

Computational ^{19}F NMR. 2. Organic Compounds

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Electronic Supporting Information

Experimental data were taken from:

(1) S. Berger, S. Braun, H.-O. Kalinowski, *NMR Spektroskopie von Nichtmetallen*, vol. 4, ^{19}F -NMR-Spektroskopie, Thieme, Stuttgart, 1994.

(2) T. S. Everett, *Nuclear Magnetic Resonance Spectroscopy of Organofluorine Compounds*, in *Chemistry of Organic Fluorine Compounds II*. Ed. M. Hudlický and A. E. Pavlath, p. 1037–1086, American Chemical Society, Washington DC, 1995.

In the cases where data were available from more than one source, noticeable differences of 1-3 ppm were commonly found.

Table S1. Experimental and calculated ^{19}F chemical shifts (ppm) of organofluorine compounds. Where necessary, the fluorine atom considered is highlighted in boldface.

(a) Fluoromethanes

Compound	δ_{exp}	σ	σ_{SO}	δ_{calc}
CFCl_3	(0.0)	120.0	4.5	0.0
CBr_2ClF	5.4	101.0	5.9	19.0
CBr_3F	6.9	91.6	7.3	28.4
CCl_2F_2	-6.8	139.1	4.0	-19.1
CBrClF_2	0.1	126.9	4.2	-6.9
CBr_2F_2	6.5	114.2	4.9	5.8
CF_2I_2	18.6	88.1	4.2	31.9
CClF_3	-27.9	170.9	3.7	-50.9
CBrF_3	-17.9	156.2	3.6	-36.2
CF_3I	-5.0	138.2	2.3	-18.2
CF_4	-61.7	213.2	3.6	-93.2
CHCl_2F	-80.8	218.3	4.2	-98.3
CHBrClF	-80.4	213.4	5.0	-93.4
CHBr_2F	-84.5	208.9	6.2	-88.9
CHClF_2	-71.8	217.4	3.9	-97.4
CHF_3	-78.3	230.5	3.7	-110.5
CH_2ClF	-168.7	327.5	3.8	-207.5
CH_2FI	-191.3	342.5	4.0	-222.5
CH_2F_2	-143.4	300.7	3.6	-180.7
CH_3F	-271.9	450.1	3.1	-330.1

(b) Fluoroethanes

Compound	δ_{exp}	σ	δ_{calc}
CF_3CHF_2	-90.2	238.8	-118.8
CF_3CHF_2	-141.9	293.9	-173.9
CHF_2CHF_2	-140.2	292.1	-172.1
$\text{CF}_3\text{CH}_2\text{F}$	-78.5	231.8	-111.8
$\text{CF}_3\text{CH}_2\text{F}$	-241.0	406.3	-286.3
$\text{CHF}_2\text{CH}_2\text{F}$	-129.9	287.8	-167.8

(c) Fluoroethylenes

Compound	δ_{exp}	σ	δ_{calc}
$\text{CH}_2=\text{CHF}$	-113.0	259.1	-139.1
<i>cis</i> - $\text{CHF}=\text{CHF}$	-165.0	314.6	-194.6
<i>trans</i> - $\text{CHF}=\text{CHF}$	-186.3	343.3	-223.3
$\text{CH}_2=\text{CF}_2$	-81.3	229.9	-109.9
$\text{CF}_2=\text{CF}_2$	-134.0	282.6	-162.6
$\text{F}_2\text{C}=\text{CHF}$ (F cis to H)	-125.7	278.4	-158.4
$\text{F}_2\text{C}=\text{CHF}$ (F trans to H)	-99.7	248.1	-128.1
$\text{F}_2\text{C}=\text{CHF}$	-205.0	361.1	-241.1
<i>trans</i> - $\text{CHF}=\text{CHCOOH}$	-106.0	249.2	-129.2
$\text{CH}_2=\text{CFCOOEt}$	-117.6	258.3	-138.3
$\text{F}_2\text{C}=\text{CHCOOEt}$ (F cis to ester)	-66.0	209.0	-89.0
$\text{F}_2\text{C}=\text{CHCOOEt}$ (F trans to ester)	-70.0	222.9	-102.9
$\text{F}_2\text{C}=\text{CFCOOCH}_3$ (F cis to ester)	-99.7	238.9	-118.9
$\text{F}_2\text{C}=\text{CFCOOCH}_3$ (F trans to ester)	-89.4	234.9	-114.9
$\text{F}_2\text{C}=\text{CFCOOCH}_3$	-187.1	333.7	-213.7

(d) Primary monofluorides

Compound	δ_{exp}	σ	δ_{calc}
CH ₃ CH ₂ F	-211.5	382.3	-262.3
CH ₃ CH ₂ CH ₂ F	-218.6	383.7	-263.7
(CH ₃) ₂ CHCH ₂ F	-220.3	387.4	-267.4
(CH ₃) ₃ CCH ₂ F	-222.8	393.5	-273.5
PhCH ₂ F	-206.3	349.8	-229.8
PhCH ₂ CH ₂ F	-216.0	379.2	-259.2
PhCH ₂ CH ₂ CH ₂ F	-220.3	385.9	-265.9
FCH ₂ COOEt	-230.2	403.1	-283.1
FCH ₂ COPh	-226.1	410.4	-290.4
FCH ₂ COCH ₃	-225.7	398.0	-278.0
FCH ₂ CONH ₂	-222.8	405.5	-285.5
FCH ₂ CH ₂ OH	-226.6	410.9	-290.9
FCH ₂ CH ₂ OCH ₃	-223.1	410.6	-290.6
FCH ₂ CH ₂ SH	-212.8	380.4	-260.4
FCH ₂ CN	-232.0	401.0	-281.0
CH ₂ =CHCH ₂ F	-216.7	368.7	-248.7
HC≡CCH ₂ F	-217.5	384.3	-264.3
BrCH ₂ CH ₂ F	-212.4	366.4	-246.4
BrCH ₂ CH ₂ CH ₂ F	-228.8	389.1	-269.1

(e) Secondary monofluorides

Compound	δ_{exp}	σ	δ_{calc}
(CH ₃) ₂ CHF	-165.2	333.2	-213.2
CH ₃ CH ₂ CHFCH ₃	-173.2	345.9	-225.9
CH ₂ =CHCHFCH ₃	-171.6	355.5	-235.5
CH ₃ CH ₂ CH ₂ CHFCH ₃	-172.8	343.0	-223.0
(CH ₃ CH ₂) ₂ CHF	-172.9	353.0	-233.0
Cyclopropyl fluoride	-212.6	381.0	-261.0
Cyclohexyl fluoride (F-ax)	-186.0	351.8	-231.8
Cyclohexyl fluoride (F-eq)	-165.5	333.8	-213.8
PhCHFCH ₃	-166.8	343.5	-223.5
PhCH ₂ CHFCH ₃	-170.8	345.9	-225.9
PhCHFCH ₂ CH ₃	-176.0	312.4	-192.4
CHF(COOEt) ₂	-195.3	352.6	-232.6
PhCHFCOOEt	-174.0	307.1	-187.1
PhCHFCH ₂ OH	-180.0	318.4	-198.4

(f) Tertiary monofluorides

Compound	δ_{exp}	σ	δ_{calc}
(CH ₃) ₃ CF	-130.8	299.3	-179.3
CH ₃ CH ₂ CF(CH ₃) ₂	-139.2	316.0	-196.0
(CH ₃ CH ₂) ₂ CFCH ₃	-149.1	304.3	-184.3
(CH ₃ CH ₂) ₃ CF	-156.2	321.2	-201.2
PhCF(CH ₃) ₂	-137.9	312.1	-192.1
Ph ₂ CFCH ₃	-135.0	270.7	-150.7
Ph ₃ CF	-126.7	272.6	-152.6
1-fluorobicyclo[2.2.1]heptane	-182.0	352.0	-232.0
1-fluorobicyclo[2.2.2]octane	-147.6	316.2	-196.2
HC≡CCF(CH ₃) ₂	-129.3	286.1	-166.1
CH ₃ CHF ₂	-110.0	268.0	-148.0
CH ₃ CH ₂ CHF ₂	-120.0	273.8	-153.8
CH ₃ CH ₂ CH ₂ CHF ₂	-116.8	272.7	-152.7
(CH ₃) ₂ CHCHF ₂	-126.7	285.7	-165.7
(CH ₃) ₃ CCHF ₂	-128.6	286.3	-166.3
PhCHF ₂	-111.2	261.9	-141.9
PhCH ₂ CHF ₂	-115.1	277.4	-157.4
CHF ₂ CH ₂ SH	-116.9	272.3	-152.3
CHF ₂ CN	-119.8	268.5	-148.5
CH ₃ CHF ₂	-110.0	268.0	-148.0
(CH ₃) ₂ CF ₂	-84.5	244.1	-124.1
CH ₃ CH ₂ CF ₂ CH ₃	-93.3	259.9	-139.9
(CH ₃ CH ₂) ₂ CF ₂	-102.4	274.8	-154.8
(CH ₃) ₃ CCF ₂ CH ₃	-102.2	259.7	-139.7
PhCF ₂ CH ₃	-87.7	249.5	-129.5
PhCH ₂ CF ₂ CH ₃	-89.6	256.0	-136.0
PhCF ₂ CH ₂ CH ₃	-97.9	265.4	-145.4
Ph ₂ CF ₂	-88.5	230.8	-110.8
CH ₃ CF ₂ CN	-85.4	235.0	-115.0
CF ₂ (COOEt) ₂	-109.0	264.7	-144.7
1,1-difluorotetramethylcyclopropane	-148.9	308.1	-188.1
1,1-difluorocyclohexane (F-ax)	-104.0	262.0	-142.0
1,1-difluorocyclohexane (F-eq)	-88.0	243.9	-123.9
2,2-difluorocyclohexanone	-111.0	265.6	-145.6

