Electronic Supplementary Material (ESI) for RSC Advances.

A novel antimicrobial target—expanded and revisited mode of action of pantothenamides

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Supplementary Information

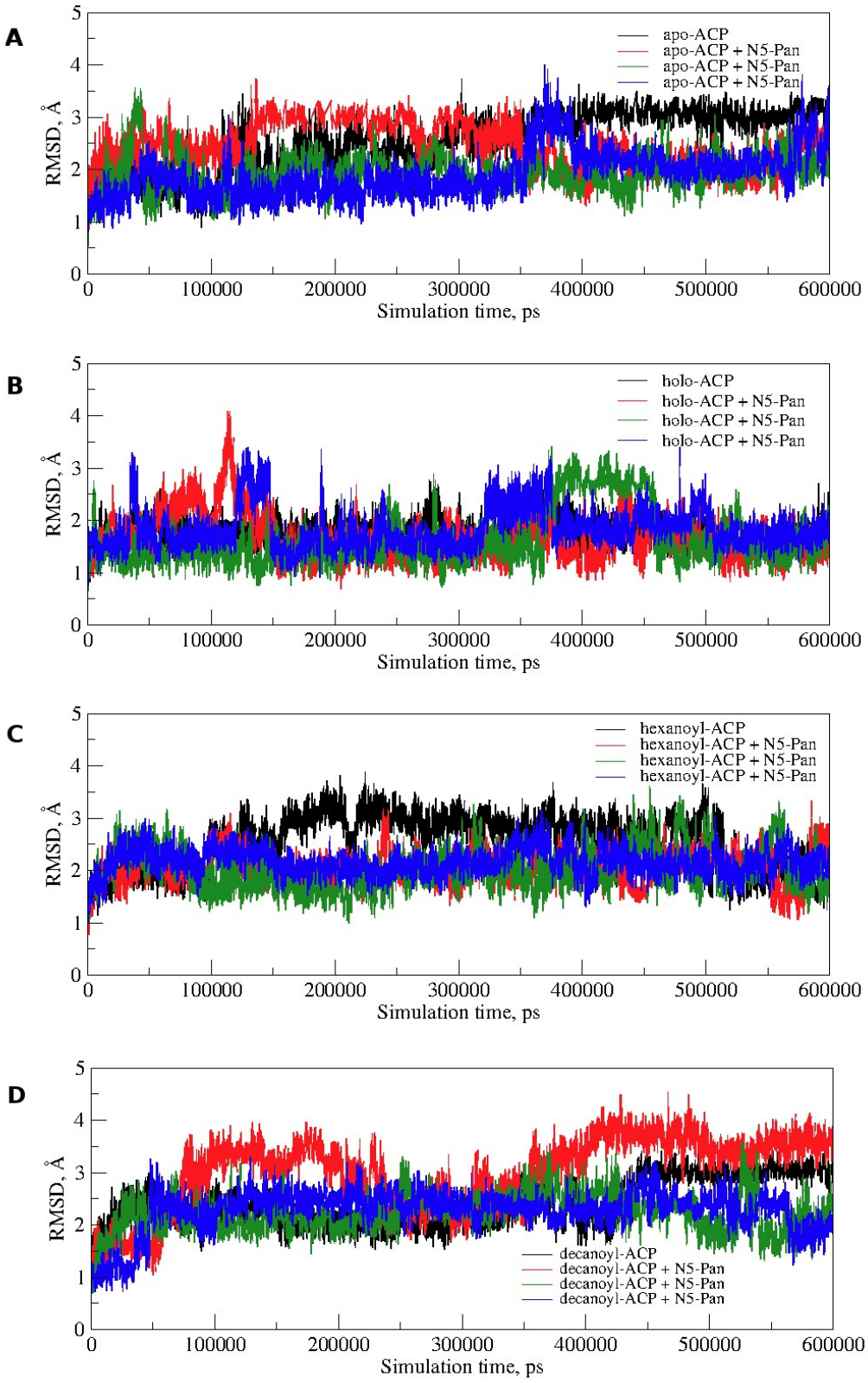

Figure S1. The root-mean-square deviations (RMSDs) of the protein backbone atoms with respect to the minimized structures. The RMSDs of the apo-ACP and its complexes with the N5-Pan (A); The RMSDs of the holo-ACP and its complexes with the N5-Pan (B); The RMSDs of the hexanoyl-ACP and its complexes with the N5-Pan (C). The RMSDs of the decanoyl-ACP and its complexes with the N5-Pan (D).

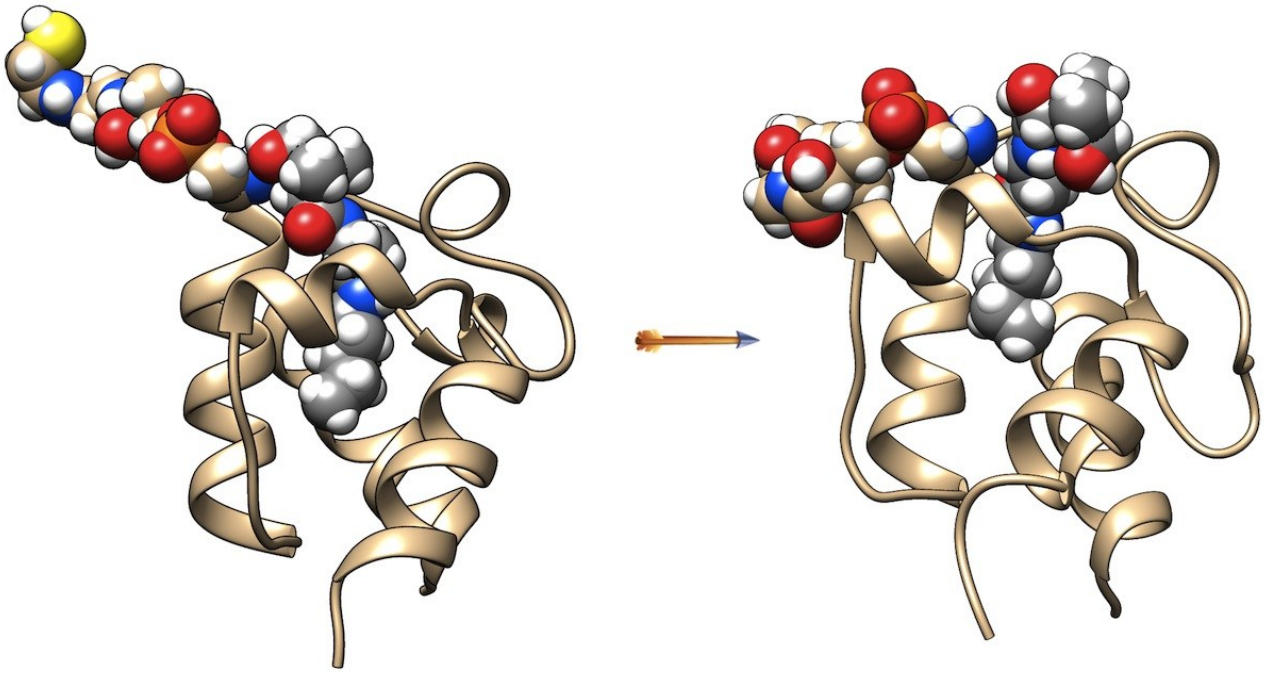

Figure S2. Starting structure of the holo-ACP+N5-Pan complex (left) and the last structure of the holo-ACP+N5-Pan complex (right) at the end of the 600 ns MD simulation.

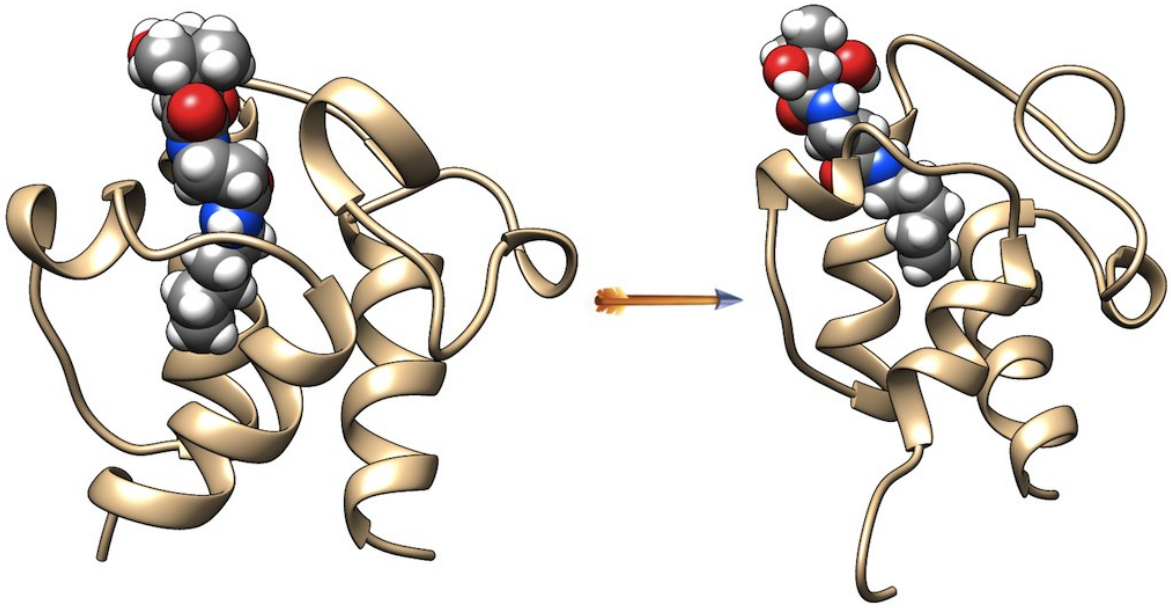

Figure S3. Starting structure of the apo-ACP+N5-Pan complex (left) and the last structure of the apo-ACP+N5-Pan complex (right) at the end of the 600 ns MD simulation.

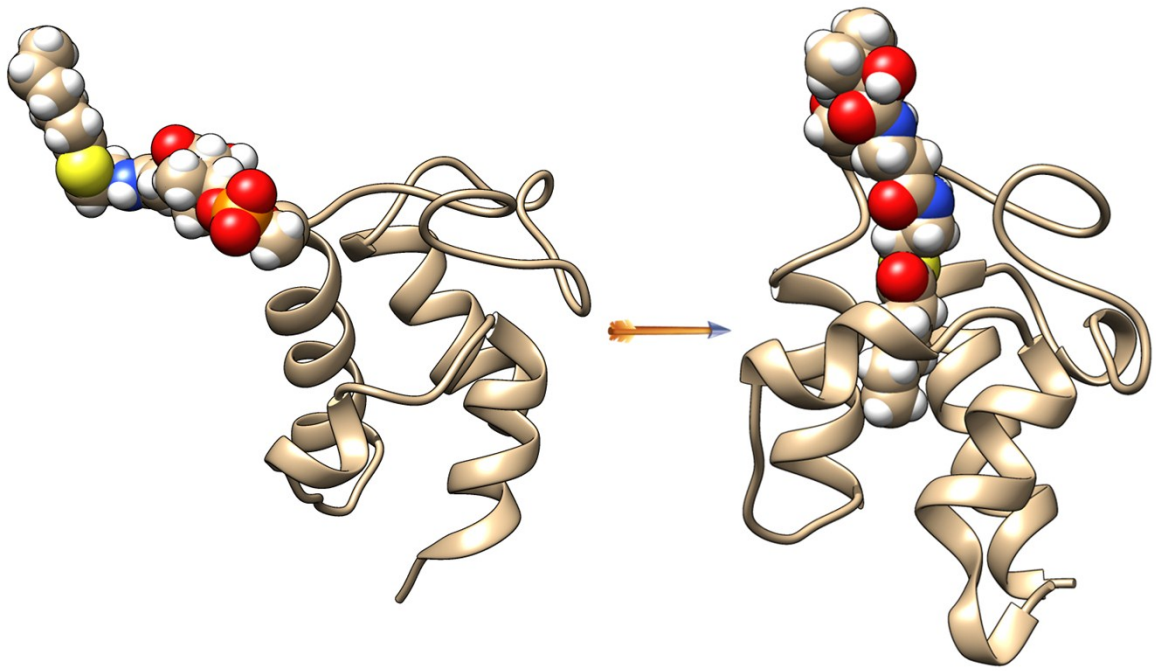

Figure S4. Transition from the solvent-exposed to the solvent-shielded hexanoyl chain. The starting structure of the hexanoyl-ACP (left) and the last structure of the hexanoyl-ACP (right) at the end of the 600 ns MD simulation.

