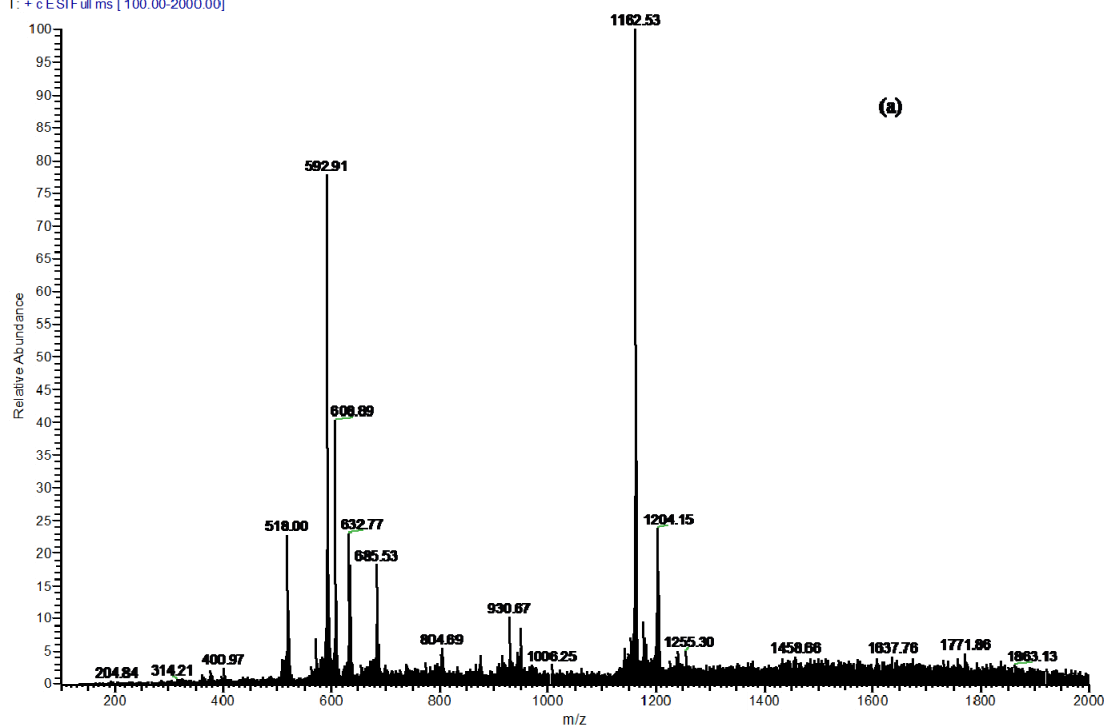
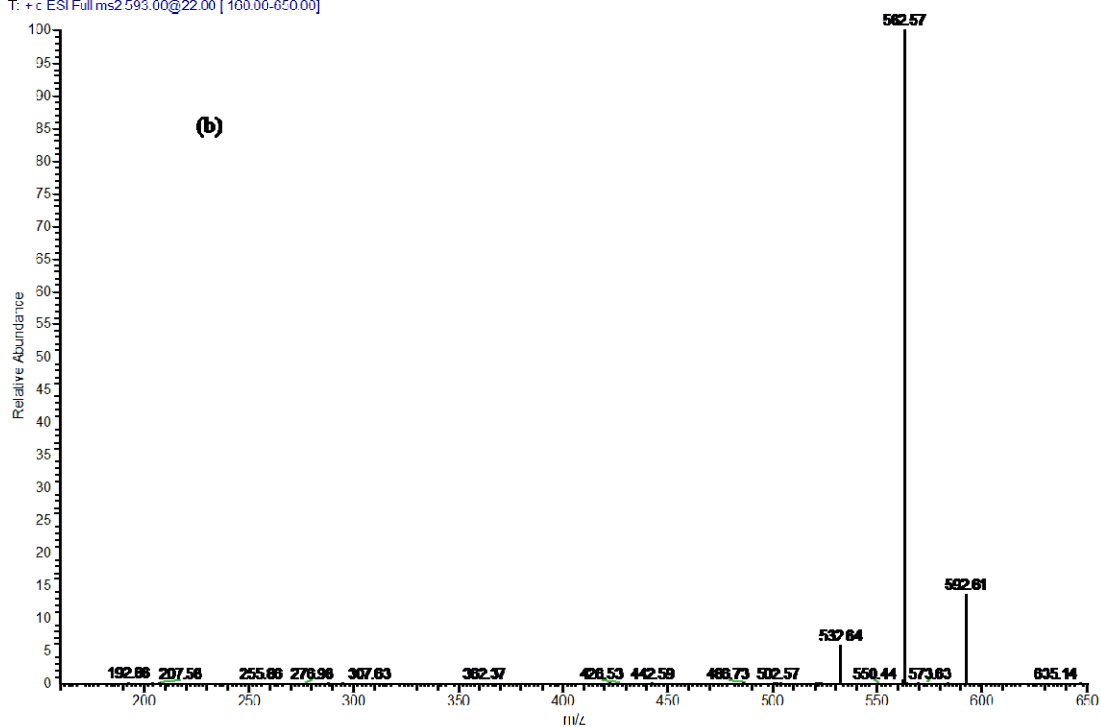