(g) Primary geminal difluorides

Compound	δ_{exp}	σ	δ_{calc}
CH ₃ CHF ₂	-110.0	268.0	-148.0
CH ₃ CH ₂ CHF ₂	-120.0	273.8	-153.8
CH ₃ CH ₂ CH ₂ CHF ₂	-116.8	272.7	-152.7
(CH ₃) ₂ CHCHF ₂	-126.7	285.7	-165.7
(CH ₃) ₃ CCHF ₂	-128.6	286.3	-166.3
PhCHF ₂	-111.2	261.9	-141.9
PhCH ₂ CHF ₂	-115.1	277.4	-157.4
CHF ₂ CH ₂ SH	-116.9	272.3	-152.3
CHF ₂ CN	-119.8	268.5	-148.5

(h) Secondary geminal difluorides

Compound	δ_{exp}	σ	δ_{calc}
(CH ₃) ₂ CF ₂	-84.5	244.1	-124.1
CH ₃ CH ₂ CF ₂ CH ₃	-93.3	259.9	-139.9
(CH ₃ CH ₂) ₂ CF ₂	-102.4	274.8	-154.8
(CH ₃) ₃ CCF ₂ CH ₃	-102.2	259.7	-139.7
PhCF ₂ CH ₃	-87.7	249.5	-129.5
PhCH ₂ CF ₂ CH ₃	-89.6	256.0	-136.0
PhCF ₂ CH ₂ CH ₃	-97.9	265.4	-145.4
Ph ₂ CF ₂	-88.5	230.8	-110.8
CH ₃ CF ₂ CN	-85.4	235.0	-115.0
CF ₂ (COOEt) ₂	-109	264.7	-144.7
1,1-difluorotetramethylcyclopropane	-148.9	308.1	-188.1
1,1-difluorocyclohexane ax	-104.0	262.0	-142.0
1,1-difluorocyclohexane eq	-88.0	243.9	-123.9
2,2-difluorocyclohexanone	-111	265.6	-145.6

(i) Trimethylsilyl (TMS) derivatives

Compound	δ_{exp}	σ	δ_{calc}
TMS-CH ₂ F	-277.0	449.7	-329.7
TMS-CHClF	-170.0	324.1	-204.1
TMS-CHF ₂	-140.0	298.4	-178.4
TMS-CF ₃	-67.0	218.8	-98.8
TMS-CClF ₂	-63.0	204.4	-84.4
TMS-CBrF ₂	-58.0	191.5	-71.5

(j) Trifluoromethyl derivatives

Compound	δ_{exp}	σ	δ_{calc}
CF ₃ CH ₂ F	-77.8	231.7	-111.7
CF ₃ CH ₂ Cl	-71.9	225.8	-105.8
CF ₃ CH ₂ Br	-69.3	223.1	-103.1
CF ₃ CH ₂ I	-65.8	219.5	-99.4
CF ₃ CH ₃	-61.1	215.4	-95.4
CF ₃ CF ₃	-89.1	237.7	-117.7
CF ₃ CH ₂ CF ₃	-63.6	216.9	-96.9
CF ₃ CH ₂ CN	-66.8	218.6	-98.6
CF ₃ CH ₂ NH ₂	-76.2	229.5	-109.5
(CF ₃ CH ₂) ₃ N	-71.5	227.0	-107.0
CF ₃ CH ₂ OH	-77.8	230.2	-110.2
CF ₃ CH ₂ OPh	-74.6	228.3	-108.3
(CF ₃ CH ₂ O) ₃ P	-75.9	230.7	-110.7
CF ₃ CHBrCl	-76.4	228.9	-108.9
CF ₃ CH=CH ₂	-66.9	221.6	-101.6
CF ₃ C≡CH	-52.1	197.1	-77.1
CF ₃ C≡CCF ₃	-53.5	199.3	-79.3
(CF ₃) ₃ CH	-64.2	214.4	-94.4
(CF ₃) ₄ C	-62.3	211.3	-91.3
CF ₃ OCF ₃	-62.0	209.4	-89.4
(CF ₃ O) ₄ C	-59.0	207.3	-87.3
CF ₃ NH ₂	-48.9	205.7	-85.7
(CF ₃) ₂ C(OH) ₂	-92.7	236.6	-116.6
PhCF ₃	-63.2	214.9	-94.9

(k) Trifluoroacetyl and trifluoromethanesulfonyl derivatives

Compound	δ_{exp}	σ	δ_{calc}
CF ₃ C(O)Cl	-75.7	227.3	-107.3
CF ₃ COOH	-76.2	226.8	-106.8
CF ₃ COOCH ₃	-75.6	227.4	-107.4
(CF ₃ CO) ₂ O	-75.5	224.3	-104.3
CF ₃ COOSiMe ₃	-76.7	229.1	-109.1
CF ₃ C(O)SEt	-76.1	226.7	-106.7
CF ₃ C(O)NH ₂	-76.8	228.9	-108.9
CF ₃ C(O)NHCH ₃	-76.5	229.6	-109.6
CF ₃ C(O)NHCH ₂ COOH	-76.4	229.7	-109.7
(CF ₃ CO) ₂ NCH ₃	-71.3	224.6	-104.6
CF ₃ SO ₂ Cl	-75.5	223.5	-103.5
CF ₃ SO ₃ H	-80.0	226.5	-106.5
CF ₃ SO ₃ CH ₃	-74.8	224.5	-104.5
CF ₃ SO ₃ CF ₃	-75.3	222.5	-102.5
CF ₃ SO ₃ CF ₃	-52.9	204.6	-84.6
(CF ₃ SO ₃) ₂ O	-72.2	218.9	-98.9
CF ₃ SO ₃ SiMe ₃	-77.5	229.3	-109.3
(CF ₃ SO ₃) ₂ Si(t-Bu) ₂	-75.9	227.5	-107.5
(CF ₃ SO ₂) ₂ NPh	-71.1	222.0	-102.0
CF ₃ C(O)CH ₃	-80.5	234.1	-114.1
CF ₃ C(O)CF ₃	-84.1	226.9	-106.9
CF ₃ C(O)Ph	-71.9	223.7	-103.7
CF ₃ CH(OH)CH ₃	-82.4	234.2	-114.2
CF ₃ CH(OH)CF ₃	-75.1	228.9	-108.9
CF ₃ CH(OH)Ph	-77.8	232.6	-112.6

(l) Ortho-substituted fluorobenzenes

Compound	δ_{exp}	σ	δ_{calc}	δ_{exp}	σ	δ_{calc}	δ_{exp}	σ	δ_{calc}
	Ortho			Meta			Para		
F	-138.9	293.9	-173.9	-110.5	264.6	-144.6	-120.1	275.5	-155.5
Cl	-116	266.9	-146.9	-111.4	265.5	-145.5	-116.5	272.5	-152.5
Br	-107.7	258.1	-138.1	-111.1	264.8	-144.8	-115.8	272.4	-152.4
I	-94.0	242.5	-122.5	-111.0	264.2	-144.2	-114.7	271.9	-151.9
NO ₂	-118.3	263.9	-143.9	-109.6	263.6	-143.6	-102.7	253.2	-133.2
OH	-141.6	308.9	-188.9	-112.2	269.1	-149.0	-124.6	282.3	-162.3
NH ₂	-135.9	298.1	-178.1	-113.7	270.9	-150.9	-127.3	285.6	-165.6
COCl	-108.7	254.1	-134.1	-111.3	264.4	-144.4	-101.4	251.3	-131.3
CN	-107.0	255.0	-135.0	-110.2	264.6	-144.6	-103.0	256.5	-136.5
NCO	-122.8	273.9	-153.9	-111.7	266.6	-146.6	-116.4	271.4	-151.4
CF ₃	-115.0	262.1	-142.1	-111.3	265.7	-145.7	-108.1	262.1	-142.1
CHO	-122.4	281.0	-161.0	-111.9	267.9	-147.9	-103.0	254.1	-134.1
COOH	-108.6	274.8	-154.8	-112.5	267.7	-147.7	-104.6	258.2	-138.2
CH ₂ Br	-117.5	269.3	-149.3	-113.0	268.1	-148.1	-113.5	265.6	-145.6
CH ₂ Cl	-118.3	271.0	-151.0	-113.0	267.8	-147.8	-113.8	266.2	-146.2
CONH ₂	-113.4	270.5	-150.5	-112.2	269.3	-149.3	-107.9	262.1	-142.1
CH ₃	-118.2	270.5	-150.5	-114.8	270.8	-150.8	-119.2	275.3	-155.3
OCH ₃	-136.1	292.6	-172.6	-112.3	269.0	-149.0	-124.9	283.3	-163.3
CH ₂ OH	-120.3	276.2	-156.2	-113.6	268.1	-148.1	-115.5	269.7	-149.7
CH ₂ NH ₂	-120.5	276.6	-156.6	-113.7	269.3	-149.3	-116.7	272.4	-152.4
CH ₂ CN	-117.8	271.0	-151.0	-112.2	264.7	-144.7	-114.5	269.9	-149.9
COCH ₃	-110.3	260.5	-140.5	-112.5	269.3	-149.3	-106.0	258.5	-138.5
CH ₂ COOH	-117.5	267.3	-147.3	-113.5	265.1	-145.1	-115.8	267.7	-147.7
NHCOCH ₃	-131.5	298.7	-178.7	-112.2	271.1	-151.1	-118.6	276.2	-156.2
COOEt	-110.2	256.5	-136.5	-113.1	268.1	-148.1	-106.6	260.7	-140.7
Ph	-118.6	275.1	-155.1	-113.2	269.9	-149.9	-116.4	272.9	-152.9
COPh	-111.7	264.2	-144.2		267.4	-147.4	-106.6	260.6	-140.6
CH=CH ₂				-114.1	270.8	-150.8	-114.9	268.3	-148.3