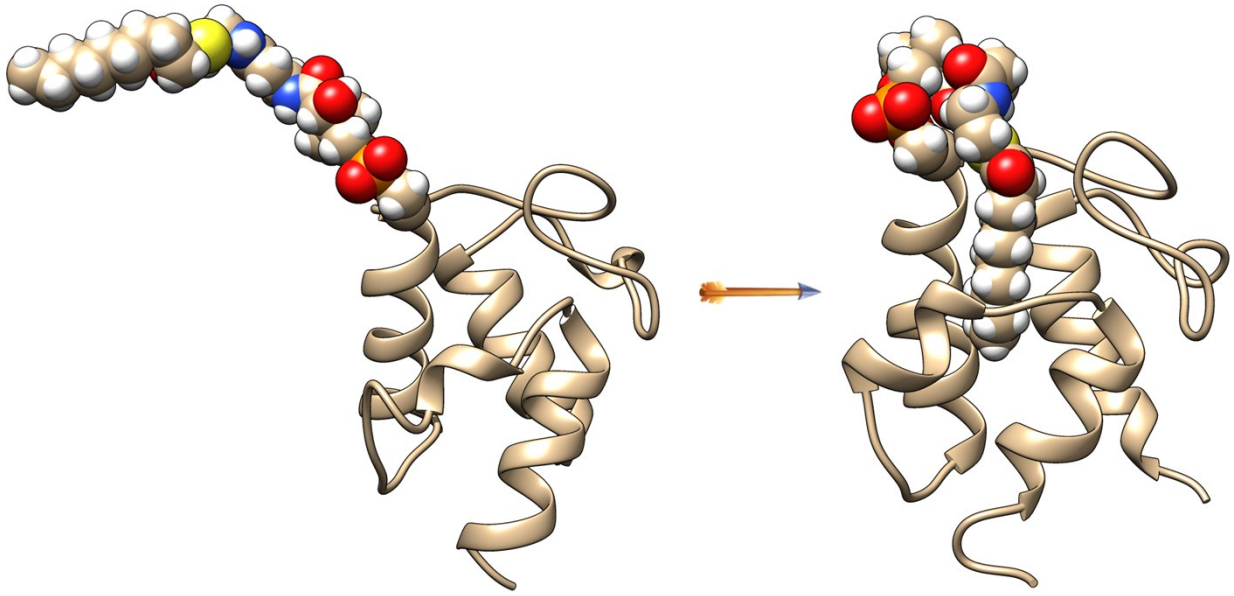

Figure S5. Transition from the solvent-exposed to the solvent-shielded decanoyl chain. The starting structure of the decanoyl-ACP (left) and the last structure of the decanoyl-ACP (right) at the end of the 600 ns MD simulation.

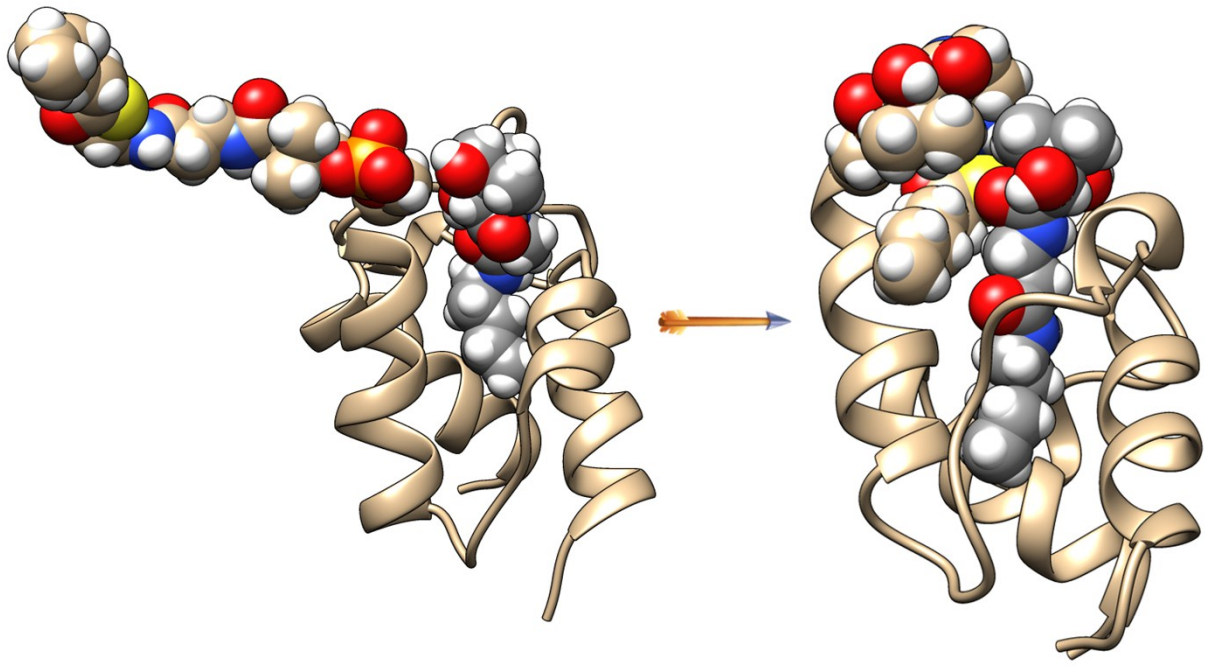

Figure S6. The starting structure of the hexanoyl-ACP+N5-Pan complex (left) and the last structure of the hexanoyl-ACP+N5-Pan complex (right) at the end of the 600 ns MD simulation.

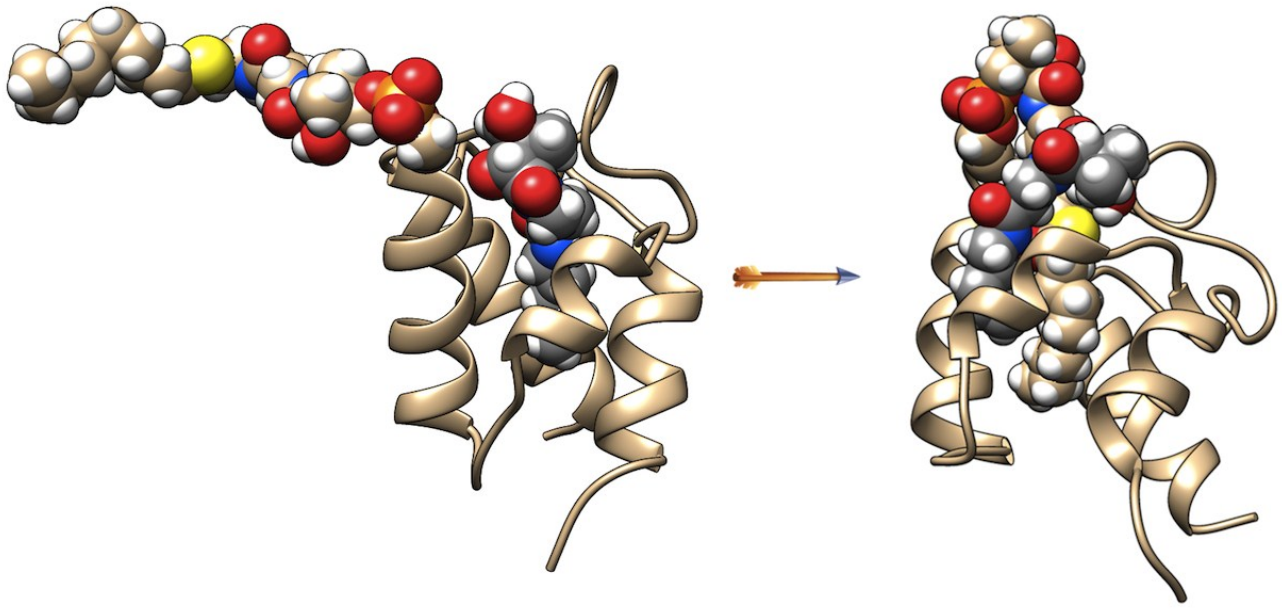

Figure S7. Transition from the solvent-exposed to the solvent-shielded decanoyl chain. The starting structure of the decanoyl-ACP+N5-Pan complex (left) and the last structure of the decanoyl-ACP+N5-Pan complex (right) at the end of the 600 ns MD simulation.