+ full ms1 DNICs sample 2 #1-85 RT: 0.02-2.97 AV: 85 NL: 5.18E5
T: + c ESI Full ms [100.00-2000.00]



+ full ms2_593 DNICs sample 2 #1-81 RT: 0.01-3.00 AV: 81 NL: 3.48E5
T: + c ESI Full ms2_593.00@22.00 [160.00-650.00]



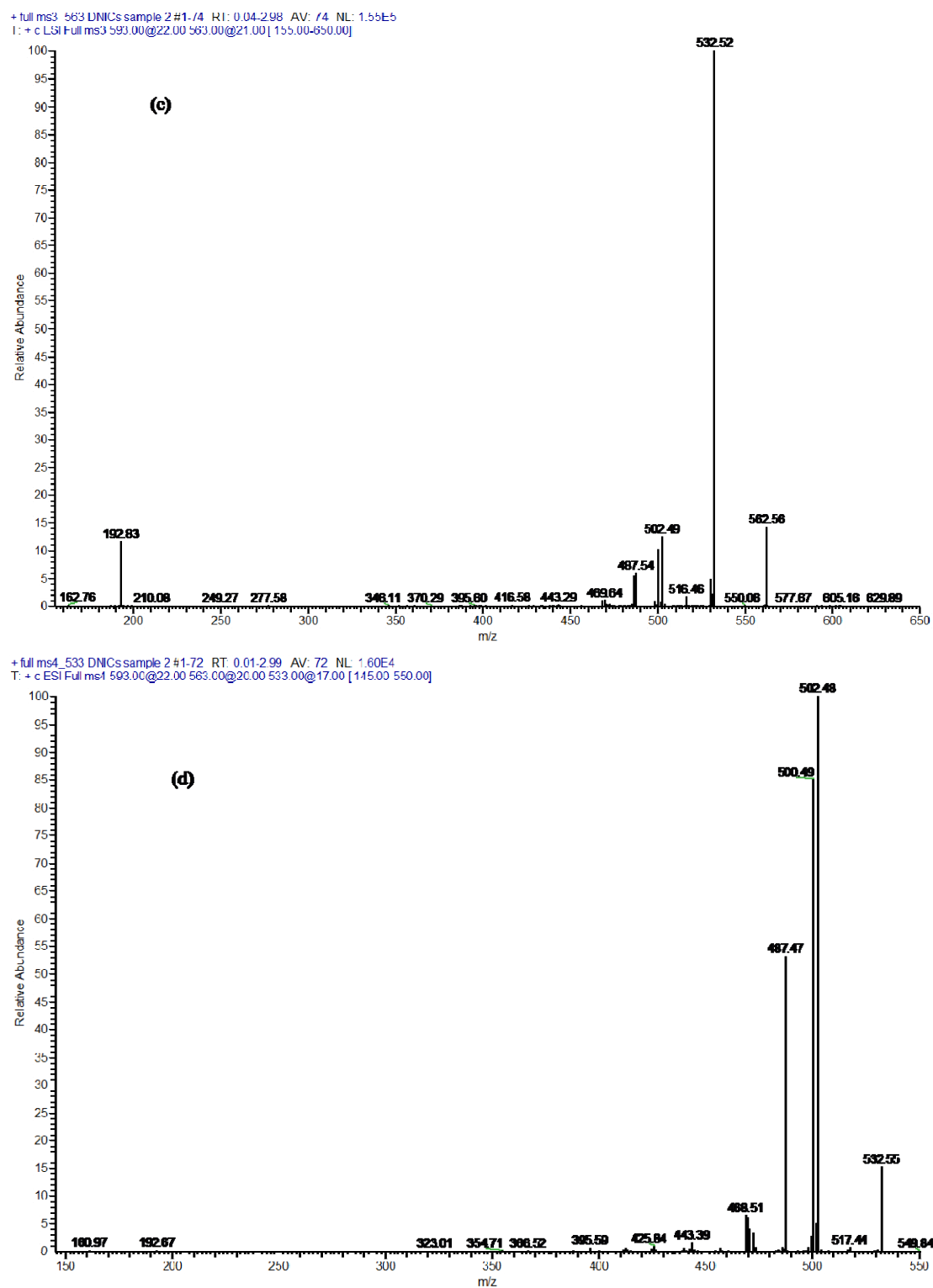


Fig. S1 Mass spectra of 1

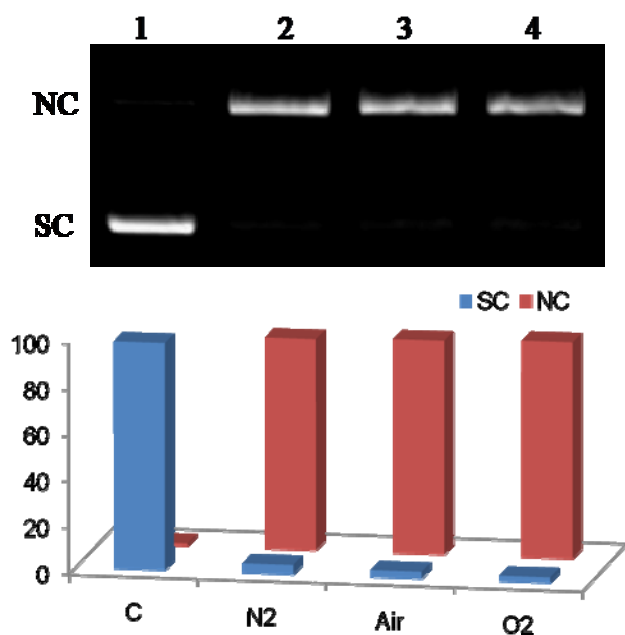


Fig. S2 Cleavage reactions in N₂, air and O₂.