(m) Other fluorobenzenes

Compound	δ_{exp}	σ	δ_{calc}
C ₆ H ₅ F	-113.5	268.5	-148.5
1,2-difluorobenzene	-138.9	293.9	-173.9
1,3-difluorobenzene	-110.5	264.6	-144.6
1,4-difluorobenzene	-120.1	275.5	-155.5
1,2,3-trifluorobenzene (F-1,3)	-135.4	290.2	-170.2
1,2,3-trifluorobenzene (F-2)	-161.8	317.8	-197.8
1,2,4-trifluorobenzene (F-1)	-143.8	299.4	-179.4
1,2,4-trifluorobenzene (F-2)	-133.8	288.0	-168.0
1,2,4-trifluorobenzene (F-4)	-116.0	270.5	-150.5
1,3,5-trifluorobenzene	-108.0	261.9	-141.9
1,2,3,4-tetrafluorobenzene (F-1,4)	-139.9	294.8	-174.8
1,2,3,4-tetrafluorobenzene (F-2,3)	-156.4	311.6	-191.6
1,2,3,5-tetrafluorobenzene (F-1,3)	-132.1	286.6	-166.6
1,2,3,5-tetrafluorobenzene (F-2)	-166.3	323.0	-203.0
1,2,3,5-tetrafluorobenzene (F-5)	-114.2	268.7	-148.7
1,2,4,5-tetrafluorobenzene	-139.7	294.4	-174.4
C ₆ HF ₅ (F-2,6)	-138.9	294.2	-174.2
C ₆ HF ₅ (F-3,5)	-162.3	318.3	-198.3
C ₆ HF ₅ (F-4)	-153.8	309.4	-189.4
C ₆ F ₆	-162.2	319.4	-199.4

(n) Miscellaneous compounds

Compound	δ_{exp}	σ	δ_{calc}
CH ₃ CF ₃	-64.5	215.3	-95.3
H ₃ SiCH ₂ F	-265.0	442.0	-322.0
H ₃ SiCHF ₂	-128.9	286.0	-166.0
H ₃ SiCF ₃	-55.2	205.2	-85.2
PhOCH ₂ F	-148.7	308.6	-188.6
PhOCHF ₂	-76.0	231.6	-111.6
PhOCF ₃	-58.3	210.9	-90.9
PhSCHF ₂	-90.0	244.5	-124.5
PhSCF ₃	-43.2	192.7	-72.7

Cartesian coordinates of fluoroalanine, steroid and taxol derivatives (ZORA scalar-BLYP/TZ2P level).

Fluoroalanine 1

F	-0.925887	-0.564071	2.440655
F	1.565887	-0.441317	3.519349
F	3.745163	0.063575	1.921463
F	3.402186	0.452675	-0.781801
F	0.906710	0.343150	-1.872694
C	-0.093232	-0.105384	0.247915
C	0.124546	-0.298494	1.617322
C	1.397755	-0.246307	2.189573
C	2.506816	0.009271	1.380777
C	2.330471	0.206962	0.009465
C	1.044265	0.147747	-0.528907
C	-1.475055	-0.171341	-0.371996
C	-2.100367	1.225353	-0.621247
C	-3.446883	1.072586	-1.352843
H	-1.416911	-0.700917	-1.328629
H	-2.145010	-0.746216	0.272618
H	-1.432713	1.821008	-1.251196
H	-2.553864	2.922633	0.484806
H	-2.995593	1.515518	1.228846
H	-4.606208	2.035783	-2.515125
O	-3.706931	2.167095	-2.146793
O	-4.231209	0.153187	-1.216919
N	-2.274993	1.955248	0.651978

Fluoroalanine 2

F	-0.981198	-0.559355	2.430265
F	1.482488	-0.463826	3.515949
F	3.346797	0.430339	-0.788695
F	0.872545	0.345135	-1.870982
C	1.003833	0.144971	-0.526527
C	-0.139666	-0.101041	0.242473
C	0.074670	-0.299223	1.610963
C	1.347384	-0.259414	2.184286
C	2.475248	-0.012030	1.392255
C	2.286774	0.190528	0.019348
C	-1.518402	-0.161028	-0.383725
C	-2.140930	1.236370	-0.634141
N	-2.324496	1.963532	0.639084
Cl	4.069201	0.040136	2.093478
C	-3.482494	1.086365	-1.376920
O	-4.261768	0.159882	-1.261886
O	-3.744419	2.192678	-2.153745
H	-1.457316	-0.688830	-1.341027
H	-2.192748	-0.735814	0.256575
H	-1.468959	1.833167	-1.258639
H	-2.605069	2.930445	0.471820
H	-3.047722	1.521389	1.210912
H	-4.640660	2.062325	-2.529793

Fluoroalanine 3

F	-1.069395	-0.565158	2.416682
F	1.379303	-0.481576	3.526540
F	3.289856	0.412640	-0.766447
F	0.827391	0.339503	-1.866470
C	0.946443	0.136636	-0.520693
C	-0.205065	-0.105146	0.237904
C	-0.004305	-0.307441	1.607838
C	1.263765	-0.273890	2.192677
C	2.396831	-0.029778	1.410111
C	2.224774	0.175420	0.037107
C	-1.578088	-0.154578	-0.400614
C	-2.187181	1.247594	-0.656863
C	-3.520092	1.107801	-1.416544
Br	4.137442	0.021082	2.195717
N	-2.382545	1.973864	0.614942
O	-4.316660	0.196822	-1.296006
O	-3.752145	2.203395	-2.217656
H	-1.512452	-0.682948	-1.357349
H	-2.262744	-0.723876	0.233771
H	-1.502738	1.840456	-1.271273
H	-2.653978	2.943106	0.446309
H	-3.115693	1.535216	1.176641
H	-4.644744	2.080198	-2.604705

Fluoroalanine 4

F	-1.174342	-0.548573	2.382213
F	1.263993	-0.477414	3.508661
F	3.210163	0.394582	-0.774731
F	0.757970	0.335921	-1.888953
C	0.866329	0.135075	-0.541687
C	-0.292558	-0.097641	0.208762
C	-0.101852	-0.297732	1.580547
C	1.164003	-0.270860	2.171201
C	2.306637	-0.036145	1.401158
C	2.139853	0.166829	0.028095
C	-1.660756	-0.145253	-0.439764
C	-2.268700	1.257428	-0.696707
C	-3.595444	1.119219	-1.467340
I	4.229236	0.005893	2.284200
N	-2.475117	1.978922	0.575927
O	-4.391129	0.205924	-1.358270
O	-3.823532	2.218885	-2.263935
H	-1.588204	-0.671628	-1.396863
H	-2.350333	-0.714993	0.188979
H	-1.580092	1.853286	-1.303577
H	-2.746131	2.948525	0.408710
H	-3.211889	1.537475	1.130629
H	-4.712904	2.096223	-2.658553

Fluoroalanine 5

F	-0.925420	-0.561160	2.419883
F	1.540211	-0.470690	3.530643
F	3.454119	0.427606	-0.728685
F	0.963382	0.354014	-1.868807
C	1.076412	0.148940	-0.522087
C	-0.073005	-0.097735	0.238024
C	0.137259	-0.298980	1.608029
C	1.402469	-0.263362	2.195889
C	2.539250	-0.016283	1.415521
C	2.346367	0.187698	0.043778
C	-1.449556	-0.150707	-0.394226
C	-2.082149	1.247747	-0.613872
C	-3.423763	1.105018	-1.356892
N	-2.270992	1.947374	0.674023
O	3.777187	0.016993	2.000353
O	-4.224592	0.200818	-1.213606
O	-3.660041	2.190071	-2.172406
H	-1.383432	-0.654205	-1.364697
H	-2.122954	-0.746364	0.227950
H	-1.414275	1.861908	-1.225576
H	-2.562792	2.914262	0.527620
H	-2.985792	1.483816	1.239063
H	-4.557257	2.063616	-2.547605
H	4.437622	0.192638	1.304671