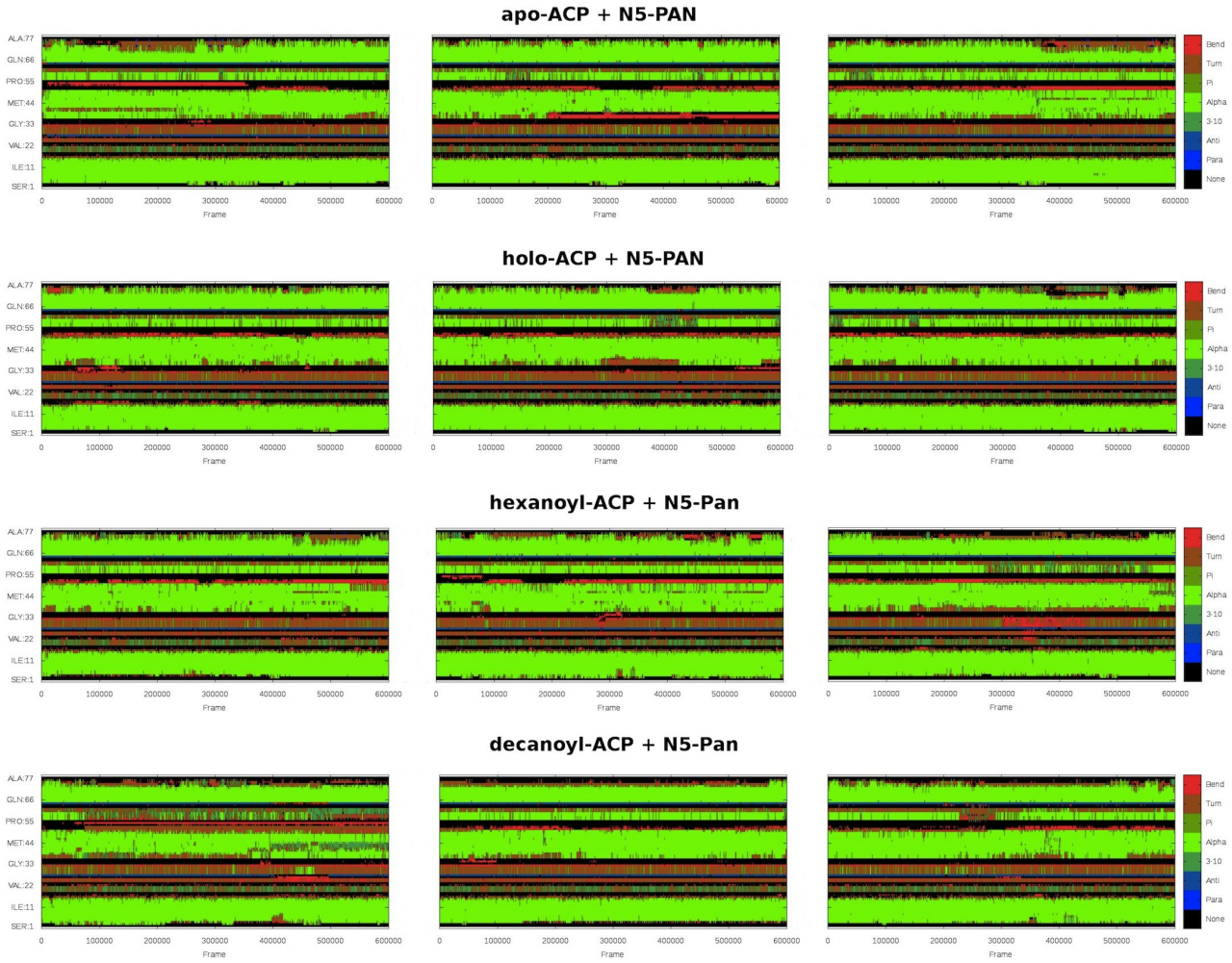

Figure S8. Analysis of the secondary structure elements during MD simulations of apo-ACP, holo-ACP, hexanoyl-ACP and decanoyl-ACP in complex with N5-Pan.

Table S1. Calculated binding free energies (ΔG_{bind}) and their components[a] obtained by the MM–PBSA method. 250 frames from the last 5 ns of the MD trajectories were used. All values are in kcal/mol. Values in parentheses represent the standard deviation. Nmode analysis was performed on 20 frames.

System	VDW	EEL	EPB	ENPOLAR	ΔH_{gas}	ΔH_{solv}	ΔH_{bind}	$T\Delta S$	ΔG_{bind}
apo-ACP	-32.0	-26.3	35.8	-4.6	-58.3	31.2	-27.1 (± 3.7)	-21.4 (± 1.8)	-5.7
apo-ACP	-33.4	-27.4	40.0	-4.8	-60.8	35.2	-25.6 (± 4.6)	-21.0 (± 2.5)	-4.6
apo-ACP	-29.4	-34.3	42.5	-4.7	-63.7	37.8	-25.9 (± 3.5)	-20.6 (± 3.1)	-5.3
holo-ACP	-35.8	-29.1	42.1	-4.9	-64.9	37.2	-27.7 (± 4.6)	-22.4 (± 2.8)	-5.3
holo-ACP	-37.1	-21.4	38.4	-4.8	-58.5	33.6	-24.9 (± 4.9)	-20.2 (± 2.7)	-4.7
holo-ACP	-30.0	-33.8	42.5	-4.6	-63.8	37.9	-25.9 (± 4.1)	-19.9 (± 3.4)	-6.0
hexanoyl-ACP	-32.5	-35.2	45.8	-4.7	-67.7	41.1	-26.6 (± 4.1)	-21.9 (± 2.6)	-4.7
hexanoyl-ACP	-37.1	-34.3	47.6	-4.7	-71.4	42.9	-28.5 (± 4.3)	-23.6 (± 3.3)	-4.9
hexanoyl-ACP	-31.4	-29.8	39.9	-4.6	-61.2	35.3	-25.9 (± 4.9)	-20.3 (± 4.6)	-5.6
decanoyl-ACP	-36.5	-21.2	34.0	-4.7	-57.7	29.3	-28.4 (± 4.1)	-22.6 (± 5.1)	-5.8

[a] VDW = van der Waals contribution from MM; EEL = electrostatic energy as calculated by the MM force field; EPB = the electrostatic contribution to the solvation free energy calculated by PB; ENPOLAR = nonpolar contribution to the solvation free energy calculated by an empirical model.

Table S2. Hydrogen bonding analysis during 600 ns of MD simulations of the apo-ACP+N5-Pan complexes.

Donor		Acceptor		Occupancy		
Residue	Group	Residue	Group	apo-ACP	apo-ACP	apo-ACP
Thr39	OG1–HG1	**N5-Pan**	O4	15%	32%	10%
N5-Pan	O2-H2	Glu60	OE1/2	17%	21%	28%
N5-Pan	N2–H22	Ile62	O	17%	14%	11%
N5-Pan	N2-H22	Ala59	O	12%	8%	20%
N5-Pan	N1-H11	Glu60	O	22%	7%	10%

Table S3. Hydrogen bonding analysis during 600 ns of MD simulations of the holo-ACP+N5-Pan complexes.

Donor		Acceptor		Occupancy		
Residue	Group	Residue	Group	holo-ACP	holo-ACP	holo-ACP
Thr39	OG1–HG1	**N5-Pan**	O4	15%	11%	14%
N5-Pan	O2-H2	Glu60	OE1/2	36%	24%	25%
N5-Pan	N2–H22	Ile62	O	30%	21%	12%
N5-Pan	N2-H22	Ala59	O	11%	13%	10%
N5-Pan	N1-H11	Glu60	O	19%	23%	12%

Table S4. Hydrogen bonding analysis during 600 ns of MD simulations of the hexanoyl-ACP+N5-Pan complexes.

Donor		Acceptor		Occupancy		
Residue	Group	Residue	Group	hexanoyl-ACP	hexanoyl-ACP	hexanoyl-ACP
Thr39	OG1–HG1	**N5-Pan**	O4	15%	10%	13%
N5-Pan	02-H2	Glu60	OE1/2	17%	19%	1%
N5-Pan	N2–H22	Ile62	O	15%	17%	23%
N5-Pan	N2-H22	Ala59	O	23%	18%	14%
N5-Pan	N1-H11	Glu60	O	11%	13%	18%

Table S5. Hydrogen bonding analysis during 600 ns of MD simulations of the decanoyl-ACP+N5-Pan complex.

Donor		Acceptor		Occupancy
Residue	Group	Residue	Group	decanoyl-ACP
Thr39	OG1–HG1	**N5-Pan**	O4	7%
N5-Pan	02-H2	Glu60	OE1/2	21%
N5-Pan	N2–H22	Ile62	O	21%
N5-Pan	N2-H22	Ala59	O	17%
N5-Pan	N1-H11	Glu60	O	22%

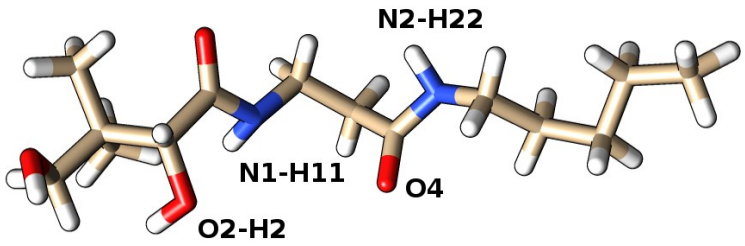

Figure S9. Chemical structure of the N-pentylpantothenamide. Atoms relevant for the discussion are highlighted.

N5-Pan.lib (N-Pentylpantothenamide)

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CT-CT-CT 63.210 110.630 same as c3-c3-c3
HC-CT-HC 39.430 108.350 same as hc-c3-hc
CT-CT-H1 46.360 110.070 same as c3-c3-h1
CT-CT-N 65.850 112.130 same as c3-c3-n
CT-N -H 46.040 116.780 same as c3-n -hn
C -N -CT 63.920 121.350 same as c -n -c3
H1-CT-H1 39.180 109.550 same as h1-c3-h1
H1-CT-N 49.820 109.320 same as h1-c3-n
N -C -O 75.830 122.030 same as n -c -o
CT-C -N 67.860 115.150 same as c3-c -n
C -N -H 49.210 118.460 same as c -n -hn
C -CT-HC 47.200 109.680 same as c -c3-hc
C -CT-CT 63.790 110.530 same as c -c3-c3
CT-C -O 68.030 123.110 same as c3-c -o
C -CT-OH 68.650 108.700 same as c -c3-oh
C -CT-H1 47.630 107.660 same as c -c3-h1
CT-OH-HO 47.090 108.160 same as c3-oh-ho
H1-CT-OH 50.970 109.880 same as h1-c3-oh
CT-CT-OH 67.720 109.430 same as c3-c3-oh

DIHE
CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3
HC-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc
CT-CT-CT-H1 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-N 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-N -H 6 0.000 0.000 2.000 same as X -c3-n -X
CT-CT-N -C 1 0.500 180.000 -4.000 same as c3-c3-n -c

CT-CT-N -C 1 0.150 180.000 -3.000 same as c3-c3-n -c
CT-CT-N -C 1 0.530 0.000 1.000 same as c3-c3-n -c
H1-CT-CT-HC 9 1.400 0.000 3.000 same as X -c3-c3-X
HC-CT-CT-N 9 1.400 0.000 3.000 same as X -c3-c3-X
O -C -N -CT 4 10.000 180.000 2.000 same as X -c -n -X
CT-C -N -CT 4 10.000 180.000 2.000 same as X -c -n -X
H1-CT-N -H 6 0.000 0.000 2.000 same as X -c3-n -X
H1-CT-N -C 6 0.000 0.000 2.000 same as X -c3-n -X
N -C -CT-HC 6 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-CT 1 0.100 0.000 -4.000 same as c3-c3-c -n
N -C -CT-CT 1 0.070 0.000 2.000 same as c3-c3-c -n
O -C -N -H 1 2.500 180.000 -2.000 same as hn-n -c -o
O -C -N -H 1 2.000 0.000 1.000 same as hn-n -c -o
CT-C -N -H 4 10.000 180.000 2.000 same as X -c -n -X
C -CT-CT-H1 9 1.400 0.000 3.000 same as X -c3-c3-X
C -CT-CT-N 9 1.400 0.000 3.000 same as X -c3-c3-X
O -C -CT-HC 1 0.800 0.000 -1.000 same as hc-c3-c -o
O -C -CT-HC 1 0.080 180.000 3.000 same as hc-c3-c -o
O -C -CT-CT 6 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-OH 6 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-H1 6 0.000 180.000 2.000 same as X -c -c3-X
C -CT-OH-HO 3 0.500 0.000 3.000 same as X -c3-oh-X
C -CT-CT-CT 9 1.400 0.000 3.000 same as X -c3-c3-X
O -C -CT-OH 6 0.000 180.000 2.000 same as X -c -c3-X
O -C -CT-H1 1 0.800 0.000 -1.000 same as h1-c3-c -o
O -C -CT-H1 1 0.080 180.000 3.000 same as h1-c3-c -o
CT-CT-CT-OH 9 1.400 0.000 3.000 same as X -c3-c3-X
H1-CT-OH-HO 3 0.500 0.000 3.000 same as X -c3-oh-X
CT-CT-OH-HO 1 0.160 0.000 -3.000 same as ho-oh-c3-c3
CT-CT-OH-HO 1 0.250 0.000 1.000 same as ho-oh-c3-c3

