62)69/h20-35,46-48,50-60,72-79,81-84,100-102,118,120H,19,36-45,49H2,1-18H3,(H,99,124)(H,103,132)(H,104,119)(H,105,121)(H,106,125)(H,107,122)(H,108,129)(H,109,130)(H,110,131)(H,111,126)(H,112,127)(H,113,128)(H,114,133)(H,115,123)(H,116,135)(H,117,134)/t58-,59-,60-,72+,73+,74+,75+,76-,77-,78-,79-,81+,82+,83-,84-/m0/s1
Chemical Structure, InChI Key	YMUHZPTUIROFMC-FNJZKDCPSA-N

Moiety (mixture component)

Name		Quantity	Undefined not 0

Moiety Characteristics

```
  -FDASRS-06071412322D

134140  0  0  1  0  0  0  0  0999 V2000
   40.2583   -8.7148    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.3784   -9.0832    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   42.0750   -8.1317    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   39.2250   -9.2875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   39.2083  -10.4250    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   38.1958  -10.9750    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   40.2333  -10.9875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.2583  -10.4291    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   42.2833  -10.9916    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   43.2958  -10.4333    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   40.2315  -12.1209    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   44.3541  -11.1125    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   40.2624   -7.5357    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.3823   -7.1767    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   41.6294   -6.0296    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   40.7579   -5.2404    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   39.6355   -5.6062    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   39.3937   -6.7524    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   27.9666   -8.5607    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   26.9334   -9.1334    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   34.1041   -8.5815    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.2243   -8.9499    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.9208   -7.9983    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   29.9899  -11.9708    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.0709   -9.1542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.0542  -10.2917    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   29.9917  -10.8333    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   25.9042  -10.8292    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   26.9250  -10.2667    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   27.9500  -10.8292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   28.9750  -10.2708    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   31.0167  -10.2917    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   32.0417  -10.8417    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   34.0792  -10.8542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.1042  -10.2958    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   36.1292  -10.8583    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   37.1417  -10.3000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   27.9584  -11.9667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   31.0226   -9.1458    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   34.0774  -11.9875    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   36.1375  -11.9916    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   37.1500   -9.1667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   31.0101  -12.5620    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   34.1083   -7.4023    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.2282   -7.0433    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   35.4753   -5.8963    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   34.6038   -5.1071    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.4813   -5.4729    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   33.2396   -6.6191    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   21.8124   -8.4357    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   22.9326   -8.8041    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   23.6292   -7.8525    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7101   -9.0375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4190   -9.0125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5000  -11.8291    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.4833  -10.6916    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    2.4208  -10.1500    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   -4.7333  -10.7334    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7083  -10.1584    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   -2.6833  -10.7250    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6667  -10.1542    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6458  -10.7166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3792  -10.1541    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4042  -10.7125    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    3.4458  -10.6917    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.4708  -10.1417    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE	6.5083 -10.1291 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.5333 -10.6875 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 8.5583 -10.1250 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 9.5708 -10.6833 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.6857 -11.8500 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0.3875 -9.0166 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3.4518 -11.8375 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 6.5065 -8.9958 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 8.5667 -8.9917 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.5792 -11.8167 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 10.5446 -10.1034 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 11.5690 -11.8000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 17.6982 -11.8250 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 20.7792 -9.0084 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 20.7625 -10.1459 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 17.7000 -10.6875 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 11.5708 -10.6791 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 12.5958 -10.1125 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.6125 -10.6833 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 14.6333 -10.1209 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 15.6583 -10.6834 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 16.6833 -10.1250 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 18.7250 -10.1458 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 19.7500 -10.6958 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 21.7875 -10.7084 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 22.8125 -10.1500 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 23.8375 -10.7125 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 24.8500 -10.1542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.5935 -8.9875 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 14.6417 -8.9875 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 15.6708 -8.4250 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 15.6667 -11.8209 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 18.7310 -9.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 21.7857 -11.8417 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 23.8459 -11.8458 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 24.8584 -9.0208 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -2.7404 -8.4756 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -4.6817 -8.4787 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.5298 -12.4037 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.5471 -13.5827 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.5422 -11.7992 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.5388 -12.3619 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.5975 -12.3588 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.6690 -8.4058 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 16.6761 -12.4129 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 18.7185 -12.4162 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 21.8166 -7.2565 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 22.9365 -6.8975 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 23.1836 -5.7504 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 22.3121 -4.9612 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 21.1897 -5.3270 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 20.9479 -6.4733 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 24.8315 -12.4052 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 24.8399 -13.5386 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 25.8089 -11.8313 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 31.0083 -13.7412 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 32.0322 -11.9740 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 37.1232 -12.5511 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 37.1316 -13.6844 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 38.1005 -11.9771 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.7472 -10.1312 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.7542 -8.9500 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 28.9756 -9.1715 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 30.0082 -8.5998 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 30.0295 -7.4174 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 29.0097 -6.8090 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 27.9813 -7.3842 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 31.0500 -6.8250 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 67 74 2 0 0 0 0 69 75 1 1 0 0 0 70 76 2 0 0 0 0 56 55 1 1 0 0 0 57 54 1 1 0 0 0 59 53 1 1 0 0 0 58 59 1 0 0 0 0 59 60 1 0 0 0 0 60 61 1 0 0 0 0 61 62 1 0 0 0 0 62 63 1 0 0 0 0

```
 63 64  1  0  0  0  0
 64 57  1  0  0  0  0
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 66 56  1  0  0  0  0
 56 67  1  0  0  0  0
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 27 32  1  0  0  0  0
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 25 21  1  0  0  0  0
  5  7  1  0  0  0  0
  7  8  1  0  0  0  0
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 21 22  2  0  0  0  0
 45 46  1  0  0  0  0
 22 23  1  0  0  0  0
 46 47  2  0  0  0  0
 23 45  1  0  0  0  0
 47 48  1  0  0  0  0
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 49 44  1  0  0  0  0
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 91100  2  0  0  0  0
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 94102  2  0  0  0  0
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 84 85  1  0  0  0  0
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 96 97  1  0  0  0  0
 87 98  2  0  0  0  0
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  9 10  1  0  0  0  0
 53104  1  0  0  0  0
  4  1  1  0  0  0  0
 55105  1  0  0  0  0