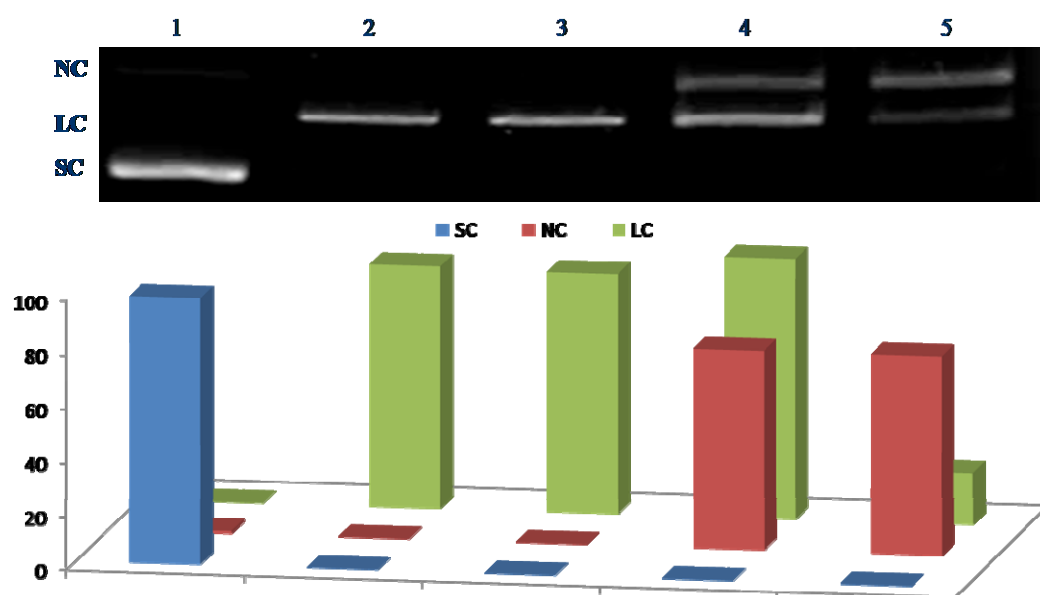


Fig. S3 Lane 1, control; lane 2, DNA cleavage product (linear plasmid pBR322) obtained from the reaction with **1** after irradiation for 8 minutes.; lane 3, DNA cleavage product with T4 ligase; lane 4, treatment of T4 ligase with DNA cleavage product and DNA cleaved by Idel enzyme; lane 5, DNA cleaved by Idel enzyme with T4 ligase.

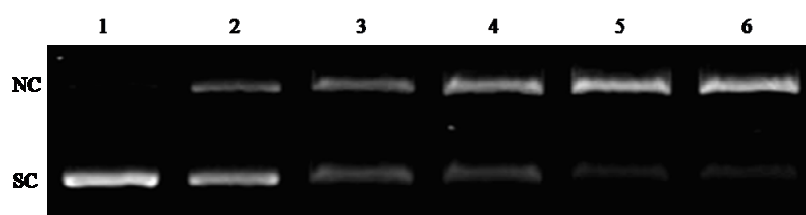


Fig. S4 Agarose gel (1%) of pBR 322 (50 ng) at 25°C and pH. 7.4 (10 mM Tris-HCl) with 20 μ M **1** with increasing time of irradiation: lane 1, DNA control; lanes 2-6, 20, 40, 60, 90, 120 sec, respectively.

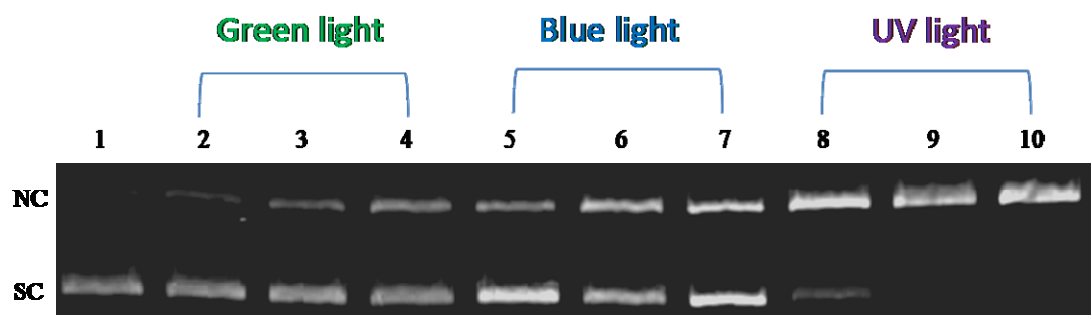


Fig. S5 Agarose gel (1%) of pBR 322 (50 ng) at 25°C with **1** then under irradiation with green (lane 2-4), blue (lane 5-7) and UV (lane 8-10) lights for 2 minutes. Lane 1, DNA control; lane 2, 5, 8: 5 μ M **1**; lane 3, 6, 9: 10 μ M **1**; lane 4, 7, 10: 15 μ M **1** in pH. 7.4 (10 mM Tris-HCl) buffer.