Fluoroalanine 6

F	-0.926422	-0.564027	2.426926
F	1.549731	-0.445600	3.533490
F	3.438010	0.459335	-0.738905
F	0.961335	0.354212	-1.862067
C	1.076307	0.145027	-0.514645
C	-0.077137	-0.106850	0.239023
C	0.134585	-0.304133	1.609237
C	1.401239	-0.257512	2.184191
C	2.553012	-0.004956	1.422246
C	2.347376	0.195133	0.047760
C	-1.452743	-0.158481	-0.393559
C	-2.081308	1.241906	-0.617955
C	-3.423269	1.104364	-1.360776
N	-2.270489	1.944956	0.668411
N	3.827378	-0.008258	1.985615
O	-4.235545	0.212027	-1.207241
O	-3.646869	2.181161	-2.192076
H	-1.389859	-0.665797	-1.362314
H	-2.129272	-0.748194	0.231185
H	-1.410116	1.852111	-1.229694
H	-2.567483	2.909967	0.519236
H	-2.983392	1.480139	1.234940
H	-4.545195	2.059032	-2.566008
H	4.534354	0.490258	1.456963
H	3.858208	0.170315	2.983125

Fluoroalanine 7

F	-0.923480	-0.573830	2.476380
F	1.557489	-0.466204	3.538439
F	3.373418	0.446860	-0.779044
F	0.894856	0.352539	-1.838256
C	1.033171	0.148868	-0.493309
C	-0.106399	-0.103862	0.280013
C	0.122765	-0.304486	1.646612
C	1.401096	-0.258240	2.200976
C	2.534624	-0.004814	1.417070
C	2.315056	0.197871	0.048217
C	-1.487058	-0.166223	-0.340416
C	-2.105222	1.231113	-0.604712
C	-3.422902	1.083031	-1.387953
N	-2.328030	1.951529	0.665899
S	4.139004	0.039441	2.184784
O	-4.224066	0.175646	-1.269396
O	-3.636673	2.165907	-2.212100
H	-1.431276	-0.704963	-1.292110
H	-2.161875	-0.731658	0.307932
H	-1.415302	1.831092	-1.205789
H	-2.603954	2.919389	0.496307
H	-3.067809	1.505005	1.212520
H	-4.520575	2.036043	-2.616539
H	4.805860	0.288906	1.036023

Steroid 8

F	1.404566	0.221890	1.949859
F	-1.692736	1.550847	-0.753336
F	-10.619420	1.989897	1.968436
C	0.307179	-0.291711	-0.146273
C	0.202786	-0.260267	1.361607
C	1.435785	0.049899	-0.798149
C	-0.957440	0.624243	1.836078
C	-2.300750	0.245714	1.158431
C	-2.141995	0.232281	-0.395109
C	-3.422968	1.229159	1.560625
C	-0.967906	-0.746368	-0.866000
C	-3.485299	0.124882	-1.197591
C	-1.228094	-2.256877	-0.497732
C	-0.815618	-0.697184	-2.372389
C	1.539129	0.042545	-2.272971
C	0.317115	-0.356848	-3.007930
H	2.326785	0.349582	-0.253177
H	0.085544	-1.281631	1.750235
H	-1.046301	0.534715	2.925103
H	-0.705622	1.665125	1.600104
H	-2.580111	-0.768383	1.473607
H	-1.686427	-1.019738	-2.940838
H	0.391605	-0.373127	-4.093323
C	-4.793857	0.888942	0.907398
C	-3.746116	1.429724	3.057698
H	-3.132659	2.207512	1.161538
H	-3.250237	0.512172	-2.198657
O	-3.867675	-1.272063	-1.316543
C	-5.697135	2.029494	1.596519
C	-4.628658	1.010166	-0.624532
C	-5.326110	-0.516365	1.311585
H	-5.556371	0.749446	-1.155777
H	-4.404270	2.051051	-0.878220
H	-0.315035	-2.824848	-0.709729
H	-1.474958	-2.389254	0.560691
H	-2.048954	-2.662089	-1.090156
H	-4.754078	-1.292758	-1.717111
C	-5.224208	1.973324	3.100822
H	-3.671268	0.489343	3.619487
H	-3.059442	2.142099	3.527807
C	-7.193485	1.751241	1.293167
O	-5.268285	3.264469	0.950457
H	-5.843606	1.215055	3.592216
C	-5.356817	3.269363	3.919245
H	-6.292828	-0.717593	0.832681
H	-4.641662	-1.299010	0.976897
H	-5.464366	-0.623847	2.392620
H	-6.397059	3.597859	4.013651
H	-4.975910	3.093746	4.933000
H	-4.767551	4.082792	3.480507
S	-8.198644	1.076278	2.699411
O	2.587319	0.341284	-2.860219
O	-7.671561	1.911386	0.191307
C	-9.791527	0.859180	1.837491
H	-9.597758	0.700297	0.773696
H	-10.301737	0.012081	2.304344
C	-5.893439	4.507258	0.820331
O	-5.305322	5.320178	0.142499
C	-7.208841	4.836383	1.524707
C	-8.252660	5.417380	0.545243
H	-7.628063	3.989523	2.071498
H	-6.948511	5.599227	2.271706
H	-9.141026	5.742889	1.098179
H	-7.835013	6.275723	0.009754
H	-8.561804	4.664930	-0.189122

Steroid 9

F	-7.201237	1.311770	1.659137
F	-5.868039	2.981565	1.074238
C	1.592255	-0.591737	-0.680869
C	0.260867	-0.128425	-0.098563
C	-1.004082	-0.415001	-0.936239
C	-0.717627	0.007530	-2.422000
C	0.613081	-0.518347	-3.007215
C	1.807059	-0.110435	-2.131672
C	0.225375	0.504573	1.085321
C	-1.023149	0.991244	1.775470
C	-2.320261	0.424052	1.158753
C	-2.220531	0.441445	-0.400994
C	-3.549952	1.236340	1.608735
C	-4.895746	0.752668	0.981004
C	-4.792154	0.890801	-0.553867
C	-3.573795	0.092328	-1.092059
C	-5.867660	1.723864	1.702329
C	-5.351134	1.876613	3.153520
C	-3.863979	1.388834	3.122970
C	-5.288855	-0.698312	1.384523
C	-1.311209	-1.944906	-0.880180
O	3.073551	-0.568472	-2.670483
H	1.167064	0.692717	1.605863
H	-1.987965	1.486010	-0.668675
H	-3.779982	-0.979057	-0.984573
H	-5.445893	2.924658	3.453463
H	-0.972481	0.737389	2.844643
H	-1.050822	2.094492	1.738524
H	-2.428322	-0.616085	1.500274
H	-3.397362	2.257145	1.220073
H	-3.490806	0.279287	-2.170096
H	-5.709758	0.533246	-1.041818
H	-4.683717	1.951399	-0.813212
H	-0.424666	-2.540552	-1.123865
H	-1.637507	-2.246787	0.122366
H	-2.094792	-2.221781	-1.596119
H	-3.760913	0.428304	3.643783
H	-3.192374	2.099093	3.616790
H	-5.974857	1.278278	3.824502
H	-6.249016	-0.963522	0.926631
H	-4.540437	-1.422133	1.048318
H	-5.398098	-0.816981	2.469027
H	3.049164	-1.541964	-2.705231
H	-1.546103	-0.324491	-3.060470
H	-0.704876	1.106790	-2.469636
H	0.591321	-1.617188	-3.088800
H	0.753880	-0.128486	-4.024171
H	1.640043	-1.694534	-0.689028
H	2.420371	-0.244836	-0.051936
H	1.902136	0.983646	-2.134947

Taxol 10 (8)