  3 14  1  0  0  0  0
105106  1  0  0  0  0
 50 51  2  0  0  0  0
105107  1  0  0  0  0
 51 52  1  0  0  0  0
 78108  1  0  0  0  0
 52114  1  0  0  0  0
 78109  1  0  0  0  0
 13  1  1  0  0  0  0
```

	96110 1 0 0 0 0 13 14 2 0 0 0 0 79111 1 0 0 0 0 79112 1 0 0 0 0 80 50 1 0 0 0 0 14 15 1 0 0 0 0 1 2 2 0 0 0 0 113114 2 0 0 0 0 15 16 2 0 0 0 0 114115 1 0 0 0 0 2 3 1 0 0 0 0 115116 2 0 0 0 0 16 17 1 0 0 0 0 116117 1 0 0 0 0 7 11 2 0 0 0 0 117118 2 0 0 0 0 118113 1 0 0 0 0 17 18 2 0 0 0 0 101119 1 0 0 0 0 18 13 1 0 0 0 0 119120 1 0 0 0 0 10 12 1 0 0 0 0 119121 1 0 0 0 0 5 4 1 1 0 0 0 43122 1 0 0 0 0 20 19 1 0 0 0 0 43123 1 0 0 0 0 44 21 1 0 0 0 0 41124 1 0 0 0 0 32 39 2 0 0 0 0 124125 1 0 0 0 0 34 40 2 0 0 0 0 124126 1 0 0 0 0 36 41 1 1 0 0 0 58127 1 0 0 0 0 37 42 2 0 0 0 0 127128 2 0 0 0 0 37 6 1 0 0 0 0 19129 2 0 0 0 0 26 25 1 1 0 0 0 129130 1 0 0 0 0 27 24 1 1 0 0 0 130131 2 0 0 0 0 28 29 1 0 0 0 0 131132 1 0 0 0 0 29 30 1 0 0 0 0 132133 2 0 0 0 0 133 19 1 0 0 0 0 65 73 2 0 0 0 0 131134 1 0 0 0 0 M END
Chemical Structures, InChI	InChI=1S/C97H139N19O18/c1-50(2)37-71(106-84(121)58(17)104-79(120)48-102-94(131)80(54(9)10)103-49-118)87(124)105-59(18)85(122)114-82(56(13)14)96(133)116-83(57(15)16)97(134)115-81(55(11)12)95(132)113-78(44-63-47-101-70-30-24-21-27-67(63)70)93(130)109-72(38-51(3)4)88(125)110-75(41-60-31-33-64(119)34-32-60)91(128)107-74(40-53(7)8)90(127)112-77(43-62-46-100-69-29-23-20-26-66(62)69)92(129)108-73(39-52(5)6)89(126)111-76(86(123)98-35-36-117)42-61-45-99-68-28-22-19-25-65(61)68/h19-34,45-47,49-59,71-78,80-83,99-101,117,119H,35-44,48H2,1-18H3,(H,98,123)(H,102,131)(H,103,118)(H,104,120)(H,105,124)(H,106,121)(H,107,128)(H,108,129)(H,109,130)(H,110,125)(H,111,126)(H,112,127)(H,113,132)(H,114,122)(H,115,134)(H,116,133)/t58-,59-,71+,72+,73+,74+,75-,76-,77-,78-,80-,81+,82+,83-/m0/s1
Chemical Structure, InChI Key	HABZTEMEEGKJMS-ZVOVLZPRSA-N

Moiety (mixture component)

Name		**Quantity**	Undefined not 0

Moiety Characteristics

	-FDASRS-060714123220

```
133139  0  0  1  0  0  0  0  0999 V2000
   17.1041   -3.2690    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.0700   -3.5375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.6625   -2.8358    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   17.1124   -2.3940    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.0697   -2.1267    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.2835   -1.2672    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5370   -0.6863    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.5688   -0.9521    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.3520   -1.8108    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   22.5291   -3.3357    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   23.5034   -3.6124    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   24.1041   -2.9025    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   21.6417   -3.7584    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   21.6333   -4.6001    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   20.7541   -5.0208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   22.5083   -5.0167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   23.3917   -4.6084    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   24.2750   -5.0208    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   25.1541   -4.6084    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   22.5107   -5.8667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   26.0541   -5.1167    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   22.5374   -2.4607    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   23.5032   -2.1934    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   23.7169   -1.3421    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   22.9621   -0.7529    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   21.9937   -1.0270    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   21.7938   -1.8774    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.0583   -3.6417    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.6940   -5.7541    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.3458   -3.6667    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.3333   -4.5000    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   13.6874   -4.9124    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   10.1750   -4.9083    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   11.0541   -4.4875    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   11.9374   -4.9083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.8207   -4.4957    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   14.5708   -4.5000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4541   -4.9167    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   17.2167   -4.9250    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.1000   -4.5041    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   18.9833   -4.9291    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   19.8458   -4.5125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.9333   -5.7500    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   14.5851   -3.6583    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   17.2107   -5.7668    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   18.9834   -5.7667    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   19.8584   -3.6708    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   14.5685   -6.1953    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.6458   -3.1273    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.6117   -3.4041    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.2041   -2.7024    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  -15.3523   -3.5751    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -10.0690   -3.5584    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -7.4208   -5.6458    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -7.4291   -4.8084    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