IMPROPER
C -CT-N -H 1.1 180.0 2.0 Same as X -X -n -hn
CT-N -C -O 10.5 180.0 2.0 Same as X -X -c -o

NONBON
CT 1.9080 0.1094 same as c3
HC 1.4870 0.0157 same as hc
H1 1.3870 0.0157 same as h1
N 1.8240 0.1700 same as n
H 0.6000 0.0157 same as hn
C 1.9080 0.0860 same as c
O 1.6612 0.2100 same as o
OH 1.7210 0.2104 same as oh
HO 0.0000 0.0000 same as ho

PNS.lib (4'-phosphopantetheine prosthetic group)

```
!!index array str
 "PNS"
!entry.PNS.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq  int elmnt  dbl chg
 "N1" "N" 0 1 131075 7 -1 -0.588025
 "H" "H" 0 1 131075 8 -1 0.268235
 "CA" "CT" 0 1 131075 9 -1 0.031996
 "C" "C" 0 1 131075 10 -1 0.586473
 "O" "O" 0 1 131075 11 -1 -0.615915
 "HA" "H1" 0 1 131075 18 -1 0.095981
 "CB" "CT" 0 1 131075 19 -1 -0.024257
 "HB2" "H1" 0 1 131075 20 -1 0.074589
 "HB3" "H1" 0 1 131075 21 -1 0.074589
 "OG" "OS" 0 1 131075 22 -1 -0.304270
 "P24" "P" 0 1 131075 23 -1 1.088199
 "O25" "O2" 0 1 131075 24 -1 -0.748502
 "O26" "O2" 0 1 131075 25 -1 -0.748502
 "O27" "OS" 0 1 131075 26 -1 -0.428188
 "C28" "CT" 0 1 131075 27 -1 0.232215
 "H281" "H1" 0 1 131075 28 -1 0.001958
 "H282" "H1" 0 1 131075 29 -1 0.001958
 "C29" "CT" 0 1 131075 30 -1 0.088126
 "C30" "CT" 0 1 131075 31 -1 -0.042345
 "H301" "HC" 0 1 131075 32 -1 0.002098
 "H302" "HC" 0 1 131075 33 -1 0.002098
 "H303" "HC" 0 1 131075 34 -1 0.002098
 "C31" "CT" 0 1 131075 35 -1 -0.042345
 "H311" "HC" 0 1 131075 36 -1 0.002098
 "H312" "HC" 0 1 131075 37 -1 0.002098
 "H313" "HC" 0 1 131075 38 -1 0.002098
 "C32" "CT" 0 1 131075 39 -1 0.124482
 "O33" "OH" 0 1 131075 40 -1 -0.697766
 "H33" "HO" 0 1 131075 41 -1 0.449914
 "H32" "H1" 0 1 131075 42 -1 0.122492
 "C34" "C" 0 1 131075 43 -1 0.556932
 "O35" "O" 0 1 131075 44 -1 -0.610871
 "N36" "N" 0 1 131075 45 -1 -0.511744
 "H36" "H" 0 1 131075 46 -1 0.308829
 "C37" "CT" 0 1 131075 47 -1 0.071666
 "H371" "H1" 0 1 131075 48 -1 0.086134
 "H372" "H1" 0 1 131075 49 -1 0.086134
 "C38" "CT" 0 1 131075 50 -1 0.082318
 "H381" "HC" 0 1 131075 51 -1 0.019296
 "H382" "HC" 0 1 131075 52 -1 0.019296
 "C39" "C" 0 1 131075 53 -1 0.458726
 "O40" "O" 0 1 131075 54 -1 -0.604788
 "N41" "N" 0 1 131075 55 -1 -0.261094
 "H41" "H" 0 1 131075 56 -1 0.254196
 "C42" "CT" 0 1 131075 57 -1 -0.097589
 "H421" "H1" 0 1 131075 58 -1 0.091890
 "H422" "H1" 0 1 131075 59 -1 0.091890
 "C43" "CT" 0 1 131075 60 -1 -0.150920
 "H431" "H1" 0 1 131075 61 -1 0.130498
 "H432" "H1" 0 1 131075 62 -1 0.130498
 "S44" "SH" 0 1 131075 63 -1 -0.382776
 "H44" "HS" 0 1 131075 64 -1 0.217799
!entry.PNS.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl pchg
```

"N1" "N" 0 -1 0.0
"H" "H" 0 -1 0.0
"CA" "CT" 0 -1 0.0
"C" "C" 0 -1 0.0
"O" "O" 0 -1 0.0
"HA" "H1" 0 -1 0.0
"CB" "CT" 0 -1 0.0
"HB2" "H1" 0 -1 0.0
"HB3" "H1" 0 -1 0.0
"OG" "OS" 0 -1 0.0
"P24" "P" 0 -1 0.0
"O25" "O2" 0 -1 0.0
"O26" "O2" 0 -1 0.0
"O27" "OS" 0 -1 0.0
"C28" "CT" 0 -1 0.0
"H281" "H1" 0 -1 0.0
"H282" "H1" 0 -1 0.0
"C29" "CT" 0 -1 0.0
"C30" "CT" 0 -1 0.0
"H301" "HC" 0 -1 0.0
"H302" "HC" 0 -1 0.0
"H202" "HC" 0 -1 0.0
"C31" "CT" 0 -1 0.0
"H311" "HC" 0 -1 0.0
"H312" "HC" 0 -1 0.0
"H313" "HC" 0 -1 0.0
"C32" "CT" 0 -1 0.0
"O33" "OH" 0 -1 0.0
"H33" "HO" 0 -1 0.0
"H32" "H1" 0 -1 0.0
"C34" "C" 0 -1 0.0
"O35" "O" 0 -1 0.0
"N36" "N" 0 -1 0.0
"H36" "H" 0 -1 0.0
"C37" "CT" 0 -1 0.0
"H371" "H1" 0 -1 0.0
"H372" "H1" 0 -1 0.0
"C38" "CT" 0 -1 0.0
"H381" "HC" 0 -1 0.0
"H382" "HC" 0 -1 0.0
"C39" "C" 0 -1 0.0
"O40" "O" 0 -1 0.0
"N41" "N" 0 -1 0.0
"H41" "H" 0 -1 0.0
"C42" "CT" 0 -1 0.0
"H421" "H1" 0 -1 0.0
"H422" "H1" 0 -1 0.0
"C43" "CT" 0 -1 0.0
"H431" "H1" 0 -1 0.0
"H432" "H1" 0 -1 0.0
"S44" "SH" 0 -1 0.0
"H44" "HS" 0 -1 0.0
!entry.PNS.unit.boundbox array dbl
-1.000000
0.0
0.0
0.0
0.0
!entry.PNS.unit.childsequence single int

```
 2
!entry.PNS.unit.connect array int
 1
 4
!entry.PNS.unit.connectivity table  int atom1x  int atom2x  int flags
 1 2 1
 1 3 1
 3 4 1
 3 6 1
 3 7 1
 4 5 1
 7 8 1
 7 9 1
 7 10 1
 10 11 1
 11 12 1
 11 13 1
 11 14 1
 14 15 1
 15 16 1
 15 17 1
 15 18 1
 18 19 1
 18 23 1
 18 27 1
 19 20 1
 19 21 1
 19 22 1
 23 24 1
 23 25 1
 23 26 1
 27 28 1
 27 30 1
 27 31 1
 28 29 1
 31 32 1
 31 33 1
 33 34 1
 33 35 1
 35 36 1
 35 37 1
 35 38 1
 38 39 1
 38 40 1
 38 41 1
 41 42 1
 41 43 1
 43 44 1
 43 45 1
 45 46 1
 45 47 1
 45 48 1
 48 49 1
 48 50 1
 48 51 1
 51 52 1
!entry.PNS.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
```

"R" 1 "A" 2
"R" 1 "A" 3
"R" 1 "A" 4
"R" 1 "A" 5
"R" 1 "A" 6
"R" 1 "A" 7
"R" 1 "A" 8
"R" 1 "A" 9
"R" 1 "A" 10
"R" 1 "A" 11
"R" 1 "A" 12
"R" 1 "A" 13
"R" 1 "A" 14
"R" 1 "A" 15
"R" 1 "A" 16
"R" 1 "A" 17
"R" 1 "A" 18
"R" 1 "A" 19
"R" 1 "A" 20
"R" 1 "A" 21
"R" 1 "A" 22
"R" 1 "A" 23
"R" 1 "A" 24
"R" 1 "A" 25
"R" 1 "A" 26
"R" 1 "A" 27
"R" 1 "A" 28
"R" 1 "A" 29
"R" 1 "A" 30
"R" 1 "A" 31
"R" 1 "A" 32
"R" 1 "A" 33
"R" 1 "A" 34
"R" 1 "A" 35
"R" 1 "A" 36
"R" 1 "A" 37
"R" 1 "A" 38
"R" 1 "A" 39
"R" 1 "A" 40
"R" 1 "A" 41
"R" 1 "A" 42
"R" 1 "A" 43
"R" 1 "A" 44
"R" 1 "A" 45
"R" 1 "A" 46
"R" 1 "A" 47
"R" 1 "A" 48
"R" 1 "A" 49
"R" 1 "A" 50
"R" 1 "A" 51
"R" 1 "A" 52
!entry.PNS.unit.name single str
"PNS"
!entry.PNS.unit.positions table dbl x dbl y dbl z
2.006354 1.263988 -1.855793
1.609213 0.523779 -1.320642
1.576407 1.321999 -3.244607
0.053820 1.498007 -3.273592
-0.417314 2.564420 -3.593713

```
 1.970393 2.232862 -3.665545
 2.124496 0.123680 -4.035808
 1.596466 0.004684 -4.973845
 3.165632 0.325677 -4.264844
 2.063470 -1.035988 -3.261043
 1.253395 -2.395987 -3.730064
-0.038712 -2.369949 -3.015004
 1.372343 -2.511948 -5.189641
 2.192299 -3.479952 -2.985126
 3.407853 -3.897834 -3.549944
 3.269765 -4.877214 -3.991119
 3.708855 -3.220876 -4.339889
 4.503868 -3.960871 -2.469954
 4.065807 -4.897957 -1.335848
 4.827108 -4.980012 -0.568552
 3.850756 -5.892018 -1.710884
 3.157965 -4.515992 -0.887910
 4.731951 -2.551626 -1.905833
 5.076934 -1.866681 -2.674751
 5.456736 -2.554661 -1.097085
 3.796632 -2.160477 -1.530677
 5.784825 -4.486885 -3.183973
 5.672811 -5.829754 -3.559948
 5.915931 -6.355002 -2.806617
 5.902865 -3.935645 -4.106341
 7.050031 -4.372921 -2.325862
 7.271052 -5.237095 -1.509752
 7.906089 -3.333909 -2.460864
 8.689240 -3.433956 -1.848763
 8.064124 -2.360838 -3.526914
 8.972716 -2.562764 -4.076684
 7.248100 -2.447809 -4.225932
 8.113173 -0.934750 -2.974856
 7.168926 -0.686667 -2.510731
 8.871036 -0.868790 -2.197015
 8.504139 0.063129 -4.052716
 9.237419 -0.256010 -4.954090
 8.036046 1.325482 -3.940670
 8.346005 1.927381 -4.672552
 7.074025 1.849510 -2.984622
 6.108656 1.371366 -3.095666
 7.417864 1.677566 -1.971081
 6.852083 3.338349 -3.195577
 6.073419 3.656221 -2.522845
 6.520953 3.523437 -4.209965
 8.382890 4.291186 -2.871609
 7.846809 5.501439 -2.965608
!entry.PNS.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int c6x
 0 51 0 0 0 0
!entry.PNS.unit.residues table  str name  int seq  int childseq  int startatomx  str restype  int imagingx
 "PNS" 1 65 1 "p" 0
!entry.PNS.unit.residuesPdbSequenceNumber array int
 0
!entry.PNS.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
```

```
!entry.PNS.unit.velocities table  dbl x  dbl y  dbl z
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 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
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 0.0 0.0 0.0
 0.0 0.0 0.0
```