F	11.619571	6.683936	0.724989
F	9.719745	7.470105	5.010074
C	5.725287	5.413313	4.074724
C	6.996909	4.944032	3.292890
C	6.650287	3.873671	2.160091
C	5.540863	4.565390	1.242185
C	4.194518	4.737393	1.976044
C	4.318908	5.320016	3.388493
C	8.205017	4.553149	4.249780
C	7.973644	3.873164	6.576386
C	7.830546	4.391283	7.972697
C	7.913045	3.462115	9.026447
C	7.796947	3.887916	10.350420
C	7.596009	5.244719	10.635662
C	7.511573	6.174118	9.591909
C	7.628583	5.753412	8.264280
C	7.855384	3.652244	1.171802
C	6.186223	2.492598	2.674563
C	4.647291	6.084614	-1.668192
C	5.103391	4.521045	5.174992
C	5.919371	7.854570	3.845410
C	6.109628	9.124019	4.657237
C	8.700382	4.865555	0.865236
C	9.789887	5.294648	1.523983
C	10.306621	6.717325	1.288936
C	10.431138	7.417904	2.700654
C	9.522731	6.800466	3.785041
C	9.647874	5.226977	3.996489
C	10.416978	4.592079	2.754718
C	9.496635	7.629568	0.360160
C	10.345957	3.040509	2.751211
C	11.946758	4.895112	2.875533
C	5.461020	3.284420	-2.767685
C	2.704763	3.698054	-1.233327
C	5.784436	1.782629	-2.549316
C	2.391745	2.252614	-0.765309
C	3.928368	6.601980	-2.942813
Si	4.542605	4.198556	-1.376595
O	7.874721	4.888421	5.638932
O	5.372026	3.810294	0.042557
O	8.032074	2.591216	0.600303
O	3.848625	4.391450	4.431599
O	5.964432	6.754661	4.658057
O	10.454244	4.964797	5.139999
O	11.104861	8.407365	2.879588
O	8.135601	2.700294	6.290251
O	5.760924	7.814451	2.634930
H	5.921566	5.567125	0.993296
H	10.216514	5.607559	5.833198
H	8.499475	7.041892	3.472570
H	7.290845	5.831897	2.729773
H	8.355302	3.475331	4.231106
H	3.777380	6.267997	3.472944
H	3.699012	3.763540	2.051581
H	3.553735	5.382874	1.364402
H	9.348385	2.611114	2.690007
H	10.809672	2.667367	3.670530
H	10.913047	2.655790	1.896313
H	8.480359	7.806568	0.728073
H	9.446845	7.191398	-0.642133
H	8.282770	5.474313	0.063172
H	10.019778	8.588350	0.295239
H	12.355353	4.322305	3.710720
H	12.195674	5.943848	3.054645
H	12.446628	4.590683	1.950932
H	5.994701	1.836231	1.822244
H	5.272791	2.564741	3.271186
H	6.958815	2.016999	3.289140
H	7.561427	6.472007	7.454384
H	7.356296	7.227289	9.812644
H	7.506559	5.576344	11.667560
H	7.864194	3.164827	11.159473
H	8.071473	2.415003	8.787466
H	5.984830	9.990743	4.005694
H	7.113460	9.136730	5.098864
H	5.386726	9.161484	5.479705
H	5.567666	3.543925	5.336639

H	4.967198	5.043444	6.128623
H	6.402498	3.831936	-2.938910
H	4.241426	6.609188	-0.788984
H	5.712544	6.364040	-1.714237
H	2.215998	4.413644	-0.552023
H	4.874870	3.409136	-3.693328
H	2.239690	3.871900	-2.217986
H	6.353315	1.377941	-3.396903
H	6.382677	1.635732	-1.643361
H	4.872763	1.180806	-2.450830
H	1.310151	2.095015	-0.659839
H	2.763152	1.507783	-1.479143
H	2.854911	2.033738	0.204429
H	2.851642	6.390779	-2.910452
H	4.045462	7.687978	-3.055261
H	4.328789	6.133291	-3.851302

Taxol 11 (9)

F	10.717258	7.221104	4.972264
Si	4.691196	4.176198	-1.415269
C	10.383932	4.777975	2.737469
C	9.534289	5.416999	1.616484
C	9.354628	6.775292	1.611907
C	9.616232	7.536272	2.852580
C	9.610909	6.744166	4.196792
C	9.686323	5.185715	4.095828
C	8.857061	4.514770	0.616940
C	7.859466	3.461250	1.237807
C	8.779277	7.587313	0.467558
C	7.987175	3.780743	6.572930
C	8.237537	4.525175	4.272644
C	10.575927	3.238810	2.655581
C	11.834566	5.363478	2.675930
C	7.064351	4.967980	3.290262
C	5.805939	5.532535	4.036253
C	4.411740	5.488752	3.321332
C	4.287976	4.900505	1.909637
C	5.637310	4.606314	1.218968
C	6.669662	3.882484	2.186013
C	5.110441	4.721263	5.155653
C	6.074081	7.952054	3.701883
C	6.075108	2.579444	2.775205
C	2.796879	3.962603	-1.288969
C	2.256172	2.618759	-0.734448
C	7.847010	4.267858	7.981096
C	7.899344	3.311778	9.012146
C	7.789794	3.707730	10.346175
C	7.626293	5.062084	10.664728
C	7.572222	6.018610	9.643679
C	7.682706	5.626765	8.306716
C	6.400485	9.250146	4.416060
C	5.069648	5.993182	-1.870937
C	4.468379	6.485686	-3.214296
C	5.488827	3.011514	-2.690342
C	5.593638	1.508706	-2.318278
O	7.978977	2.304239	0.885819
O	9.669805	8.764270	2.911847
O	7.867737	4.811064	5.657111
O	8.151829	2.614896	6.262171
O	10.453876	4.662564	5.190275
O	3.881412	4.596447	4.368786
O	6.124292	6.881973	4.562197
O	5.817297	7.863681	2.512159
O	5.448962	3.804966	0.046316
H	6.088809	5.566664	0.932330
H	10.952403	5.406105	5.576810
H	8.722634	7.048160	4.759359
H	7.413013	5.825810	2.719640
H	8.380817	3.445998	4.207645
H	3.907106	6.457063	3.386066
H	3.711982	3.971548	1.980458
H	3.722000	5.590116	1.272950
H	9.660601	2.651611	2.730824
H	11.226897	2.931404	3.479205
H	11.067067	2.964719	1.714566
H	7.722763	7.834780	0.634747
H	8.874638	7.072971	-0.491975
H	8.281658	5.098040	-0.109080
H	9.317660	8.539120	0.407313
H	12.450028	4.912392	3.461644
H	11.871203	6.450965	2.784485
H	12.282021	5.112603	1.705694
H	5.802144	1.900727	1.964245
H	5.183838	2.778149	3.374730
H	6.807071	2.060184	3.403280
H	7.643132	6.367356	7.515335
H	7.446955	7.070282	9.889682
H	7.542565	5.370766	11.704269
H	7.833375	2.963158	11.137257
H	8.030366	2.266906	8.747875
H	5.773416	10.046237	4.004819
H	7.447424	9.506103	4.205168
H	6.261319	9.170785	5.496932
H	5.526712	3.738376	5.389526
H	4.958289	5.300612	6.073618

H	6.500113	3.402881	-2.889868
H	4.718100	6.647263	-1.057484
H	6.164637	6.115672	-1.897778
H	2.408172	4.791717	-0.675566
H	4.937557	3.123359	-3.638636
H	2.384837	4.132316	-2.297811
H	6.109051	0.944257	-3.106784
H	6.153262	1.370700	-1.386372
H	4.604860	1.053457	-2.184161
H	1.161323	2.635804	-0.651721
H	2.522034	1.777248	-1.385235
H	2.659749	2.400734	0.261635
H	3.372069	6.431713	-3.207777
H	4.743056	7.529339	-3.417101
H	4.822734	5.882984	-4.060906
H	9.572372	3.900268	0.060864

Taxol 12 (3a)

F	6.402237	5.868634	0.230502
C	10.560089	7.040820	1.699864
C	10.112107	5.577187	1.665345
C	10.623652	4.729030	2.846233
C	9.779537	5.197023	4.094109
C	9.828362	6.752269	4.243455
C	9.931989	7.647517	2.992300
C	9.163416	5.189414	0.800376
C	8.252754	3.998009	0.851953
O	8.317459	3.070261	0.062083
C	10.534965	3.195842	2.620372
C	12.145076	4.998223	3.101711
C	8.292840	4.609053	4.100175
O	7.826214	4.860446	5.480385
C	7.712537	3.774780	6.331498
O	7.777672	2.613534	5.969320
O	10.452268	4.607339	5.237866
H	10.737962	6.979133	4.819245
O	9.575925	8.814041	3.045782
C	10.256076	7.907168	0.467556
C	7.502507	4.206378	7.750434
C	7.482737	3.207668	8.741680
C	7.315376	3.552208	10.083772
C	7.160024	4.895647	10.449127
C	7.170144	5.893699	9.467201
C	7.342220	5.554797	8.122368
C	7.214296	5.124114	3.041320
C	6.991401	4.113916	1.828083
C	5.902135	4.670628	0.845607
C	4.530310	4.993668	1.440067
C	4.532265	5.508604	2.883868
C	5.867090	5.566356	3.712042
C	6.547092	2.684992	2.244098
O	3.974069	4.509115	3.815036
C	5.135254	4.616589	4.694359
O	6.078387	6.862171	4.383484
C	6.041566	8.017575	3.626633
O	5.821796	8.045940	2.431895
C	6.336019	9.235202	4.483022
H	8.842006	5.877789	0.019574
H	10.011156	4.927654	6.044048
H	8.988041	7.116702	4.843951
H	7.591860	6.042030	2.584019
H	8.389355	3.528289	4.021424
H	3.969651	6.442085	2.968174
H	3.906998	4.090605	1.423630
H	4.063197	5.722981	0.768167
H	5.799359	3.951387	0.025089
H	9.535146	2.819068	2.401806
H	10.888847	2.678415	3.517861
H	11.175152	2.912389	1.777015
H	9.180204	8.019498	0.300811
H	10.709773	7.466868	-0.427131
H	10.667619	8.909968	0.610697
H	12.526470	4.276864	3.827999
H	12.364151	5.995015	3.493355
H	12.696576	4.869510	2.162085
H	6.510662	2.043886	1.358555
H	5.557358	2.693799	2.711353
H	7.248075	2.230107	2.950704
H	7.343680	6.326171	7.359460
H	7.044221	6.935985	9.749559
H	7.030540	5.163677	11.495113
H	7.307409	2.776003	10.844826
H	7.605730	2.171763	8.440842
H	5.741070	10.076925	4.118148
H	7.396441	9.488169	4.352325
H	6.135923	9.053155	5.542160
H	5.583560	3.634247	4.864703
H	4.889288	5.097009	5.649104
H	11.645003	7.080482	1.872120

