Indexing - Substance

Food and Drug Administration
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LEUCOVORIN CALCIUM (RPR1R4C0P4)

Alias Name

Name	Name Type	Assigning Territory	Assigning Organization	Reference Document	Citation	Policy
leucovorin calcium	primary name					

Substance Information

Mapping	Definition Hash:	e0e29887-0ca6-325d-6927-d60c55c9bf26

Moiety (mixture component)

Name		Quantity	1

Moiety Characteristics

```
C20H21CaN7O7
  -FDASRS-09061311012D

 44 45  0  0  0  0  0  0  0  0999 V2000
   17.6947   -9.7491    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   17.0529   -9.3720    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.4064   -9.7448    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   17.0529   -8.6279    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   17.6926   -8.2478    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.3374   -8.6286    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.9812   -8.2559    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.9812   -7.5131    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   19.6248   -8.6359    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   16.4064   -8.2527    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   15.7706   -8.6317    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.7706   -9.3734    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   15.1240   -8.2608    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.1240   -7.5226    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.4547   -7.1559    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.8173   -7.5394    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.8173   -8.2935    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.4838   -8.6476    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.1630   -7.1810    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.5297   -7.5726    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.8797   -7.2142    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   11.8797   -6.4727    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.2255   -6.0976    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   10.5880   -6.4726    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9381   -6.0976    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.2881   -6.4727    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.6339   -6.1143    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.2881   -7.2142    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.9381   -7.5934    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9381   -8.3351    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   10.5880   -7.2227    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.2255   -7.5934    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   11.2255   -8.3351    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.5838   -8.7144    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.6495   -9.6017    0.0000 Ca  0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE	<pre>16.6519 -8.8588 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	16.4037 -7.7900 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	13.1508 -6.7184 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	11.8847 -7.6769 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	11.2229 -5.6349 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	9.9381 -5.6349 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	8.6235 -5.6517 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	8.2385 -6.3546 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	11.6274 -8.5644 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	2 3 2 0 0 0 0
	2 4 1 0 0 0 0
	4 5 1 0 0 0 0
	5 6 1 0 0 0 0
	6 7 1 0 0 0 0
	7 8 2 0 0 0 0
	7 9 1 0 0 0 0
	4 10 1 1 0 0 0
	10 11 1 0 0 0 0
	11 12 2 0 0 0 0
	11 13 1 0 0 0 0
	13 14 1 0 0 0 0
	14 15 2 0 0 0 0
	15 16 1 0 0 0 0
	16 17 2 0 0 0 0
	17 18 1 0 0 0 0
	13 18 2 0 0 0 0
	16 19 1 0 0 0 0
	19 20 1 0 0 0 0
	21 20 1 6 0 0 0
	21 22 1 0 0 0 0
	22 23 1 0 0 0 0
	23 24 1 0 0 0 0
	24 25 1 0 0 0 0
	25 26 1 0 0 0 0
	26 27 1 0 0 0 0
	26 28 2 0 0 0 0
	28 29 1 0 0 0 0
	29 30 2 0 0 0 0
	29 31 1 0 0 0 0
	31 32 1 0 0 0 0
	32 33 1 0 0 0 0
	33 34 2 0 0 0 0
	21 32 1 0 0 0 0
	24 31 2 0 0 0 0
	1 2 1 0 0 0 0
	4 36 1 0 0 0 0
	10 37 1 0 0 0 0
	19 38 1 0 0 0 0
	21 39 1 0 0 0 0
	23 40 1 0 0 0 0
	25 41 1 0 0 0 0
	27 42 1 0 0 0 0
	27 43 1 0 0 0 0
	33 44 1 0 0 0 0
	M CHG 3 1 -1 9 -1 35 2
	M END</pre>

Chemical Structures, InChI	InChI=1S/C20H23N7O7.Ca/c21-20-25-16-15(18(32)26-20)27(9-28)12(8-23-16)7-22-11-3-1-10(2-4-11)17(31)24-13(19(33)34)5-6-14(29)30;/h1-4,9,12-13,22H,5-8H2,(H,24,31)(H,29,30)(H,33,34)(H4,21,23,25,26,32);/q;+2/p-2/t12-,13-;/m0./s1