  -10.0624   -4.4001    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  -16.2374   -4.8334    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  -15.3541   -4.4042    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
  -14.4708   -4.8291    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -13.5874   -4.4041    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  -12.7208   -4.8167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -11.8208   -4.4041    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -10.9541   -4.8168    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -9.1791   -4.8084    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -8.2957   -4.4000    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -6.5458   -4.3917    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.6542   -4.8001    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7709   -4.3834    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   -3.8959   -4.8000    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -14.4685   -5.6624    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  -11.8167   -3.5584    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -9.1768   -5.6583    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -6.5524   -3.5457    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7709   -3.5375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8876   -5.6333    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0638   -4.3702    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1810   -5.6291    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE	3.1023 -5.6458 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5.7583 -3.5500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5.7374 -4.4000 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 3.1041 -4.8041 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 -2.1709 -4.7875 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 -1.2876 -4.3708 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.4166 -4.8000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0.4708 -4.3834 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 1.3541 -4.8000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2.2250 -4.3917 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 3.9874 -4.4000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.8707 -4.8084 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 6.6208 -4.8167 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.5041 -4.4041 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 8.3874 -4.8208 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 9.2624 -4.4041 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.2983 -3.5375 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0.4624 -3.5334 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1.3540 -3.1168 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1.3583 -5.6417 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3.9935 -3.5500 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 6.6190 -5.6583 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 8.3958 -5.6624 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.2667 -3.5667 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -14.5095 -3.1589 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -16.1849 -3.1620 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -6.5256 -6.0786 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -6.5096 -6.9535 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.6496 -5.6283 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.3487 -6.0453 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -3.0234 -6.0422 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.3728 -3.1101 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2.2177 -6.0838 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3.9767 -6.0870 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.6540 -2.2523 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.6114 -1.9850 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.8252 -1.1338 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.0787 -0.5446 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.1021 -0.8188 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5.8937 -1.6691 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.2441 -6.0761 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.2523 -6.9261 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.0839 -5.6521 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.5708 -7.0703 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 15.4531 -5.7532 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 19.8356 -6.1844 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 19.8441 -7.0261 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 20.6755 -5.7605 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -17.1028 -4.3937 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -17.1041 -3.5124 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 11.7792 -3.2125 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.5109 -3.6252 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.2312 -3.1967 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.2204 -2.3569 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.4831 -1.9475 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.7658 -2.3783 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 64 72 2 0 0 0 0 66 73 2 0 0 0 0 68 74 1 1 0 0 0 69 75 2 0 0 0 0 55 54 1 1 0 0 0 56 53 1 1 0 0 0 58 52 1 1 0 0 0 57 58 1 0 0 0 0 58 59 1 0 0 0 0 59 60 1 0 0 0 0 60 61 1 0 0 0 0 61 62 1 0 0 0 0 62 63 1 0 0 0 0 63 56 1 0 0 0 0 56 64 1 0 0 0 0 64 65 1 0 0 0 0 65 55 1 0 0 0 0 55 66 1 0 0 0 0 66 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 59 70 2 0 0 0 0 62 71 2 0 0 0 0