Taxol 13 (11)

F	10.749333	7.142010	5.287947
F	6.591018	5.834175	0.179182
C	7.464172	3.145742	8.720324
C	7.533413	4.156355	7.743467
C	7.401780	5.502436	8.131356
C	7.205538	5.828110	9.476171
C	7.139742	4.817700	10.443194
C	7.268608	3.475699	10.062421
C	7.770507	3.739735	6.326423
C	8.294205	4.598710	4.114893
C	7.253348	5.115668	3.018126
C	7.004200	4.083922	1.826795
C	5.982468	4.688885	0.804343
C	4.620668	5.123094	1.353050
C	4.605240	5.630397	2.799444
C	5.916337	5.628836	3.660197
C	8.251692	3.778687	0.873356
C	9.400472	4.797055	0.555185
C	9.929041	5.609961	1.703889
C	10.601224	4.855871	2.867617
C	9.768421	5.211664	4.157144
C	9.728500	6.760188	4.357814
C	9.911906	7.638075	3.083425
C	9.776003	6.968191	1.770749
C	10.703330	3.316606	2.687009
C	12.077553	5.349016	3.019963
C	9.344827	7.867212	0.628280
C	6.433947	2.717560	2.304390
C	6.206125	8.073917	3.565240
C	6.490137	9.288412	4.431198
C	5.114306	4.734922	4.638216
O	7.914463	2.585160	5.964396
O	6.175820	6.923344	4.324260
O	7.770065	4.820284	5.462118
O	10.382617	4.589019	5.297010
O	9.998943	8.855322	3.235410
O	3.980733	4.657214	3.715281
O	8.233640	2.749437	0.222240
O	6.045214	8.103276	2.359530
H	8.978637	5.443897	-0.219611
H	10.177992	4.181596	0.090228
H	10.853640	5.286897	5.789098
H	8.788605	7.057579	4.833595
H	7.657759	6.005340	2.539684
H	8.420716	3.521229	4.013233
H	4.081261	6.587895	2.870651
H	3.925463	4.275227	1.304731
H	4.242321	5.891961	0.669412
H	5.845745	3.964350	-0.006099
H	9.750720	2.806923	2.521061
H	11.145813	2.888648	3.591502
H	11.357186	3.073123	1.841525
H	8.263922	8.057248	0.654010
H	9.598015	7.444205	-0.347293
H	9.846578	8.834444	0.732591
H	12.575440	4.792016	3.821153
H	12.153609	6.418162	3.237861
H	12.619472	5.161989	2.084238
H	6.329251	2.039265	1.454256
H	5.454355	2.842017	2.773850
H	7.101337	2.238087	3.027624
H	7.455553	6.284563	7.381917
H	7.108200	6.870097	9.770885
H	6.991223	5.075057	11.489430
H	7.219798	2.689467	10.811773
H	7.571658	2.111199	8.408928
H	5.924387	10.139350	4.041893
H	7.558127	9.530619	4.348388
H	6.244776	9.111599	5.481341
H	5.512708	3.740310	4.852115
H	4.855700	5.250845	5.570125

Taxol 14 (12)

F	10.823911	7.085455	5.066956
C	10.391777	4.699921	2.771227
C	9.604278	5.419377	1.657606
C	9.493381	6.783057	1.679083
C	9.773949	7.500715	2.941219
C	9.708621	6.678377	4.264414
C	9.713477	5.119985	4.133722
C	8.930923	4.584025	0.600471
C	7.891618	3.507439	1.070828
O	7.836187	2.478491	0.420942
C	8.973352	7.641295	0.541669
O	9.897231	8.721053	3.031655
C	8.249888	4.509540	4.288931
O	7.835795	4.854866	5.648671
C	7.881410	3.851517	6.600224
O	8.006801	2.669684	6.332431
O	10.448054	4.544179	5.225677
C	10.460976	3.154673	2.641565
C	11.880949	5.178070	2.738968
C	7.119558	4.904759	3.239608
C	5.849757	5.517938	3.917970
C	4.523703	5.529163	3.100217
C	4.545010	4.886499	1.755242
C	5.551781	4.108467	1.347457
C	6.785442	3.748394	2.190602
C	5.052291	4.733946	4.985438
O	3.859772	4.685008	4.135098
O	6.183812	6.847988	4.475878
C	6.222418	7.940630	3.639725
O	6.052288	7.891119	2.434702
C	6.474651	2.363216	2.845342
H	5.489764	3.600860	0.385785
C	7.725088	4.391175	7.987182
C	7.734344	3.471955	9.052564
C	7.616082	3.919108	10.369598
C	7.485775	5.288097	10.636709
C	7.472573	6.207917	9.581172
C	7.592400	5.764911	8.261151
C	6.525117	9.211085	4.414703
H	10.984427	5.255983	5.621693
H	8.825943	7.009956	4.819836
H	7.480446	5.730760	2.629162
H	8.385544	3.429328	4.284617
H	4.042475	6.510599	3.073191
H	3.673332	5.028753	1.117654
H	9.492862	2.648430	2.625063
H	11.015431	2.758294	3.497688
H	10.996632	2.869803	1.728464
H	7.900670	7.847946	0.651243
H	9.146381	7.180078	-0.434483
H	8.376063	5.222416	-0.097596
H	9.488183	8.607009	0.567023
H	12.458066	4.648091	3.504474
H	11.991204	6.254148	2.900550
H	12.315266	4.943595	1.758826
H	6.245192	1.636583	2.062883
H	5.604217	2.446575	3.500574
H	7.318190	1.975586	3.425981
H	7.584228	6.476682	7.442953
H	7.372827	7.270805	9.787211
H	7.396677	5.636692	11.663135
H	7.628036	3.203071	11.187642
H	7.841060	2.414970	8.828525
H	5.917430	10.023805	4.006282
H	7.579549	9.471961	4.255082
H	6.339912	9.095938	5.485265
H	5.409921	3.730271	5.233156
H	4.880105	5.310544	5.901821
H	9.649766	4.007963	0.006703

Taxol 15 (13)

F	6.579568	5.905931	0.279782
F	9.180138	5.343229	-0.624868
C	7.449062	3.068130	8.697063
C	7.490399	4.102367	7.743633
C	7.336377	5.437450	8.163452
C	7.148909	5.728233	9.517455
C	7.116280	4.694737	10.461434
C	7.265600	3.364428	10.048585
C	7.720110	3.722839	6.313197
C	8.319705	4.641203	4.124655
C	7.256771	5.152991	3.052612
C	6.998354	4.117275	1.866125
C	5.980351	4.740177	0.849094
C	4.611601	5.137433	1.408702
C	4.602406	5.655171	2.852160
C	5.921034	5.661225	3.705042
C	8.237468	3.773500	0.919607
C	9.508150	4.705464	0.589620
C	9.950733	5.631061	1.681856
C	10.613696	4.904051	2.886570
C	9.774720	5.291899	4.151201
C	9.768853	6.831789	4.312351
C	9.856924	7.678522	3.027896
C	9.772865	6.984349	1.704039
C	10.739713	3.354553	2.760885
C	12.087407	5.414937	3.015673
C	9.374106	7.881724	0.545816
C	6.414819	2.757158	2.350910
C	6.186489	8.109626	3.610445
C	6.501148	9.320628	4.470260
C	5.125709	4.768191	4.691021
O	7.805939	2.576000	5.911152
O	6.186378	6.953392	4.366978
O	7.823534	4.837474	5.499894
O	10.475397	4.697975	5.275094
O	9.882138	8.904978	3.135608
O	3.986099	4.685159	3.779168
O	8.197734	2.752221	0.262949
O	5.978000	8.144115	2.413810
H	10.285843	3.979059	0.337189
H	10.058268	5.021780	6.092323
H	8.877127	7.166474	4.855839
H	10.630059	7.115425	4.928366
H	7.653193	6.044348	2.569772
H	8.454786	3.566182	4.014998
H	4.075883	6.610652	2.921256
H	3.938271	4.271612	1.372821
H	4.207259	5.892472	0.724540
H	5.853844	4.038264	0.016704
H	9.803479	2.823530	2.567272
H	11.141198	2.966108	3.700913
H	11.442297	3.087531	1.963431
H	8.284552	7.907200	0.421517
H	9.813459	7.555747	-0.395938
H	9.702508	8.899659	0.774297
H	12.590322	4.905273	3.843512
H	12.151938	6.494635	3.175351
H	12.626574	5.189787	2.087128
H	6.277540	2.084455	1.501021
H	5.447985	2.898120	2.840653
H	7.089058	2.264244	3.058584
H	7.356748	6.237188	7.430637
H	7.029239	6.760637	9.836391
H	6.974932	4.925028	11.514858
H	7.240573	2.560759	10.780211
H	7.568735	2.042913	8.360464
H	5.908047	10.168093	4.115327
H	7.561110	9.572006	4.332404
H	6.309945	9.135448	5.530266
H	5.524631	3.773749	4.905353
H	4.873295	5.288049	5.622914