PNS.frcmod (4'-phosphopantetheine prosthetic group)

remark goes here
MASS
CT 12.010 0.878 same as c3
HC 1.008 0.135 same as hc
C 12.010 0.616 same as c
O 16.000 0.434 same as o
N 14.010 0.530 same as n
H 1.008 0.161 same as hn
H1 1.008 0.135 same as hc
OS 16.000 0.465 same as os
P 30.970 1.538 same as p4
O2 16.000 0.434 same as o
OH 16.000 0.465 same as oh
HO 1.008 0.135 same as ho
SH 32.060 2.900 same as sh
HS 1.008 0.135 same as hs

BOND
CT-HC 337.30 1.092 same as c3-hc
CT-C 328.30 1.508 same as c -c3
C -O 648.00 1.214 same as c -o
C -N 478.20 1.345 same as c -n
N -H 410.20 1.009 same as hn-n
N -CT 330.60 1.460 same as c3-n
CT-H1 337.30 1.092 same as c3-hc
CT-CT 303.10 1.535 same as c3-c3
CT-OS 301.50 1.439 same as c3-os
OS-P 311.60 1.636 same as os-p4
P -O2 456.40 1.503 same as o -p4
CT-OH 314.10 1.426 same as c3-oh
OH-HO 369.60 0.974 same as ho-oh
CT-SH 225.30 1.822 same as c3-sh
SH-HS 302.20 1.337 same as hs-sh

ANGLE
CT-C -O 68.030 123.110 same as c3-c -o
CT-C -N 67.860 115.150 same as c3-c -n
HC-CT-HC 39.430 108.350 same as hc-c3-hc
HC-CT-C 47.200 109.680 same as c -c3-hc
C -N -H 49.210 118.460 same as c -n -hn
C -N -CT 63.920 121.350 same as c -n -c3
O -C -N 75.830 122.030 same as n -c -o
N -CT-C 66.670 111.560 same as c -c3-n
N -CT-H1 49.780 109.500 same as hc-c3-n
N -CT-CT 65.850 112.130 same as c3-c3-n
H -N -CT 46.040 116.780 same as c3-n -hn
CT-CT-H1 46.370 110.050 same as c3-c3-hc
CT-CT-OS 67.780 108.420 same as c3-c3-os
C -CT-H1 47.200 109.680 same as c -c3-hc
C -CT-CT 63.790 110.530 same as c -c3-c3
H1-CT-H1 39.430 108.350 same as hc-c3-hc
CT-OS-P 77.590 117.480 same as c3-os-p4
H1-CT-OS 50.870 108.700 same as hc-c3-os
OS-P -O2 43.100 116.670 same as o -p4-os
OS-P -OS 44.740 100.340 same as os-p4-os
O2-P -O2 45.060 117.220 same as o -p4-o

CT-CT-CT 63.210 110.630 same as c3-c3-c3
CT-CT-HC 46.490 109.490 Calculated with empirical approach
CT-CT-OH 67.720 109.430 same as c3-c3-oh
CT-OH-HO 47.090 108.160 same as c3-oh-ho
OH-CT-H1 51.070 109.500 same as hc-c3-oh
OH-CT-C 68.650 108.700 same as c -c3-oh
CT-CT-SH 60.980 113.020 same as c3-c3-sh
CT-SH-HS 44.940 96.600 same as c3-sh-hs
H1-CT-SH 42.660 107.870 same as hc-c3-sh

DIHE
CT-C -N -H 1 2.500 180.000 2.000 same as X -c -n -X
CT-C -N -CT 1 2.500 180.000 2.000 same as X -c -n -X
HC-CT-C -O 1 0.800 0.000 -1.000 same as hc-c3-c -o
HC-CT-C -O 1 0.080 180.000 3.000 same as hc-c3-c -o
HC-CT-C -N 1 0.000 180.000 2.000 same as X -c -c3-X
C -N -CT-C 1 0.850 180.000 -2.000 same as c -n -c3-c
C -N -CT-C 1 0.800 0.000 1.000 same as c -n -c3-c
C -N -CT-H1 1 0.000 0.000 2.000 same as X -c3-n -X
C -N -CT-CT 1 0.500 180.000 -4.000 same as c3-c3-n -c
C -N -CT-CT 1 0.150 180.000 -3.000 same as c3-c3-n -c
C -N -CT-CT 1 0.530 0.000 1.000 same as c3-c3-n -c
O -C -N -H 1 2.500 180.000 -2.000 same as hn-n -c -o
O -C -N -H 1 2.000 0.000 1.000 same as hn-n -c -o
O -C -N -CT 1 2.500 180.000 2.000 same as X -c -n -X
N -CT-C -O 1 0.000 180.000 2.000 same as X -c -c3-X
N -CT-C -N 1 1.700 180.000 -1.000 same as n -c3-c -n
N -CT-C -N 1 2.000 180.000 2.000 same as n -c3-c -n
N -CT-CT-H1 1 0.156 0.000 3.000 same as X -c3-c3-X
N -CT-CT-OS 1 0.156 0.000 3.000 same as X -c3-c3-X
H -N -CT-C 1 0.000 0.000 2.000 same as X -c3-n -X
H -N -CT-H1 1 0.000 0.000 2.000 same as X -c3-n -X
H -N -CT-CT 1 0.000 0.000 2.000 same as X -c3-n -X
CT-CT-OS-P 1 0.383 0.000 3.000 same as X -c3-os-X
C -CT-CT-H1 1 0.156 0.000 3.000 same as X -c3-c3-X
C -CT-CT-OS 1 0.156 0.000 3.000 same as X -c3-c3-X
O -C -CT-H1 1 0.800 0.000 -1.000 same as hc-c3-c -o
O -C -CT-H1 1 0.080 180.000 3.000 same as hc-c3-c -o
O -C -CT-CT 1 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-H1 1 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-CT 1 0.100 0.000 -4.000 same as c3-c3-c -n
N -C -CT-CT 1 0.070 0.000 2.000 same as c3-c3-c -n
H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc
H1-CT-CT-OS 1 0.000 0.000 -3.000 same as hc-c3-c3-os
H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os
CT-OS-P -O2 1 1.050 180.000 2.000 same as X -os-p4-X
CT-OS-P -OS 1 1.050 180.000 2.000 same as X -os-p4-X
H1-CT-OS-P 1 0.383 0.000 3.000 same as X -c3-os-X
OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-CT-CT-OH 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-CT-CT-C 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-OH-HO 1 0.160 0.000 -3.000 same as ho-oh-c3-c3
CT-CT-OH-HO 1 0.250 0.000 1.000 same as ho-oh-c3-c3
OH-CT-C -O 1 0.000 180.000 2.000 same as X -c -c3-X
OH-CT-C -N 1 0.000 180.000 2.000 same as X -c -c3-X
HO-OH-CT-H1 1 0.167 0.000 3.000 same as X -c3-oh-X
HO-OH-CT-C 1 0.167 0.000 3.000 same as X -c3-oh-X

N -CT-CT-HC	1	0.156	0.000	3.000 same as X -c3-c3-X
N -CT-CT-C	1	0.156	0.000	3.000 same as X -c3-c3-X
H1-CT-CT-HC	1	0.150	0.000	3.000 same as hc-c3-c3-hc
N -CT-CT-SH	1	0.156	0.000	3.000 same as X -c3-c3-X
CT-CT-SH-HS	1	0.250	0.000	3.000 same as X -c3-sh-X
H1-CT-CT-SH	1	0.156	0.000	3.000 same as X -c3-c3-X
H1-CT-SH-HS	1	0.250	0.000	3.000 same as X -c3-sh-X

IMPROPER

CT-N -C -O	1.1	180.0	2.0	Using default value
C -CT-N -H	1.1	180.0	2.0	Using default value

NONBON

CT	1.9080	0.1094	same as c3
HC	1.4870	0.0157	same as hc
C	1.9080	0.0860	same as c
O	1.6612	0.2100	same as o
N	1.8240	0.1700	same as n
H	0.6000	0.0157	same as hn
H1	1.4870	0.0157	same as hc
OS	1.6837	0.1700	same as os
P	2.1000	0.2000	same as p4
O2	1.6612	0.2100	same as o
OH	1.7210	0.2104	same as oh
HO	0.0000	0.0000	same as ho
SH	2.0000	0.2500	same as sh
HS	0.6000	0.0157	same as hs