```
 14 16  1  0  0  0  0
 69 76  1  0  0  0  0
 16 17  1  0  0  0  0
 37 44  2  0  0  0  0
 39 45  2  0  0  0  0
 41 46  1  1  0  0  0
 42 47  2  0  0  0  0
 42 15  1  0  0  0  0
 31 30  1  1  0  0  0
 32 29  1  1  0  0  0
 33 34  1  0  0  0  0
 34 35  1  0  0  0  0
 35 36  1  0  0  0  0
 36 32  1  0  0  0  0
 32 37  1  0  0  0  0
 37 38  1  0  0  0  0
 38 31  1  0  0  0  0
 31 39  1  0  0  0  0
 39 40  1  0  0  0  0
 40 41  1  0  0  0  0
 41 42  1  0  0  0  0
 34 28  1  1  0  0  0
 35 43  2  0  0  0  0
 17 18  1  0  0  0  0
 29 48  1  0  0  0  0
 88 98  2  0  0  0  0
 90 99  2  0  0  0  0
 92100  1  1  0  0  0
 93101  2  0  0  0  0
 93 33  1  0  0  0  0
 80 79  1  1  0  0  0
 81 78  1  1  0  0  0
 82 77  1  1  0  0  0
 76 82  1  0  0  0  0
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 81 88  1  0  0  0  0
 88 89  1  0  0  0  0
 89 80  1  0  0  0  0
 80 90  1  0  0  0  0
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 92 93  1  0  0  0  0
 83 94  2  0  0  0  0
 85 95  1  1  0  0  0
 95 96  1  0  0  0  0
 86 97  2  0  0  0  0
112 49  1  0  0  0  0
 52102  1  0  0  0  0
 52103  1  0  0  0  0
 18 19  1  0  0  0  0
 54104  1  0  0  0  0
104105  1  0  0  0  0
 49 50  2  0  0  0  0
104106  1  0  0  0  0
 50 51  1  0  0  0  0
 77107  1  0  0  0  0
 51113  1  0  0  0  0
 77108  1  0  0  0  0
 13 10  1  0  0  0  0
 95109  1  0  0  0  0
 78110  1  0  0  0  0
 12 23  1  0  0  0  0
 78111  1  0  0  0  0
 79 49  1  0  0  0  0
 22 10  1  0  0  0  0
112113  2  0  0  0  0
113114  1  0  0  0  0
114115  2  0  0  0  0
 22 23  2  0  0  0  0
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116117  2  0  0  0  0
117112  1  0  0  0  0
 23 24  1  0  0  0  0
100118  1  0  0  0  0
```

	10 11 2 0 0 0 0 118119 1 0 0 0 0 24 25 2 0 0 0 0 118120 1 0 0 0 0 11 12 1 0 0 0 0 48121 1 0 0 0 0 25 26 1 0 0 0 0 48122 1 0 0 0 0 16 20 2 0 0 0 0 46123 1 0 0 0 0 26 27 2 0 0 0 0 123124 1 0 0 0 0 27 22 1 0 0 0 0 123125 1 0 0 0 0 57126 1 0 0 0 0 19 21 1 0 0 0 0 126127 2 0 0 0 0 14 13 1 1 0 0 0 15 14 1 0 0 0 0 7 8 1 0 0 0 0 8 9 2 0 0 0 0 9 4 1 0 0 0 0 4 1 1 0 0 0 0 1 2 2 0 0 0 0 1 30 1 0 0 0 0 28128 1 0 0 0 0 2 3 1 0 0 0 0 128129 2 0 0 0 0 3 5 1 0 0 0 0 129130 1 0 0 0 0 4 5 2 0 0 0 0 130131 2 0 0 0 0 5 6 1 0 0 0 0 131132 1 0 0 0 0 6 7 2 0 0 0 0 132133 2 0 0 0 0 133128 1 0 0 0 0 M END
Chemical Structures, InChI	InChI=1S/C97H139N19O17/c1-51(2)38-71(106-84(120)59(17)104-79(119)49-102-94(130)80(55(9)10)103-50-118)87(123)105-60(18)85(121)114-82(57(13)14)96(132)116-83(58(15)16)97(133)115-81(56(11)12)95(131)113-78(45-64-48-101-70-35-27-24-32-67(64)70)93(129)109-72(39-52(3)4)88(124)110-75(42-61-28-20-19-21-29-61)91(127)107-74(41-54(7)8)90(126)112-77(44-63-47-100-69-34-26-23-31-66(63)69)92(128)108-73(40-53(5)6)89(125)111-76(86(122)98-36-37-117)43-62-46-99-68-33-25-22-30-65(62)68/h19-35,46-48,50-60,71-78,80-83,99-101,117H,36-45,49H2,1-18H3,(H,98,122)(H,102,130)(H,103,118)(H,104,119)(H,105,123)(H,106,120)(H,107,127)(H,108,128)(H,109,129)(H,110,124)(H,111,125)(H,112,126)(H,113,131)(H,114,121)(H,115,133)(H,116,132)/t59-,60-,71+,72+,73+,74+,75-,76-,77-,78-,80-,81+,82+,83-/m0/s1
Chemical Structure, InChI Key	LQSMEVHEYXACJP-DSHASFMGSA-N

Moiety (mixture component)

Name		Quantity	Undefined not 0

Moiety Characteristics

-FDASRS-06071412322D

136143 0 0 1 0 0 0 0 0999 V2000
15.6083 -3.7065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
16.1243 -3.8666 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
16.4500 -3.4525 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
15.1251 -3.9500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
15.1167 -4.4417 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
14.6500 -4.6792 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
15.5917 -4.6834 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
16.0667 -4.4458 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
16.5417 -4.6875 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
17.0125 -4.4458 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
15.5941 -5.1750 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0

```
17.5000   -4.7416    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
15.6083   -3.1981    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
16.1282   -3.0433    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
16.2378   -2.5463    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
15.8371   -2.2071    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
15.3146   -2.3646    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
15.2063   -2.8608    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 9.9124   -3.6398    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
10.4284   -3.7999    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
10.7500   -3.3859    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 9.4292   -3.8833    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 9.9124   -3.1315    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
10.4323   -2.9767    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
10.5461   -2.4796    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