Chemical Structure, InChI Key	KVUAALJSMIVURS-QNTKWALQSA-L

Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

	C20H21CaN7O7 -FDASRS-09061311012D

Chemical Structure, MOLFILE	44 45 0 0 0 0 0 0 0 0999 V2000
	  17.6947 -9.7491 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	  17.0529 -9.3720 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  16.4064 -9.7448 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	  17.0529 -8.6279 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
	  17.6926 -8.2478 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  18.3374 -8.6286 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  18.9812 -8.2559 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  18.9812 -7.5131 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	  19.6248 -8.6359 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	  16.4064 -8.2527 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	  15.7706 -8.6317 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  15.7706 -9.3734 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	  15.1240 -8.2608 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  15.1240 -7.5226 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  14.4547 -7.1559 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  13.8173 -7.5394 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  13.8173 -8.2935 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  14.4838 -8.6476 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  13.1630 -7.1810 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	  12.5297 -7.5726 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  11.8797 -7.2142 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
	  11.8797 -6.4727 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  11.2255 -6.0976 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	  10.5880 -6.4726 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	   9.9381 -6.0976 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	   9.2881 -6.4727 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	   8.6339 -6.1143 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	   9.2881 -7.2142 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	   9.9381 -7.5934 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	   9.9381 -8.3351 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	  10.5880 -7.2227 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  11.2255 -7.5934 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
	  11.2255 -8.3351 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
	  10.5838 -8.7144 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
	   5.6495 -9.6017 0.0000 Ca 0 0 0 0 0 0 0 0 0 0 0 0
	  16.6519 -8.8588 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	  16.4037 -7.7900 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	  13.1508 -6.7184 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	  11.8847 -7.6769 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	  11.2229 -5.6349 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	   9.9381 -5.6349 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	   8.6235 -5.6517 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	   8.2385 -6.3546 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	  11.6274 -8.5644 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
	 2 3 2 0 0 0 0
	 2 4 1 0 0 0 0
	 4 5 1 0 0 0 0
	 5 6 1 0 0 0 0
	 6 7 1 0 0 0 0
	 7 8 2 0 0 0 0
	 7 9 1 0 0 0 0
	 4 10 1 0 0 0 0
	10 11 1 0 0 0 0
	11 12 2 0 0 0 0
	11 13 1 0 0 0 0
	13 14 1 0 0 0 0
	14 15 2 0 0 0 0
	15 16 1 0 0 0 0
	16 17 2 0 0 0 0
	17 18 1 0 0 0 0
	13 18 2 0 0 0 0
	16 19 1 0 0 0 0
	19 20 1 0 0 0 0
	21 20 1 0 0 0 0
	21 22 1 0 0 0 0
	22 23 1 0 0 0 0
	23 24 1 0 0 0 0
	24 25 1 0 0 0 0
	25 26 1 0 0 0 0
	26 27 1 0 0 0 0
	26 28 2 0 0 0 0
	28 29 1 0 0 0 0
	29 30 2 0 0 0 0
	29 31 1 0 0 0 0
	31 32 1 0 0 0 0
	32 33 1 0 0 0 0
	33 34 2 0 0 0 0
	21 32 1 0 0 0 0

	24 31 2 0 0 0 0 1 2 1 0 0 0 0 4 36 1 6 0 0 0 10 37 1 0 0 0 0 19 38 1 0 0 0 0 21 39 1 6 0 0 0 23 40 1 0 0 0 0 25 41 1 0 0 0 0 27 42 1 0 0 0 0 27 43 1 0 0 0 0 33 44 1 0 0 0 0 M CHG 3 1 -1 9 -1 35 2 M END
Chemical Structures, InChI	InChI=1S/C20H23N7O7.Ca/c21-20-25-16-15(18(32)26-20)27(9-28)12(8-23-16)7-22-11-3-1-10(2-4-11)17(31)24-13(19(33)34)5-6-14(29)30;/h1-4,9,12-13,22H,5-8H2,(H,24,31)(H,29,30)(H,33,34)(H4,21,23,25,26,32);/q;+2/p-2/t12-,13+;/m1./s1
Chemical Structure, InChI Key	KVUAALJSMIVURS-KZCZEQIWSA-L

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	**Item Code (Source)**	RPR1R4C0P4

Labeler - Food and Drug Administration (927645523)

Revised: 9/2013 Food and Drug Administration