HEX.lib (hexanoyl acyl chain bound to the phosphopantetheine prosthetic group)

```
!!index array str
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!entry.HEX.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq  int elmnt  dbl chg
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 "H2" "H" 0 1 131075 8 -1 0.257181
 "CA" "CT" 0 1 131075 9 -1 0.013960
 "C" "C" 0 1 131075 10 -1 0.657576
 "O" "O" 0 1 131075 11 -1 -0.644337
 "H1" "H1" 0 1 131075 18 -1 0.074804
 "CB" "CT" 0 1 131075 19 -1 0.051668
 "H3" "H1" 0 1 131075 20 -1 0.079424
 "H4" "H1" 0 1 131075 21 -1 0.079424
 "OG" "OS" 0 1 131075 22 -1 -0.439764
 "P02" "P" 0 1 131075 23 -1 1.004347
 "O01" "O2" 0 1 131075 24 -1 -0.742611
 "O04" "O2" 0 1 131075 25 -1 -0.742611
 "O05" "OS" 0 1 131075 26 -1 -0.354359
 "C06" "CT" 0 1 131075 27 -1 0.148994
 "H5" "H1" 0 1 131075 28 -1 0.034743
 "H6" "H1" 0 1 131075 29 -1 0.034743
 "C09" "CT" 0 1 131075 30 -1 0.115199
 "C14" "CT" 0 1 131075 31 -1 -0.120111
 "H7" "HC" 0 1 131075 32 -1 0.029409
 "H8" "HC" 0 1 131075 33 -1 0.029409
 "H9" "HC" 0 1 131075 34 -1 0.029409
 "C10" "CT" 0 1 131075 35 -1 -0.120138
 "H10" "HC" 0 1 131075 36 -1 0.029409
 "H11" "HC" 0 1 131075 37 -1 0.029409
 "H12" "HC" 0 1 131075 38 -1 0.029409
 "C18" "CT" 0 1 131075 39 -1 -0.006848
 "O20" "OH" 0 1 131075 40 -1 -0.694970
 "H14" "HO" 0 1 131075 41 -1 0.435436
 "H13" "H1" 0 1 131075 42 -1 0.098017
 "C22" "C" 0 1 131075 43 -1 0.616259
 "O23" "O" 0 1 131075 44 -1 -0.597818
 "N24" "N" 0 1 131075 45 -1 -0.431486
 "H15" "H" 0 1 131075 46 -1 0.334159
 "C26" "CT" 0 1 131075 47 -1 -0.064155
 "H16" "H1" 0 1 131075 48 -1 0.088976
 "H17" "H1" 0 1 131075 49 -1 0.088976
 "C29" "CT" 0 1 131075 50 -1 -0.069252
 "H18" "HC" 0 1 131075 51 -1 0.047188
 "H19" "HC" 0 1 131075 52 -1 0.047188
 "C32" "C" 0 1 131075 53 -1 0.551746
 "O33" "O" 0 1 131075 54 -1 -0.546511
 "N34" "N" 0 1 131075 55 -1 -0.537284
 "H20" "H" 0 1 131075 56 -1 0.321808
 "C36" "CT" 0 1 131075 57 -1 0.035919
 "H21" "H1" 0 1 131075 58 -1 0.070851
 "H22" "H1" 0 1 131075 59 -1 0.070851
 "C39" "CT" 0 1 131075 60 -1 0.124148
 "H23" "H1" 0 1 131075 61 -1 0.032529
 "H24" "H1" 0 1 131075 62 -1 0.032529
 "S1" "S" 0 1 131075 63 -1 -0.312013
 "C95" "C" 0 1 131075 64 -1 0.549337
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"O47" "O" 0 1 131075 65 -1 -0.495142
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"H93" "HC" 0 1 131075 73 -1 0.002078
"H94" "HC" 0 1 131075 74 -1 0.002078
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"H95" "HC" 0 1 131075 76 -1 -0.020179
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"C60" "CT" 0 1 131075 78 -1 -0.022852
"H97" "HC" 0 1 131075 79 -1 0.002229
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"C" "C" 0 -1 0.0
"O" "O" 0 -1 0.0
"H1" "H1" 0 -1 0.0
"CB" "CT" 0 -1 0.0
"H3" "H1" 0 -1 0.0
"H4" "H1" 0 -1 0.0
"OG" "OS" 0 -1 0.0
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"O01" "O2" 0 -1 0.0
"O04" "O2" 0 -1 0.0
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"C14" "CT" 0 -1 0.0
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"C26" "CT" 0 -1 0.0
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"H23" "H1" 0 -1 0.0
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!entry.HEX.unit.childsequence single int
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!entry.HEX.unit.connect array int
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!entry.HEX.unit.connectivity table int atom1x int atom2x int flags
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11 12 1
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11 14 1
14 15 1
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0.874166 -0.879688 -3.133244
0.974173 -1.554958 -4.128663
2.530399 -1.766889 -2.197857
0.805545 -2.299598 -1.068022
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-0.884164 -0.833607 0.372937
-0.577043 0.525759 -0.168196
-0.345227 -1.290595 1.652841
-2.487640 -1.041607 0.355916
-3.246776 -0.587472 -0.725326
-3.136731 0.488576 -0.822316
-2.874874 -1.056379 -1.629135
-4.729044 -0.947468 -0.506312
-4.886083 -2.474283 -0.486336
-4.637031 -2.909386 -1.448564
-5.903392 -2.764326 -0.236282
-4.222015 -2.897388 0.255769
-5.186175 -0.350255 0.834112
-4.559944 -0.734441 1.628441
-6.218628 -0.590308 1.046190
-5.092127 0.732665 0.831107
-5.528020 -0.313414 -1.681364
-5.052095 -0.713380 -2.949144
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-8.851681 -1.867264 -2.692526
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-9.002662 -2.322171 -3.660340
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-9.137628 -2.375097 -0.628630
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-11.061565 -3.002982 0.218261
-12.889293 -3.647909 -0.602109
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-16.460104 2.071013 -0.174916
-15.976107 3.187206 -1.415553
-17.374559 1.740900 -2.120741
-18.162588 2.479001 -1.986729
-17.056540 1.825881 -3.158799
-17.976675 0.346801 -1.903711
-18.694427 0.168882 -2.700420
-17.212474 -0.417464 -2.019751
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!entry.HEX.unit.residuesPdbSequenceNumber array int
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HEX.frcmod (hexanoyl acyl chain bound to the phosphopantetheine prosthetic group)

Remark line goes here
MASS
CT 12.010 0.878 same as c3
HC 1.008 0.135 same as hc
C 12.010 0.616 same as c
O 16.000 0.434 same as o
N 14.010 0.530 same as n
H 1.008 0.161 same as hn
H1 1.008 0.135 same as h1
OS 16.000 0.465 same as os
P 30.970 1.538 same as p5
O2 16.000 0.434 same as o
OH 16.000 0.465 same as oh
HO 1.008 0.135 same as ho
S 32.060 2.900 same as ss

BOND
CT-HC 337.30 1.092 same as c3-hc
C -CT 328.30 1.508 same as c-c3
C -O 648.00 1.214 same as c- o
C -N 478.20 1.345 same as c- n
H -N 410.20 1.009 same as hn- n
CT-N 330.60 1.460 same as c3- n
CT-H1 335.90 1.093 same as c3-h1
CT-CT 303.10 1.535 same as c3-c3
CT-OS 301.50 1.439 same as c3-os
OS-P 342.50 1.602 same as os-p5
O2-P 487.70 1.481 same as o-p5
CT-OH 314.10 1.426 same as c3-oh
HO-OH 369.60 0.974 same as ho-oh
CT-S 225.80 1.821 same as c3-ss
C -S 261.90 1.762 same as c-ss

ANGLE
CT-C -O 68.030 123.110 same as c3-c -o
CT-C -N 67.860 115.150 same as c3-c -n
HC-CT-HC 39.430 108.350 same as hc-c3-hc
C -CT-HC 47.200 109.680 same as c -c3-hc
C -N -H 49.210 118.460 same as c -n -hn
C -N -CT 63.920 121.350 same as c -n -c3
N -C -O 75.830 122.030 same as n -c -o
C -CT-N 66.670 111.560 same as c -c3-n
H1-CT-N 49.820 109.320 same as h1-c3-n
CT-CT-N 65.850 112.130 same as c3-c3-n
CT-N -H 46.040 116.780 same as c3-n -hn
CT-CT-H1 46.360 110.070 same as c3-c3-h1
CT-CT-OS 67.780 108.420 same as c3-c3-os
C -CT-H1 47.630 107.660 same as c -c3-h1
C -CT-CT 63.790 110.530 same as c -c3-c3
H1-CT-H1 39.180 109.550 same as h1-c3-h1
CT-OS-P 78.480 118.000 same as c3-os-p5
H1-CT-OS 50.840 108.820 same as h1-c3-os
O2-P -OS 44.010 116.090 same as o -p5-os
OS-P -OS 45.370 101.770 same as os-p5-os
O2-P -O2 46.010 115.800 same as o -p5-o

CT-CT-CT 63.210 110.630 same as c3-c3-c3
CT-CT-HC 46.370 110.050 same as c3-c3-hc
CT-CT-OH 67.720 109.430 same as c3-c3-oh
CT-OH-HO 47.090 108.160 same as c3-oh-ho
H1-CT-OH 50.970 109.880 same as h1-c3-oh
C -CT-OH 68.650 108.700 same as c -c3-oh
CT-CT-S 61.100 112.690 same as c3-c3-ss
C -S -CT 61.480 100.290 same as c -ss-c3
H1-CT-S 42.400 109.340 same as h1-c3-ss
O -C -S 64.620 122.290 same as o -c -ss
CT-C -S 62.410 114.320 same as c3-c -ss

DIHE
CT-C -N -H 4 10.000 180.000 2.000 same as X -c -n -X
CT-C -N -CT 4 10.000 180.000 2.000 same as X -c -n -X
O -C -CT-HC 1 0.800 0.000 -1.000 same as hc-c3-c -o
O -C -CT-HC 1 0.080 180.000 3.000 same as hc-c3-c -o
N -C -CT-HC 6 0.000 180.000 2.000 same as X -c -c3-X
C -CT-N -C 1 0.850 180.000 -2.000 same as c -n -c3-c
C -CT-N -C 1 0.800 0.000 1.000 same as c -n -c3-c
H1-CT-N -C 6 0.000 0.000 2.000 same as X -c3-n -X
CT-CT-N -C 1 0.500 180.000 -4.000 same as c3-c3-n -c
CT-CT-N -C 1 0.150 180.000 -3.000 same as c3-c3-n -c
CT-CT-N -C 1 0.530 0.000 1.000 same as c3-c3-n -c
O -C -N -H 1 2.500 180.000 -2.000 same as hn-n -c -o
O -C -N -H 1 2.000 0.000 1.000 same as hn-n -c -o
O -C -N -CT 4 10.000 180.000 2.000 same as X -c -n -X
O -C -CT-N 6 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-N 1 1.700 180.000 -1.000 same as n -c3-c -n
N -C -CT-N 1 2.000 180.000 2.000 same as n -c3-c -n
H1-CT-CT-N 9 1.400 0.000 3.000 same as X -c3-c3-X
N -CT-CT-OS 9 1.400 0.000 3.000 same as X -c3-c3-X
C -CT-N -H 6 0.000 0.000 2.000 same as X -c3-n -X
H1-CT-N -H 6 0.000 0.000 2.000 same as X -c3-n -X
CT-CT-N -H 6 0.000 0.000 2.000 same as X -c3-n -X
CT-CT-OS-P 3 1.150 0.000 3.000 same as X -c3-os-X
C -CT-CT-H1 9 1.400 0.000 3.000 same as X -c3-c3-X
C -CT-CT-OS 9 1.400 0.000 3.000 same as X -c3-c3-X
O -C -CT-H1 1 0.800 0.000 -1.000 same as h1-c3-c -o
O -C -CT-H1 1 0.080 180.000 3.000 same as h1-c3-c -o
O -C -CT-CT 6 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-H1 6 0.000 180.000 2.000 same as X -c -c3-X
N -C -CT-CT 1 0.100 0.000 -4.000 same as c3-c3-c -n
N -C -CT-CT 1 0.070 0.000 2.000 same as c3-c3-c -n
H1-CT-CT-H1 9 1.400 0.000 3.000 same as X -c3-c3-X
H1-CT-CT-OS 1 0.000 0.000 -3.000 same as h1-c3-c3-os
H1-CT-CT-OS 1 0.250 0.000 1.000 same as h1-c3-c3-os
CT-OS-P -O2 3 2.400 0.000 2.000 same as X -os-p5-X
CT-OS-P -OS 1 0.250 0.000 -3.000 same as os-p5-os-c3
CT-OS-P -OS 1 1.200 0.000 2.000 same as os-p5-os-c3
H1-CT-OS-P 3 1.150 0.000 3.000 same as X -c3-os-X
CT-CT-CT-OS 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-CT-CT-OH 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-H1 9 1.400 0.000 3.000 same as X -c3-c3-X
C -CT-CT-CT 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-OH-HO 1 0.160 0.000 -3.000 same as ho-oh-c3-c3
CT-CT-OH-HO 1 0.250 0.000 1.000 same as ho-oh-c3-c3
O -C -CT-OH 6 0.000 180.000 2.000 same as X -c -c3-X

N -C -CT-OH 6 0.000 180.000 2.000 same as X -c -c3-X
H1-CT-OH-HO 3 0.500 0.000 3.000 same as X -c3-oh-X
C -CT-OH-HO 3 0.500 0.000 3.000 same as X -c3-oh-X
HC-CT-CT-N 9 1.400 0.000 3.000 same as X -c3-c3-X
C -CT-CT-N 9 1.400 0.000 3.000 same as X -c3-c3-X
H1-CT-CT-HC 9 1.400 0.000 3.000 same as X -c3-c3-X
N -CT-CT-S 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-S -C 3 1.000 0.000 3.000 same as X -c3-ss-X
H1-CT-CT-S 9 1.400 0.000 3.000 same as X -c3-c3-X
O -C -S -CT 2 6.200 180.000 2.000 same as X -c -ss-X
CT-C -S -CT 2 6.200 180.000 2.000 same as X -c -ss-X
H1-CT-S -C 3 1.000 0.000 3.000 same as X -c3-ss-X
S -C -CT-HC 6 0.000 180.000 2.000 same as X -c -c3-X
S -C -CT-CT 6 0.000 180.000 2.000 same as X -c -c3-X
C -CT-CT-HC 9 1.400 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3
HC-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc

IMPROPER
CT-N -C -O 10.5 180.0 2.0 Same as X -X -c -o
C -CT-N -H 1.1 180.0 2.0 Same as X -X -n -hn
CT-O -C -S 1.1 180.0 2.0 Using the default value

NONBON
CT 1.9080 0.1094 same as c3
HC 1.4870 0.0157 same as hc
C 1.9080 0.0860 same as c
O 1.6612 0.2100 same as o
N 1.8240 0.1700 same as n
H 0.6000 0.0157 same as hn
H1 1.3870 0.0157 same as h1
OS 1.6837 0.1700 same as os
P 2.1000 0.2000 same as p5
O2 1.6612 0.2100 same as o
OH 1.7210 0.2104 same as oh
HO 0.0000 0.0000 same as ho
S 2.0000 0.2500 same as ss

decacyl.lib (decanoyl acyl chain bound to the phosphopantetheine prosthetic group)