Taxol 16 (14)

F	6.236747	5.686528	0.288509
F	8.892747	5.672804	-0.486874
F	10.479858	4.198586	-0.082160
C	7.319747	3.086096	8.682428
C	7.439843	4.115538	7.730406
C	7.356552	5.457572	8.148307
C	7.160260	5.759693	9.498460
C	7.048089	4.730418	10.440821
C	7.127140	3.393426	10.030160
C	7.674822	3.721813	6.304662
C	8.346337	4.610304	4.121929
C	7.292405	5.091250	3.029453
C	7.074572	4.019437	1.866594
C	5.895338	4.460746	0.926425
C	4.557394	4.648686	1.628238
C	4.622182	5.620589	2.820123
C	5.951920	5.624313	3.651457
C	8.275862	3.821968	0.841920
C	9.444946	4.903319	0.522603
C	9.963261	5.711333	1.685526
C	10.616122	4.910143	2.849099
C	9.796259	5.257481	4.143751
C	9.799113	6.790793	4.371058
C	9.940571	7.692300	3.133962
C	9.825791	7.066422	1.771644
C	10.714865	3.366706	2.663900
C	12.099289	5.391155	2.990053
C	9.467817	8.041476	0.665646
C	6.726914	2.591167	2.390715
C	6.296065	8.079589	3.475374
C	6.526308	9.314936	4.329190
C	5.119179	4.857078	4.709998
O	7.721173	2.571500	5.906838
O	6.208545	6.949943	4.263392
O	7.837826	4.829248	5.489466
O	10.509007	4.617113	5.234315
O	10.035280	8.907517	3.295084
O	3.874858	5.106685	3.980580
O	8.276419	2.849071	0.122795
O	6.219009	8.082139	2.262623
H	10.098927	4.904237	6.068683
H	8.891227	7.111859	4.896189
H	10.639684	7.040365	5.028534
H	7.687145	5.974317	2.529151
H	8.489263	3.535422	4.036806
H	4.271195	6.614714	2.541401
H	4.197888	3.677318	1.988414
H	3.831177	5.002858	0.886534
H	5.808350	3.714838	0.127990
H	9.768666	2.863793	2.446813
H	11.099382	2.938820	3.593907
H	11.406855	3.120024	1.855505
H	8.382161	8.095471	0.517816
H	9.930777	7.774625	-0.284189
H	9.807657	9.034767	0.972095
H	12.598028	4.833970	3.788758
H	12.183540	6.460587	3.204570
H	12.624373	5.201503	2.046760
H	6.423256	1.947998	1.560697
H	5.917366	2.625560	3.122900
H	7.585055	2.115909	2.872706
H	7.439044	6.255071	7.417538
H	7.095628	6.797478	9.815442
H	6.899883	4.969287	11.491344
H	7.040946	2.593120	10.760692
H	7.386512	2.055516	8.347790
H	5.968581	10.149212	3.894358
H	7.593644	9.569348	4.287959
H	6.232383	9.158879	5.369959
H	5.330770	3.783963	4.789615
H	5.108433	5.317386	5.701901

Taxol 17 (30a)

F	11.701953	6.697883	0.888008
F	9.881623	7.311343	5.147828
C	10.412495	4.522710	2.756225
C	9.820290	5.302320	1.559736
C	10.338186	6.740112	1.390709
C	10.437341	7.426078	2.823556
C	9.559502	6.728861	3.878987
C	9.668510	5.148756	4.013993
C	8.733705	4.909685	0.872767
C	7.874258	3.693368	1.115629
C	9.595877	7.607294	0.374720
C	8.203199	4.513477	4.249956
C	7.965574	3.902118	6.594720
C	10.246631	2.976783	2.702000
C	11.966363	4.692766	2.874001
C	7.010471	4.927299	3.276558
C	5.729645	5.383665	4.055633
C	4.321914	5.268318	3.376463
C	4.201781	4.706772	1.957178
C	5.548202	4.572676	1.216660
C	6.673096	3.878769	2.118037
C	5.124827	4.480546	5.157075
C	6.224695	2.481547	2.603530
C	5.867556	7.822887	3.804411
C	2.694774	3.642255	-1.220566
C	2.446722	2.182358	-0.758409
C	7.849325	4.466682	7.976629
C	7.912221	3.569001	9.058366
C	7.819168	4.039022	10.369264
C	7.661555	5.409528	10.613264
C	7.598013	6.307955	9.541307
C	7.692168	5.842733	8.226679
C	6.083233	9.103868	4.591261
C	4.532029	6.109880	-1.659011
C	3.753718	6.615522	-2.903068
C	5.430921	3.361996	-2.817384
C	5.798199	1.864833	-2.641452
Si	4.509441	4.217368	-1.390685
O	10.031351	8.810620	2.818018
O	7.870477	4.887535	5.629643
O	8.028584	2.663736	0.482676
O	8.100484	2.716743	6.346161
O	10.462732	4.808792	5.151512
O	3.877290	4.315066	4.408594
O	5.954976	6.731344	4.627863
O	5.657852	7.767649	2.603302
O	5.383530	3.839533	0.002022
H	5.912291	5.584456	0.986399
H	10.323467	5.498283	5.826617
H	8.524106	7.025858	3.698218
H	7.317588	5.826283	2.738585
H	8.319450	3.431702	4.254091
H	3.761017	6.202795	3.479933
H	3.724878	3.722636	2.018209
H	3.547368	5.350533	1.358513
H	9.225914	2.607759	2.642427
H	10.693791	2.549516	3.605757
H	10.780961	2.583408	1.830189
H	8.569822	7.824080	0.685723
H	9.591597	7.109720	-0.599714
H	8.319330	5.556163	0.099765
H	10.120558	8.559546	0.269061
H	12.333260	4.033739	3.663725
H	12.309113	5.698445	3.108422
H	12.425487	4.399895	1.924153
H	6.021246	1.847554	1.737008
H	5.322192	2.533880	3.218874
H	7.009143	1.992493	3.192020
H	7.643516	6.537083	7.394648
H	7.476958	7.371924	9.729737
H	7.590033	5.775692	11.634914
H	7.870615	3.339764	11.200216
H	8.036770	2.510608	8.850826
H	5.819081	9.957809	3.964585
H	7.138695	9.182494	4.879552
H	5.484629	9.101146	5.508214
H	5.611638	3.515736	5.325298

H	4.970871	5.004246	6.107610
H	6.354445	3.939551	-2.987614
H	4.134581	6.606675	-0.760189
H	5.583845	6.430633	-1.733190
H	2.189575	4.332768	-0.525580
H	4.827594	3.493383	-3.731095
H	2.206656	3.804364	-2.196086
H	6.367952	1.497495	-3.505474
H	6.410681	1.712084	-1.746124
H	4.904472	1.235671	-2.548615
H	1.373924	1.981092	-0.637351
H	2.836402	1.457407	-1.482919
H	2.933311	1.976013	0.202534
H	2.687299	6.362675	-2.840104
H	3.825709	7.706679	-3.003910
H	4.142304	6.174372	-3.830403
H	11.482619	7.361404	3.134088
H	10.818214	9.360848	2.672333

Taxol 18 (30b)