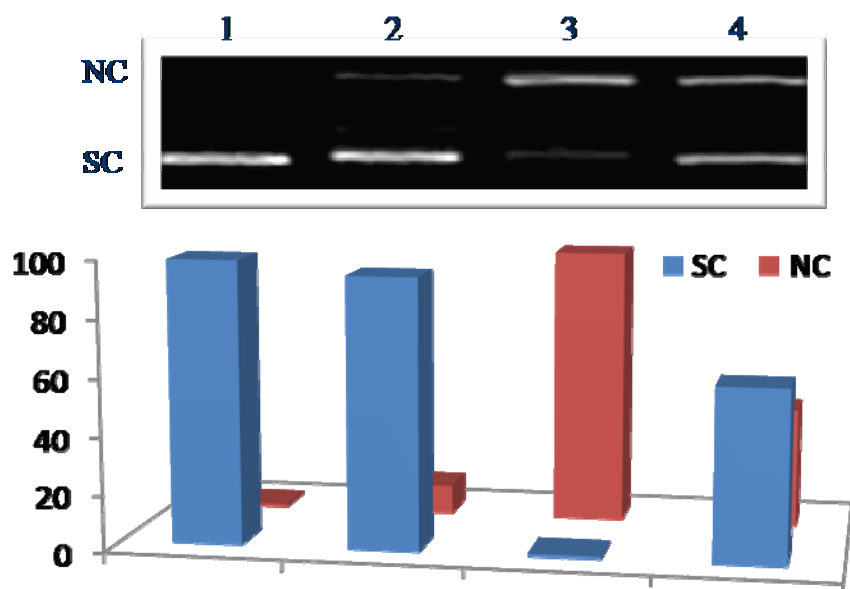


Fig. S6 Comparison the cleavage reactions of control (lane 1), **1** (lane 3), **2** (lane 4), and **3** (lane 2).

Table S1 Crystallographic Data of [(C₆H₅)₃CS(CH₂)₂P(CH₂OH)₂.

chem formula	C23 H25 O3 P S
fw	412.46
cryst syst	Monoclinic
space group	P 21/n
λ , Å(Mo K α)	0.71073
a , Å	7.00660(10)
b , Å	34.1821(7)
c , Å	9.0994(2)
β , deg	112.9130(10)
Z	4
d_{calcd} , Mg m ⁻³	1.365
μ , mm ⁻¹	0.263
T , K	200(2)
R	0.0524 ^a
R_{wF^2}	0.1259 ^b
GOF	1.129

$$^a R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| \quad ^b wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [(C₆H₅)₃CS(CH₂)₂P(CH₂OH)₂.. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7744(1)	1488(1)	8548(1)	28(1)

P(1)	8504(1)	2243(1)	5986(1)	27(1)
O(1)	5911(4)	2785(1)	6183(3)	42(1)
O(2)	12203(3)	2645(1)	6800(3)	38(1)
O(3)	6955(4)	2088(1)	4442(2)	35(1)
C(1)	7249(5)	2490(1)	7136(4)	33(1)
C(2)	10228(5)	2590(1)	5592(4)	38(1)
C(3)	10169(5)	1876(1)	7263(4)	30(1)
C(4)	9114(5)	1479(1)	7215(4)	31(1)
C(5)	6054(5)	1047(1)	7932(3)	26(1)
C(6)	4050(5)	1123(1)	6456(3)	25(1)
C(7)	3775(5)	1441(1)	5438(4)	32(1)
C(8)	1932(5)	1488(1)	4111(4)	36(1)
C(9)	335(5)	1223(1)	3770(4)	39(1)
C(10)	596(5)	906(1)	4769(4)	35(1)
C(11)	2410(5)	858(1)	6096(4)	31(1)
C(12)	7314(5)	705(1)	7673(4)	26(1)
C(13)	6628(5)	480(1)	6297(4)	31(1)
C(14)	7773(6)	165(1)	6132(4)	38(1)
C(15)	9635(5)	68(1)	7328(4)	39(1)
C(16)	10372(5)	297(1)	8693(4)	36(1)
C(17)	9238(5)	610(1)	8859(4)	30(1)
C(18)	5473(5)	981(1)	9386(3)	26(1)
C(19)	5829(5)	632(1)	10243(4)	32(1)
C(20)	5258(5)	597(1)	11543(4)	41(1)
C(21)	4324(6)	901(1)	11994(4)	42(1)
C(22)	3952(6)	1248(1)	11145(4)	42(1)
C(23)	4503(5)	1284(1)	9853(4)	33(1)

Table S3. Bond lengths [Å] and angles [°] for [(C₆H₅)₃CS(CH₂)₂P(CH₂OH)₂.