```
!!index array str
 "DEC"
!entry.DEC.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq  int elmnt  dbl chg
 "N" "N" 0 1 131075 7 -1 -0.539900
 "H2" "H" 0 1 131075 8 -1 0.346500
 "CA" "CT" 0 1 131075 9 -1 -0.010300
 "H1" "H1" 0 1 131075 10 -1 0.106700
 "C" "C" 0 1 131075 11 -1 0.662100
 "O" "O" 0 1 131075 18 -1 -0.643100
 "CB" "CT" 0 1 131075 19 -1 0.165400
 "H3" "H1" 0 1 131075 20 -1 0.044700
 "H4" "H1" 0 1 131075 21 -1 0.044700
 "OG" "OS" 0 1 131075 22 -1 -0.597201
 "P02" "P" 0 1 131075 23 -1 1.432800
 "O01" "O2" 0 1 131075 24 -1 -0.822000
 "O04" "O2" 0 1 131075 25 -1 -0.822000
 "O05" "OS" 0 1 131075 26 -1 -0.559200
 "C06" "CT" 0 1 131075 27 -1 0.198400
 "H5" "H1" 0 1 131075 28 -1 0.034200
 "H6" "H1" 0 1 131075 29 -1 0.034200
 "C09" "CT" 0 1 131075 30 -1 -0.098000
 "C14" "CT" 0 1 131075 31 -1 -0.093600
 "H7" "HC" 0 1 131075 32 -1 0.044367
 "H8" "HC" 0 1 131075 33 -1 0.044367
 "H9" "HC" 0 1 131075 34 -1 0.044367
 "C10" "CT" 0 1 131075 35 -1 -0.093600
 "H10" "HC" 0 1 131075 36 -1 0.044367
 "H11" "HC" 0 1 131075 37 -1 0.044367
 "H12" "HC" 0 1 131075 38 -1 0.044367
 "C18" "CT" 0 1 131075 39 -1 0.078100
 "H13" "H1" 0 1 131075 40 -1 0.110700
 "O20" "OH" 0 1 131075 41 -1 -0.591800
 "H14" "HO" 0 1 131075 42 -1 0.402000
 "C22" "C" 0 1 131075 43 -1 0.638100
 "O23" "O" 0 1 131075 44 -1 -0.605100
 "N24" "N" 0 1 131075 45 -1 -0.564900
 "H15" "H" 0 1 131075 46 -1 0.303500
 "C26" "CT" 0 1 131075 47 -1 0.096000
 "H16" "H1" 0 1 131075 48 -1 0.065700
 "H17" "H1" 0 1 131075 49 -1 0.065700
 "C29" "CT" 0 1 131075 50 -1 -0.186400
 "H18" "HC" 0 1 131075 51 -1 0.078200
 "H19" "HC" 0 1 131075 52 -1 0.078200
 "C32" "C" 0 1 131075 53 -1 0.663100
 "O33" "O" 0 1 131075 54 -1 -0.607100
 "N34" "N" 0 1 131075 55 -1 -0.584900
 "H20" "H" 0 1 131075 56 -1 0.324500
 "C36" "CT" 0 1 131075 57 -1 0.098000
 "H21" "H1" 0 1 131075 58 -1 0.065200
 "H22" "H1" 0 1 131075 59 -1 0.065200
 "C39" "CT" 0 1 131075 60 -1 -0.043300
 "H23" "H1" 0 1 131075 61 -1 0.085700
```

"H24" "H1" 0 1 131075 62 -1 0.085700
"S1" "S" 0 1 131075 63 -1 -0.248700
"C95" "C" 0 1 131075 64 -1 0.582700
"O47" "O" 0 1 131075 65 -1 -0.548100
"C48" "CT" 0 1 131075 66 -1 -0.169400
"H79" "HC" 0 1 131075 67 -1 0.077700
"H90" "HC" 0 1 131075 68 -1 0.077700
"C51" "CT" 0 1 131075 69 -1 -0.074400
"H92" "HC" 0 1 131075 70 -1 0.059200
"H91" "HC" 0 1 131075 71 -1 0.059200
"C54" "CT" 0 1 131075 72 -1 -0.080400
"H93" "HC" 0 1 131075 73 -1 0.039700
"H94" "HC" 0 1 131075 74 -1 0.039700
"C57" "CT" 0 1 131075 75 -1 -0.077400
"H96" "HC" 0 1 131075 76 -1 0.041700
"H95" "HC" 0 1 131075 77 -1 0.041700
"C60" "CT" 0 1 131075 78 -1 -0.079400
"H97" "HC" 0 1 131075 79 -1 0.040200
"H99" "HC" 0 1 131075 80 -1 0.040200
"C63" "CT" 0 1 131075 81 -1 -0.079400
"H87" "HC" 0 1 131075 82 -1 0.039700
"H88" "HC" 0 1 131075 83 -1 0.039700
"C66" "CT" 0 1 131075 84 -1 -0.079400
"H85" "HC" 0 1 131075 85 -1 0.040200
"H86" "HC" 0 1 131075 86 -1 0.040200
"C69" "CT" 0 1 131075 87 -1 -0.080400
"H83" "HC" 0 1 131075 88 -1 0.038200
"H84" "HC" 0 1 131075 89 -1 0.038200
"C72" "CT" 0 1 131075 90 -1 -0.092100
"H80" "HC" 0 1 131075 91 -1 0.032033
"H82" "HC" 0 1 131075 92 -1 0.032033
"H81" "HC" 0 1 131075 93 -1 0.032033
!entry.DEC.unit.atomspertinfo table str pname str ptype int ptypex int pelmnt dbl pchg
"N" "N" 0 -1 0.0
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"CA" "CT" 0 -1 0.0
"H1" "H1" 0 -1 0.0
"C" "C" 0 -1 0.0
"O" "O" 0 -1 0.0
"CB" "CT" 0 -1 0.0
"H3" "H1" 0 -1 0.0
"H4" "H1" 0 -1 0.0
"OG" "OS" 0 -1 0.0
"P02" "P" 0 -1 0.0
"O01" "O2" 0 -1 0.0
"O04" "O2" 0 -1 0.0
"O05" "OS" 0 -1 0.0
"C06" "CT" 0 -1 0.0
"H5" "H1" 0 -1 0.0
"H6" "H1" 0 -1 0.0
"C09" "CT" 0 -1 0.0
"C14" "CT" 0 -1 0.0
"H7" "HC" 0 -1 0.0
"H8" "HC" 0 -1 0.0
"H9" "HC" 0 -1 0.0
"C10" "CT" 0 -1 0.0
"H10" "HC" 0 -1 0.0
"H11" "HC" 0 -1 0.0
"H12" "HC" 0 -1 0.0

"C18" "CT" 0 -1 0.0
"H13" "H1" 0 -1 0.0
"O20" "OH" 0 -1 0.0
"H14" "HO" 0 -1 0.0
"C22" "C" 0 -1 0.0
"O23" "O" 0 -1 0.0
"N24" "N" 0 -1 0.0
"H15" "H" 0 -1 0.0
"C26" "CT" 0 -1 0.0
"H16" "H1" 0 -1 0.0
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"H19" "HC" 0 -1 0.0
"C32" "C" 0 -1 0.0
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"C36" "CT" 0 -1 0.0
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!entry.DEC.unit.childsequence single int
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!entry.DEC.unit.connect array int
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5
!entry.DEC.unit.connectivity table int atom1x int atom2x int flags
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3 4 1
3 5 1
3 7 1
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7 8 1
7 9 1
7 10 1
10 11 1
11 12 1
11 13 1
11 14 1
14 15 1
15 16 1
15 17 1
15 18 1
18 19 1
18 23 1
18 27 1
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78 81 1
!entry.DEC.unit.hierarchy table str abovetype int abovex str belowtype int belowx
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!entry.DEC.unit.name single str
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2.036589 0.061021 1.600497
1.053837 1.761775 2.679286

0.936900 2.657535 2.250403
1.662791 1.946732 4.065139
1.399871 2.939607 4.740057
-0.289121 1.036874 2.788293
-0.768041 1.042894 1.910455
-0.868953 1.468796 3.479117
-0.109138 -0.318377 3.168376
-0.473245 -1.432573 2.174212
0.414758 -1.292623 0.848215
-1.900157 -1.013546 2.054200
-0.149317 -2.793457 2.969162
1.064729 -3.034506 3.699201
1.739696 -2.374578 3.372223
0.868668 -2.851417 4.662549
1.602746 -4.463705 3.534211
1.962836 -4.698820 2.063810
1.765941 -3.868129 1.544980
1.417543 -5.458192 1.711658
2.937104 -4.918918 1.997789
0.493995 -5.495412 3.796171
0.362941 -6.049595 2.972941
-0.353968 -5.013393 4.021154
0.766058 -6.080576 4.561393
2.905749 -4.592744 4.382229
3.639467 -4.461841 3.715504
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2.333016 -2.964744 5.368312
3.018710 -5.890855 5.133336
2.968675 -6.971784 4.576401
3.251635 -5.793864 6.541917
3.334670 -4.906845 6.993916
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3.958634 -7.646779 6.782804
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1.426395 -7.461862 6.552288
1.435361 -7.128944 8.144570
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3.237117 -8.602876 9.541848
3.309225 -10.719084 9.194167
3.085277 -11.282891 8.400461
4.289246 -10.792125 9.379164
2.482338 -11.115978 10.410006
2.982510 -11.786258 10.958232
2.294408 -10.311104 10.972910
1.077933 -11.766104 9.834868
-0.017231 -11.621013 11.266101
-0.678274 -10.347793 11.232081
-0.952260 -12.934937 11.615132
-0.989283 -13.576867 10.849262
-0.461293 -13.554939 12.227136
-2.331124 -12.820875 12.316078
-2.906266 -12.221705 11.760913
-2.739092 -13.734701 12.338093
-2.336089 -12.270813 13.764114
-1.462185 -12.483802 14.201067
-3.073272 -12.706875 14.280264

-2.543968 -10.753222 13.791059
-2.468967 -10.378262 12.867056
-1.858049 -10.320295 14.375942
-3.943932 -10.501155 14.349044
-4.484044 -10.011052 13.664881