10.1413   -2.1404    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 9.6230   -2.2979    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 9.5104   -2.7941    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.7541   -3.6482    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
13.2743   -3.8083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
13.5959   -3.3983    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
10.8482   -5.1083    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.2750   -3.8959    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.2667   -4.3834    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
10.8458   -4.6167    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
 8.9542   -4.6208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 9.4291   -4.3751    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
 9.9041   -4.6167    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
10.3791   -4.3750    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
11.3208   -4.3875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
11.7958   -4.6250    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
12.7417   -4.6292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
13.2167   -4.3875    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
13.6917   -4.6292    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
14.1583   -4.3875    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 9.9042   -5.1084    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
11.3268   -3.8917    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
12.7399   -5.1167    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
13.6959   -5.1208    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
14.1626   -3.9000    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
11.3185   -5.3662    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.7583   -3.1398    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
13.2740   -2.9850    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
13.3878   -2.4879    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.9871   -2.1487    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.4647   -2.3062    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
12.3521   -2.8025    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 7.0583   -3.5856    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 7.5784   -3.7457    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 7.9000   -3.3359    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
-4.7643   -3.8417    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-1.9268   -3.8334    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-0.4999   -5.0500    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-0.5083   -4.5583    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
-1.9250   -4.3250    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
-5.2417   -4.5750    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
-4.7667   -4.3292    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
-4.2917   -4.5709    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-3.8208   -4.3291    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
-3.3458   -4.5708    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-2.8708   -4.3291    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-2.3958   -4.5667    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
-1.4500   -4.5583    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-0.9750   -4.3208    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
-0.0333   -4.3166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 0.4417   -4.5542    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 0.9167   -4.3125    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
 1.3875   -4.5542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
-4.2899   -5.0584    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
-2.8666   -3.8375    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
-1.4482   -5.0500    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
-0.0309   -3.8250    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 0.9208   -3.8251    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 1.3917   -5.0458    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
 1.8404   -4.3076    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
 2.3149   -5.0374    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 5.1523   -5.0499    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 6.5792   -3.8292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 6.5750   -4.3208    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
 5.1541   -4.5583    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE	2.3125 -4.5541 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 2.7875 -4.3084 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3.2625 -4.5542 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 3.7334 -4.3125 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 4.2084 -4.5542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.6834 -4.3166 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 5.6291 -4.3208 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.1041 -4.5583 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 7.0500 -4.5667 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.5250 -4.3249 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 8.0000 -4.5708 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 8.4666 -4.3291 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2.7893 -3.8209 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3.7375 -3.8209 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.2124 -3.5792 