S(1)-C(4)	1.816(3)
S(1)-C(5)	1.863(3)
P(1)-O(3)	1.499(2)
P(1)-C(3)	1.798(3)
P(1)-C(1)	1.814(3)
P(1)-C(2)	1.825(3)
O(1)-C(1)	1.421(4)
O(1)-H(1')	0.9016
O(2)-C(2)	1.405(4)
O(2)-H(2')	0.8499
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.536(4)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(12)	1.537(4)
C(5)-C(18)	1.545(4)
C(5)-C(6)	1.541(4)
C(6)-C(7)	1.391(4)
C(6)-C(11)	1.399(4)
C(7)-C(8)	1.392(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.380(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.380(5)
C(9)-H(9)	0.9300
C(10)-C(11)	1.381(4)
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-C(13)	1.386(4)
C(12)-C(17)	1.398(4)
C(13)-C(14)	1.385(5)

C(13)-H(13)	0.9300
C(14)-C(15)	1.375(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.384(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.378(4)
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
C(18)-C(23)	1.393(4)
C(18)-C(19)	1.393(4)
C(19)-C(20)	1.394(4)
C(19)-H(19)	0.9300
C(20)-C(21)	1.374(5)
C(20)-H(20)	0.9300
C(21)-C(22)	1.385(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.378(4)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300

C(4)-S(1)-C(5)	103.00(14)
O(3)-P(1)-C(3)	114.09(14)
O(3)-P(1)-C(1)	111.64(15)
C(3)-P(1)-C(1)	106.84(14)
O(3)-P(1)-C(2)	109.85(14)
C(3)-P(1)-C(2)	105.55(15)
C(1)-P(1)-C(2)	108.55(16)
C(1)-O(1)-H(1')	106.7
C(2)-O(2)-H(2')	109.7
O(1)-C(1)-P(1)	109.3(2)
O(1)-C(1)-H(1A)	109.8
P(1)-C(1)-H(1A)	109.8
O(1)-C(1)-H(1B)	109.8
P(1)-C(1)-H(1B)	109.8
H(1A)-C(1)-H(1B)	108.3
O(2)-C(2)-P(1)	117.3(2)
O(2)-C(2)-H(2A)	108.0
P(1)-C(2)-H(2A)	108.0

O(2)-C(2)-H(2B)	108.0
P(1)-C(2)-H(2B)	108.0
H(2A)-C(2)-H(2B)	107.2
C(4)-C(3)-P(1)	114.5(2)
C(4)-C(3)-H(3A)	108.6
P(1)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3B)	108.6
P(1)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6
C(3)-C(4)-S(1)	109.9(2)
C(3)-C(4)-H(4A)	109.7
S(1)-C(4)-H(4A)	109.7
C(3)-C(4)-H(4B)	109.7
S(1)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
C(12)-C(5)-C(18)	112.2(2)
C(12)-C(5)-C(6)	112.2(2)
C(18)-C(5)-C(6)	108.4(2)
C(12)-C(5)-S(1)	109.0(2)
C(18)-C(5)-S(1)	102.12(19)
C(6)-C(5)-S(1)	112.5(2)
C(7)-C(6)-C(11)	117.5(3)
C(7)-C(6)-C(5)	123.7(3)
C(11)-C(6)-C(5)	118.8(3)
C(6)-C(7)-C(8)	120.7(3)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(9)-C(8)-C(7)	121.0(3)
C(9)-C(8)-H(8)	119.5
C(7)-C(8)-H(8)	119.5
C(8)-C(9)-C(10)	118.8(3)
C(8)-C(9)-H(9)	120.6
C(10)-C(9)-H(9)	120.6
C(11)-C(10)-C(9)	120.7(3)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(10)-C(11)-C(6)	121.4(3)
C(10)-C(11)-H(11)	119.3

C(6)-C(11)-H(11)	119.3
C(13)-C(12)-C(17)	117.3(3)
C(13)-C(12)-C(5)	122.9(3)
C(17)-C(12)-C(5)	119.8(3)
C(14)-C(13)-C(12)	121.2(3)
C(14)-C(13)-H(13)	119.4
C(12)-C(13)-H(13)	119.4
C(15)-C(14)-C(13)	120.8(3)
C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6
C(14)-C(15)-C(16)	118.9(3)
C(14)-C(15)-H(15)	120.6
C(16)-C(15)-H(15)	120.6
C(17)-C(16)-C(15)	120.5(3)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(12)	121.3(3)
C(16)-C(17)-H(17)	119.3
C(12)-C(17)-H(17)	119.3
C(23)-C(18)-C(19)	117.9(3)
C(23)-C(18)-C(5)	118.3(3)
C(19)-C(18)-C(5)	123.8(3)
C(20)-C(19)-C(18)	120.1(3)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(21)-C(20)-C(19)	121.0(3)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(20)-C(21)-C(22)	119.4(3)
C(20)-C(21)-H(21)	120.3
C(22)-C(21)-H(21)	120.3
C(23)-C(22)-C(21)	119.8(3)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(18)	121.8(3)
C(22)-C(23)-H(23)	119.1
C(18)-C(23)-H(23)	119.1