-4.373890 -11.379956 14.556033
-3.830933 -9.679394 15.597619
-2.889689 -9.087297 15.602610
-3.818964 -10.349563 16.484904
-4.988911 -8.737330 15.744600
-4.804931 -7.789630 15.194747
-5.933227 -9.187445 15.367496
-5.181900 -8.401256 17.193672
-4.778905 -7.391366 17.426613
-4.639114 -9.139016 17.822491
-6.630637 -8.439181 17.580614
-7.190779 -7.600929 17.111444
-7.108856 -9.397518 17.281549
-6.723660 -8.338100 18.684096
!entry.DEC.unit.residueconnect table int c1x int c2x int c3x int c4x int c5x int c6x
0 78 0 0 0 0
!entry.DEC.unit.residues table str name int seq int childseq int startatomx str restype int imagingx
"DEC" 1 94 1 "p" 0
!entry.DEC.unit.residuesPdbSequenceNumber array int
0
!entry.DEC.unit.solventcap array dbl
-1.000000
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!entry.DEC.unit.velocities table dbl x dbl y dbl z
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decacyl.frcmod (decanoyl acyl chain bound to the phosphopantetheine prosthetic group)

remark goes here
MASS
CT 12.010 0.878 same as c3
HC 1.008 0.135 same as hc
C 12.010 0.616 same as c
O 16.000 0.434 same as o
N 14.010 0.530 same as n
H 1.008 0.161 same as hn
H1 1.008 0.135 same as hc
OS 16.000 0.465 same as os
P 30.970 1.538 same as p4
O2 16.000 0.434 same as o
OH 16.000 0.465 same as oh
HO 1.008 0.135 same as ho
S 32.060 2.900 same as ss

BOND
CT-HC 337.30 1.092 same as c3-hc
CT-C 328.30 1.508 same as c -c3
C -O 648.00 1.214 same as c -o
C -N 478.20 1.345 same as c -n
N -H 410.20 1.009 same as hn-n
N -CT 330.60 1.460 same as c3-n
CT-H1 337.30 1.092 same as c3-hc
CT-CT 303.10 1.535 same as c3-c3
CT-OS 301.50 1.439 same as c3-os
OS-P 311.60 1.636 same as os-p4
P -O2 456.40 1.503 same as o -p4
CT-OH 314.10 1.426 same as c3-oh
OH-HO 369.60 0.974 same as ho-oh
CT-S 225.80 1.821 same as c3-ss
S -C 261.90 1.762 same as c -ss

ANGLE
CT-C -O 68.030 123.110 same as c3-c -o
CT-C -N 67.860 115.150 same as c3-c -n
HC-CT-HC 39.430 108.350 same as hc-c3-hc
HC-CT-C 47.200 109.680 same as c -c3-hc
C -N -H 49.210 118.460 same as c -n -hn
C -N -CT 63.920 121.350 same as c -n -c3
O -C -N 75.830 122.030 same as n -c -o
N -CT-H1 49.780 109.500 same as hc-c3-n
N -CT-C 66.670 111.560 same as c -c3-n
N -CT-CT 65.850 112.130 same as c3-c3-n
H -N -CT 46.040 116.780 same as c3-n -hn
CT-CT-H1 46.370 110.050 same as c3-c3-hc
CT-CT-OS 67.780 108.420 same as c3-c3-os
H1-CT-C 47.200 109.680 same as c -c3-hc
C -CT-CT 63.790 110.530 same as c -c3-c3
H1-CT-H1 39.430 108.350 same as hc-c3-hc
CT-OS-P 77.590 117.480 same as c3-os-p4
H1-CT-OS 50.870 108.700 same as hc-c3-os
OS-P -O2 43.100 116.670 same as o -p4-os

OS-P -OS 44.740 100.340 same as os-p4-os
O2-P -O2 45.060 117.220 same as o -p4-o
CT-CT-CT 63.210 110.630 same as c3-c3-c3
CT-CT-HC 46.490 109.490 Calculated with empirical approach
CT-CT-OH 67.720 109.430 same as c3-c3-oh
CT-OH-HO 47.090 108.160 same as c3-oh-ho
H1-CT-OH 51.070 109.500 same as hc-c3-oh
OH-CT-C 68.650 108.700 same as c -c3-oh
CT-CT-S 61.100 112.690 same as c3-c3-ss
CT-S -C 61.480 100.290 same as c -ss-c3
H1-CT-S 42.510 108.760 same as hc-c3-ss
S -C -O 64.620 122.290 same as o -c -ss
S -C -CT 62.410 114.320 same as c3-c -ss

DIHE
CT-C -N -H 1 2.500 180.000 2.000 same as X -c -n -X
CT-C -N -CT 1 2.500 180.000 2.000 same as X -c -n -X
HC-CT-C -O 1 0.800 0.000 -1.000 same as hc-c3-c -o
HC-CT-C -O 1 0.080 180.000 3.000 same as hc-c3-c -o
HC-CT-C -N 1 0.000 180.000 2.000 same as X -c -c3-X
C -N -CT-H1 1 0.000 0.000 2.000 same as X -c3-n -X
C -N -CT-C 1 0.850 180.000 -2.000 same as c -n -c3-c
C -N -CT-C 1 0.800 0.000 1.000 same as c -n -c3-c
C -N -CT-CT 1 0.500 180.000 -4.000 same as c3-c3-n -c
C -N -CT-CT 1 0.150 180.000 -3.000 same as c3-c3-n -c
C -N -CT-CT 1 0.530 0.000 1.000 same as c3-c3-n -c
O -C -N -H 1 2.500 180.000 -2.000 same as hn-n -c -o
O -C -N -H 1 2.000 0.000 1.000 same as hn-n -c -o
O -C -N -CT 1 2.500 180.000 2.000 same as X -c -n -X
N -CT-C -N 1 1.700 180.000 -1.000 same as n -c3-c -n
N -CT-C -N 1 2.000 180.000 2.000 same as n -c3-c -n
N -CT-C -O 1 0.000 180.000 2.000 same as X -c -c3-X
N -CT-CT-H1 1 0.156 0.000 3.000 same as X -c3-c3-X
N -CT-CT-OS 1 0.156 0.000 3.000 same as X -c3-c3-X
H -N -CT-H1 1 0.000 0.000 2.000 same as X -c3-n -X
H -N -CT-C 1 0.000 0.000 2.000 same as X -c3-n -X
H -N -CT-CT 1 0.000 0.000 2.000 same as X -c3-n -X
CT-CT-OS-P 1 0.383 0.000 3.000 same as X -c3-os-X
H1-CT-C -N 1 0.000 180.000 2.000 same as X -c -c3-X
H1-CT-C -O 1 0.800 0.000 -1.000 same as hc-c3-c -o
H1-CT-C -O 1 0.080 180.000 3.000 same as hc-c3-c -o
H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc
H1-CT-CT-OS 1 0.000 0.000 -3.000 same as hc-c3-c3-os
H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os
C -CT-CT-H1 1 0.156 0.000 3.000 same as X -c3-c3-X
C -CT-CT-OS 1 0.156 0.000 3.000 same as X -c3-c3-X
N -C -CT-CT 1 0.100 0.000 -4.000 same as c3-c3-c -n
N -C -CT-CT 1 0.070 0.000 2.000 same as c3-c3-c -n
O -C -CT-CT 1 0.000 180.000 2.000 same as X -c -c3-X
CT-OS-P -O2 1 1.050 180.000 2.000 same as X -os-p4-X
CT-OS-P -OS 1 1.050 180.000 2.000 same as X -os-p4-X
H1-CT-OS-P 1 0.383 0.000 3.000 same as X -c3-os-X
OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-CT-CT-OH 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-C 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-OH-HO 1 0.160 0.000 -3.000 same as ho-oh-c3-c3
CT-CT-OH-HO 1 0.250 0.000 1.000 same as ho-oh-c3-c3

H1-CT-OH-HO 1 0.167 0.000 3.000 same as X -c3-oh-X
OH-CT-C -O 1 0.000 180.000 2.000 same as X -c -c3-X
OH-CT-C -N 1 0.000 180.000 2.000 same as X -c -c3-X
HO-OH-CT-C 1 0.167 0.000 3.000 same as X -c3-oh-X
N -CT-CT-HC 1 0.156 0.000 3.000 same as X -c3-c3-X
N -CT-CT-C 1 0.156 0.000 3.000 same as X -c3-c3-X
H1-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc
N -CT-CT-S 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-S -C 1 0.333 0.000 3.000 same as X -c3-ss-X
H1-CT-CT-S 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-S -C -O 1 3.100 180.000 2.000 same as X -c -ss-X
CT-S -C -CT 1 3.100 180.000 2.000 same as X -c -ss-X
H1-CT-S -C 1 0.333 0.000 3.000 same as X -c3-ss-X
S -C -CT-HC 1 0.000 180.000 2.000 same as X -c -c3-X
S -C -CT-CT 1 0.000 180.000 2.000 same as X -c -c3-X
C -CT-CT-HC 1 0.156 0.000 3.000 same as X -c3-c3-X
CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3
HC-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc

IMPROPER
CT-N -C -O 1.1 180.0 2.0 Using default value
C -CT-N -H1 1.1 180.0 2.0 Using default value
C -CT-N -H 1.1 180.0 2.0 Using default value
CT-O -C -S 1.1 180.0 2.0 Using default value

NONBON
CT 1.9080 0.1094 same as c3
HC 1.4870 0.0157 same as hc
C 1.9080 0.0860 same as c
O 1.6612 0.2100 same as o
N 1.8240 0.1700 same as n
H 0.6000 0.0157 same as hn
H1 1.4870 0.0157 same as hc
OS 1.6837 0.1700 same as os
P 2.1000 0.2000 same as p4
O2 1.6612 0.2100 same as o
OH 1.7210 0.2104 same as oh
HO 0.0000 0.0000 same as ho
S 2.0000 0.2500 same as ss