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.2083 -5.0458 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 5.6310 -3.8292 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 7.0482 -5.0542 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 8.0000 -5.0542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.4709 -3.8375 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -4.3153 -3.6005 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.2151 -3.6036 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.0244 -5.2995 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.0154 -5.8077 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0.4463 -5.0366 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2.7638 -5.2786 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1.8641 -5.2755 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3.2856 -3.5725 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.6802 -5.3004 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5.6268 -5.3036 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.0624 -3.0774 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.5823 -2.9225 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.6919 -2.4254 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.2912 -2.0862 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.7688 -2.2437 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.6604 -2.7399 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.4566 -5.2969 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.4607 -5.7885 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.9089 -5.0522 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.3208 -5.8745 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.7948 -5.1115 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.1523 -5.3594 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.1566 -5.8511 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.6047 -5.1146 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.7096 -4.3187 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.7125 -3.8042 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 16 17 1 0 0 0 0 7 11 2 0 0 0 0 17 18 2 0 0 0 0 18 13 1 0 0 0 0 23 19 1 0 0 0 0 10 12 1 0 0 0 0 5 4 1 1 0 0 0 6 5 1 0 0 0 0 19 20 2 0 0 0 0 20 21 1 0 0 0 0 21 24 1 0 0 0 0 5 7 1 0 0 0 0 22 19 1 0 0 0 0 7 8 1 0 0 0 0 8 9 1 0 0 0 0 73 81 2 0 0 0 0 75 82 2 0 0 0 0 77 83 1 1 0 0 0 78 84 2 0 0 0 0 64 63 1 1 0 0 0 65 62 1 1 0 0 0 67 61 1 1 0 0 0 66 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 69 70 1 0 0 0 0 70 71 1 0 0 0 0 71 72 1 0 0 0 0 72 65 1 0 0 0 0 65 73 1 0 0 0 0 73 74 1 0 0 0 0 74 64 1 0 0 0 0 64 75 1 0 0 0 0

```
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 77 78  1  0  0  0  0
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 71 80  2  0  0  0  0
 23 24  2  0  0  0  0
 78 85  1  0  0  0  0
 40 47  2  0  0  0  0
 42 48  2  0  0  0  0
 44 49  1  1  0  0  0
 45 50  2  0  0  0  0
 45  6  1  0  0  0  0
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 35 32  1  1  0  0  0
 36 37  1  0  0  0  0
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 38 39  1  0  0  0  0
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 41 34  1  0  0  0  0
 34 42  1  0  0  0  0
 42 43  1  0  0  0  0
 43 44  1  0  0  0  0
 44 45  1  0  0  0  0
 37 22  1  1  0  0  0
 38 46  2  0  0  0  0
  9 10  1  0  0  0  0
 32 51  1  0  0  0  0
 33 29  1  0  0  0  0
 24 25  1  0  0  0  0
  4  1  1  0  0  0  0
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101102  1  0  0  0  0
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104105  1  0  0  0  0
 95106  2  0  0  0  0
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 61111  1  0  0  0  0
 25 26  2  0  0  0  0
 61112  1  0  0  0  0
 53 54  1  0  0  0  0
 63113  1  0  0  0  0
  3 14  1  0  0  0  0
113114  1  0  0  0  0
 54 55  2  0  0  0  0
113115  1  0  0  0  0
 26 27  1  0  0  0  0
 86116  1  0  0  0  0
 55 56  1  0  0  0  0
 86117  1  0  0  0  0
 13  1  1  0  0  0  0
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 57 52  1  0  0  0  0
 87120  1  0  0  0  0
 88 58  1  0  0  0  0
```

	121 58 1 0 0 0 0
	 27 28 2 0 0 0 0
	121122 2 0 0 0 0
	 28 23 1 0 0 0 0
	122123 1 0 0 0 0
	 52 29 1 0 0 0 0
	123124 2 0 0 0 0
	 58 59 2 0 0 0 0
	124125 1 0 0 0 0
	 59 60 1 0 0 0 0
	125126 2 0 0 0 0
	126121 1 0 0 0 0
	 60122 1 0 0 0 0
	109127 1 0 0 0 0
	 13 14 2 0 0 0 0
	127128 1 0 0 0 0
	127129 1 0 0 0 0
	 14 15 1 0 0 0 0
	 51130 1 0 0 0 0
	 29 30 2 0 0 0 0
	 51131 1 0 0 0 0
	 30 31 1 0 0 0 0
	 49132 1 0 0 0 0
	 31 53 1 0 0 0 0
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	  1 2 2 0 0 0 0
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	  2 3 1 0 0 0 0
	135136 2 0 0 0 0
	M END

Chemical Structures, InChI	InChI=1S/C99H140N20O17/c1-51(2)37-73(109-86(123)59(17)107-81(122)49-105-96(133)82(55(9)10)106-50-121)89(126)108-60(18)87(124)117-84(57(13)14)98(135)119-85(58(15)16)99(136)118-83(56(11)12)97(134)116-80(44-64-48-104-72-34-26-22-30-68(64)72)95(132)112-76(40-54(7)8)92(129)115-79(43-63-47-103-71-33-25-21-29-67(63)71)94(131)111-75(39-53(5)6)91(128)114-78(42-62-46-102-70-32-24-20-28-66(62)70)93(130)110-74(38-52(3)4)90(127)113-77(88(125)100-35-36-120)41-61-45-101-69-31-23-19-27-65(61)69/h19-34,45-48,50-60,73-80,82-85,101-104,120H,35-44,49H2,1-18H3,(H,100,125)(H,105,133)(H,106,121)(H,107,122)(H,108,126)(H,109,123)(H,110,130)(H,111,131)(H,112,132)(H,113,127)(H,114,128)(H,115,129)(H,116,134)(H,117,124)(H,118,136)(H,119,135)/t59-,60-,73+,74+,75+,76+,77-,78-,79-,80-,82-,83+,84+,85-/m0/s1
Chemical Structure, InChI Key	ZWCXYZRRTRDGQE-LUPIJMBPSA-N

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	**Item Code (Source)**	5IE62321P4

Labeler - Food and Drug Administration (927645523)