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[(\text{C}_6\text{H}_5)_3\text{CS}(\text{CH}_2)_2\text{P}(\text{CH}_2\text{OH})_2]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	30(1)	26(1)	31(1)	-2(1)	14(1)	-2(1)
P(1)	26(1)	30(1)	25(1)	2(1)	10(1)	-1(1)
O(1)	39(1)	41(1)	48(2)	9(1)	18(1)	12(1)
O(2)	32(1)	50(2)	32(1)	-4(1)	11(1)	-5(1)
O(3)	34(1)	43(1)	25(1)	-1(1)	6(1)	-4(1)
C(1)	33(2)	31(2)	34(2)	3(1)	13(2)	6(1)
C(2)	38(2)	46(2)	28(2)	5(2)	9(2)	-6(2)
C(3)	24(2)	35(2)	33(2)	2(1)	14(1)	-1(1)
C(4)	28(2)	31(2)	35(2)	0(1)	14(1)	2(1)
C(5)	26(2)	24(2)	28(2)	2(1)	11(1)	1(1)
C(6)	25(2)	28(2)	25(2)	-1(1)	13(1)	4(1)
C(7)	34(2)	31(2)	34(2)	1(1)	17(2)	2(1)
C(8)	37(2)	41(2)	28(2)	7(2)	11(2)	10(2)
C(9)	30(2)	56(2)	28(2)	-3(2)	8(1)	9(2)
C(10)	28(2)	40(2)	38(2)	-9(2)	14(2)	-3(2)
C(11)	31(2)	32(2)	31(2)	1(1)	14(1)	1(1)
C(12)	27(2)	23(2)	30(2)	5(1)	14(1)	2(1)
C(13)	30(2)	32(2)	31(2)	1(1)	12(1)	4(1)
C(14)	45(2)	32(2)	39(2)	-5(2)	21(2)	3(2)
C(15)	38(2)	29(2)	55(2)	5(2)	24(2)	10(2)
C(16)	29(2)	32(2)	48(2)	7(2)	15(2)	7(2)
C(17)	28(2)	29(2)	31(2)	0(1)	10(1)	0(1)
C(18)	22(2)	30(2)	27(2)	0(1)	9(1)	1(1)
C(19)	34(2)	31(2)	35(2)	6(1)	16(2)	5(2)
C(20)	41(2)	45(2)	35(2)	14(2)	13(2)	3(2)
C(21)	41(2)	61(2)	28(2)	6(2)	17(2)	4(2)
C(22)	46(2)	46(2)	41(2)	-2(2)	24(2)	7(2)
C(23)	34(2)	34(2)	33(2)	4(1)	14(2)	5(2)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[(\text{C}_6\text{H}_5)_3\text{CS}(\text{CH}_2)_2\text{P}(\text{CH}_2\text{OH})_2]$.

	x	y	z	U(eq)
H(1')	4696	2759	6298	50
H(2')	12092	2760	7591	46
H(1A)	6459	2303	7470	39
H(1B)	8287	2606	8083	39
H(2A)	10408	2505	4637	46
H(2B)	9538	2842	5357	46
H(3A)	11337	1837	6960	36
H(3B)	10707	1972	8352	36
H(4A)	10149	1273	7537	37
H(4B)	8147	1425	6135	37
H(7)	4832	1623	5647	38
H(8)	1775	1703	3444	43
H(9)	-895	1256	2884	47
H(10)	-461	723	4546	42
H(11)	2545	645	6765	37
H(13)	5378	541	5470	37
H(14)	7275	17	5202	45
H(15)	10387	-146	7223	47
H(16)	11641	237	9503	43
H(17)	9763	762	9779	36
H(19)	6450	422	9948	39
H(20)	5512	363	12113	49
H(21)	3945	874	12861	51
H(22)	3333	1457	11445	50
H(23)	4221	1516	9278	40