F	11.634318	6.694433	0.813656
F	9.737407	7.461019	5.007925
C	7.693568	5.808792	8.245325
C	7.898129	4.442062	7.978526
C	8.011926	3.537143	9.050073
C	7.923923	3.991170	10.366982
C	7.719931	5.352456	10.627480
C	7.604393	6.257973	9.565847
C	8.011892	3.894556	6.589487
O	8.167679	2.715296	6.326641
O	7.895154	4.889583	5.635235
C	8.213479	4.531160	4.245885
C	6.987403	4.900641	3.296915
C	5.713455	5.329801	4.098715
C	4.299270	5.202968	3.436627
C	4.168248	4.642252	2.017919
C	5.506132	4.512123	1.261020
C	6.652576	3.838436	2.151085
C	5.136290	4.410950	5.201199
O	3.877324	4.243361	4.472684
O	5.921394	6.676229	4.687197
C	5.825165	7.778032	3.884356
C	5.981784	9.047669	4.705280
O	5.319294	3.763467	0.060108
Si	4.597413	4.215968	-1.396078
C	5.429717	3.147812	-2.730102
C	5.562495	1.627620	-2.449087
C	7.840291	3.672106	1.129667
O	7.997355	2.643768	0.495251
C	6.233404	2.437157	2.648868
C	8.674443	4.900415	0.854647
C	9.768450	5.322153	1.512253
C	10.395193	4.580791	2.719881
C	9.652004	5.220878	3.972129
C	9.462021	6.782649	3.763979
C	10.257783	7.549187	2.665456
C	10.285102	6.752467	1.275469
C	10.260768	3.030942	2.694126
C	11.942046	4.797984	2.819216
C	9.555451	7.569989	0.204002
H	9.688312	8.475166	2.484059
O	10.475670	4.956336	5.106881
O	5.645210	7.745725	2.676868
C	2.703573	3.973205	-1.316276
C	2.175486	2.589731	-0.854770
C	4.957362	6.064519	-1.724647
C	4.375105	6.631792	-3.046813
H	5.858962	5.524340	1.015070
H	10.217647	5.570835	5.817009
H	8.407002	6.988594	3.581632
H	7.255688	5.800436	2.740414
H	8.369242	3.454858	4.246599
H	3.730123	6.132013	3.548114
H	3.697536	3.655364	2.083057
H	3.503977	5.281602	1.424899
H	9.249526	2.633351	2.646576
H	10.726230	2.629409	3.600601
H	10.800251	2.637179	1.825881
H	8.514494	7.773551	0.475979
H	9.585033	7.055323	-0.761032
H	8.247100	5.516954	0.063980
H	10.077173	8.526834	0.096849
H	12.326798	4.188497	3.640692
H	12.241319	5.829540	2.989219
H	12.402257	4.458180	1.885203
H	6.043777	1.791085	1.788249
H	5.328822	2.475600	3.262293
H	7.028002	1.971337	3.242728
H	7.601810	6.508190	7.421133
H	7.445915	7.314624	9.767248
H	7.652242	5.706074	11.653764
H	8.015321	3.286463	11.189789
H	8.171508	2.486039	8.830022
H	5.865488	9.915386	4.053373
H	6.969845	9.068594	5.180202
H	5.232286	9.075322	5.504334
H	5.635669	3.449320	5.350512

H	4.994376	4.922959	6.159865
H	6.435010	3.569028	-2.893509
H	4.578928	6.661036	-0.879528
H	6.050865	6.203283	-1.721895
H	2.294272	4.756596	-0.657271
H	4.883879	3.306943	-3.674960
H	2.302658	4.200636	-2.318117
H	6.089861	1.122996	-3.269484
H	6.126410	1.447361	-1.527401
H	4.582859	1.145356	-2.344362
H	1.079304	2.584675	-0.788419
H	2.464689	1.794616	-1.552256
H	2.568378	2.316634	0.132040
H	3.279888	6.560644	-3.066750
H	4.636238	7.690368	-3.178109
H	4.756401	6.089205	-3.921787
O	11.578928	7.911471	3.069907
H	11.523078	8.155530	4.012434

Taxol 19 (31)

F	6.630218	5.849720	0.245340
F	9.159799	5.103162	-0.583232
C	9.733802	6.900830	1.621362
C	9.952481	5.554395	1.690630
C	10.681147	4.976369	2.944408
C	9.786420	5.384298	4.166945
C	9.722384	6.928840	4.237970
C	9.811176	7.688835	2.898644
C	9.490194	4.534568	0.680232
C	8.288002	3.608028	1.136303
O	7.933224	2.825407	-0.021492
C	10.993210	3.448060	2.955689
C	12.100353	5.637718	3.036724
C	8.347466	4.679810	4.129249
O	7.844539	4.829202	5.508586
C	7.762408	3.691896	6.290172
O	7.895190	2.558827	5.860641
O	10.478802	4.875371	5.334670
O	9.820782	8.919232	2.920661
C	9.293660	7.721199	0.422945
C	7.491225	4.023959	7.725164
C	7.458039	2.962157	8.648085
C	7.236296	3.214341	10.002820
C	7.041423	4.527757	10.449450
C	7.066044	5.588423	9.535796
C	7.290493	5.341782	8.178592
C	7.256527	5.169091	3.072122
C	6.968172	4.112711	1.906045
C	5.985561	4.738944	0.883678
C	4.635263	5.231548	1.426688
C	4.626187	5.730183	2.875595
C	5.940384	5.708977	3.732660
C	6.317730	2.792211	2.431172
O	3.990420	4.764125	3.796529
C	5.123278	4.834584	4.717308
O	6.230410	7.001321	4.389207
C	6.238152	8.153348	3.627177
O	6.028241	8.185501	2.430374
C	6.565916	9.368260	4.477077
H	10.296798	3.829246	0.446652
H	9.997894	5.183019	6.122847
H	8.807634	7.264009	4.740697
H	10.560061	7.279596	4.851201
H	7.650961	6.043641	2.557708
H	8.520123	3.612365	4.001949
H	4.111770	6.691706	2.952691
H	3.898107	4.420531	1.364184
H	4.299663	6.024611	0.748961
H	5.807002	4.013555	0.082956
H	10.125208	2.791289	3.026812
H	11.611979	3.236418	3.831435
H	11.568930	3.162447	2.068083
H	8.200563	7.795727	0.374362
H	9.648858	7.303039	-0.516776
H	9.682159	8.736566	0.548872
H	12.611360	5.301779	3.944409
H	12.073944	6.729715	3.030046
H	12.693238	5.324716	2.168076
H	6.248764	2.067693	1.612997
H	5.310862	2.955944	2.825280
H	6.924487	2.343829	3.226066
H	7.304094	6.162565	7.469140
H	6.910967	6.607622	9.880866
H	6.870818	4.723824	11.505452
H	7.217170	2.389597	10.710800
H	7.613721	1.950779	8.285405
H	5.936082	10.202684	4.155162
H	7.610653	9.645854	4.284653
H	6.431058	9.177301	5.544561
H	5.504891	3.835268	4.940708
H	4.871258	5.363074	5.644839
H	7.910573	3.439665	-0.779121
H	8.740869	2.884369	1.814689

Taxol 20 (32)

F	6.529810	5.995187	0.258531
F	9.035300	5.323013	-0.590671
F	10.413395	3.764433	0.117595
C	9.727730	6.946106	1.566727
C	9.940359	5.594921	1.621667
C	10.669393	5.012146	2.876921
C	9.759162	5.403675	4.098306
C	9.679977	6.946338	4.186126
C	9.809980	7.719991	2.863376
C	9.391070	4.652660	0.564254
C	8.137606	3.697688	0.913924
O	8.588978	2.426859	1.390090
C	11.004196	3.492851	2.910688
C	12.075092	5.701713	2.980804
C	8.329866	4.678270	4.044997
O	7.830022	4.787726	5.430108
C	7.756956	3.632290	6.186857
O	7.878847	2.509793	5.730989
O	10.449796	4.902327	5.268873
O	9.860796	8.947233	2.895575
C	9.314446	7.801139	0.382460
C	7.506945	3.935269	7.633292
C	7.483973	2.854389	8.533936
C	7.280926	3.077923	9.896678
C	7.094433	4.381670	10.374044
C	7.109468	5.461456	9.483015
C	7.315674	5.243282	8.117994
C	7.230053	5.200131	3.013764
C	6.899914	4.173833	1.829484
C	5.896421	4.857518	0.852161
C	4.557734	5.324541	1.435410
C	4.596021	5.815980	2.886971
C	5.931522	5.750388	3.708500
C	6.204679	2.871147	2.335583
O	3.953636	4.866303	3.817287
C	5.120338	4.876917	4.699650
O	6.250298	7.027280	4.383040
C	6.256513	8.194020	3.644103
O	6.041675	8.250701	2.449254
C	6.581910	9.392662	4.518381
H	9.943783	5.181684	6.051799
H	8.749859	7.271409	4.666168
H	10.497515	7.294540	4.827091
H	7.628928	6.079883	2.510447
H	8.511723	3.618398	3.873739
H	4.113866	6.792516	2.978405
H	3.832483	4.502249	1.392010
H	4.189508	6.115578	0.772495
H	5.702956	4.172296	0.016332
H	10.134477	2.840319	2.879904
H	11.540748	3.294939	3.842120
H	11.662425	3.232117	2.077488
H	8.234129	7.751327	0.205397
H	9.823593	7.502101	-0.533520
H	9.564999	8.838976	0.617904
H	12.586547	5.360534	3.886061
H	12.037876	6.794131	2.991067
H	12.673404	5.406088	2.110724
H	6.045363	2.176699	1.502943
H	5.231153	3.095725	2.777893
H	6.816796	2.351985	3.075660
H	7.322047	6.079562	7.426698
H	6.961394	6.473420	9.851784
H	6.938083	4.555447	11.436166
H	7.270117	2.238229	10.587065
H	7.633183	1.850827	8.147631
H	5.924769	10.220513	4.235732
H	7.613884	9.700699	4.306811
H	6.478882	9.171083	5.583345
H	5.477587	3.860987	4.883269
H	4.916426	5.387814	5.647975
H	9.351604	2.172457	0.839985
H	7.712935	3.558478	-0.092538