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Supporting Information

Disulfide Bond Creates a Small Connecting Loop in Aminoxy Peptide Backbone

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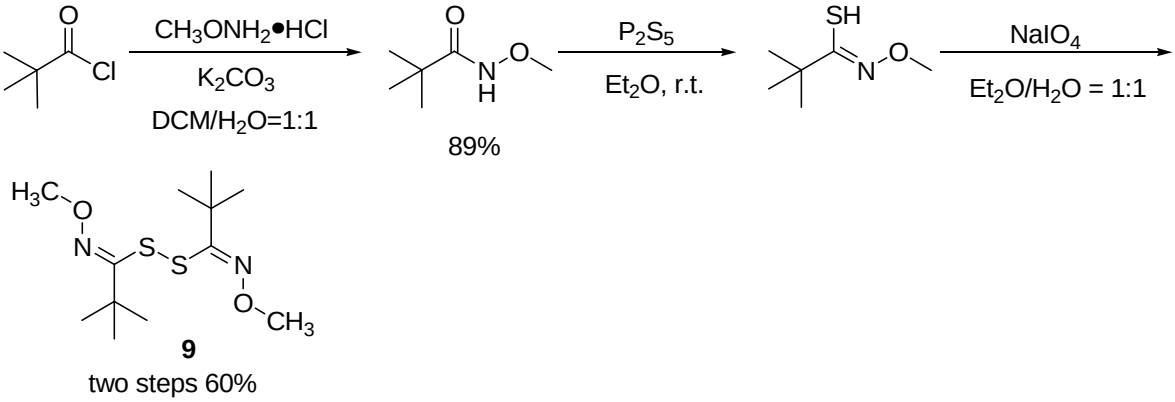
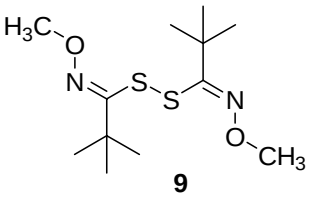
Synthesis of compound 9:



Scheme S1. Synthetic route to compound **9**.

For references: see (a) J. E. Johnson, A. Ghafouripour, Y. K. Haug, A. W. Cordes, W. T. Pennington, O. Exner *J. Org. Chem.* **1985**, *60*, 993; (b) V. Polshettiwar, M. P. Kaushik, *Tetrahedron Lett.* **2006,** *47*, 2315; (c) M. A. Shalaby, C. W. Grote, H. Rapoport, *J. Org. Chem.* **1996**, *61*, 9045; (d) M. Montazerozohori, S. Joohari, B. Karami, N. Haghighat, *Molecules* **2007**, *12*, 694.

Characterization data of compound 9:



9

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.94 (s, 6H, MeO–), 1.20 (s, 18H, Me_3C–); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 61.9, 39.6, 28.1; LRMS *m/z* 293 (M^+ + 1, 100), 294 (16), 295 (9).

IR (CH_2Cl_2) data of (*Z*)-*N*-methoxy-2,2-dimethylpropanethioimidic acid: 2972, 2941, 2902, 2871, 2574 (SH), 1605 (C=N) cm^{-1}.

^{1}H NMR dilution studies and DMSO-d_6 addition studies of compounds 8a and **8b:**

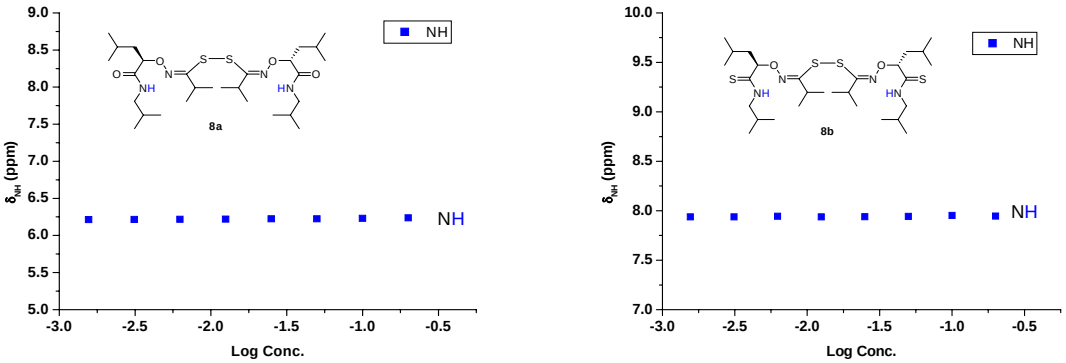


Figure S1. Amide proton chemical shift as a function of logarithm of concentration for compounds **8a** and **8b** (in $CDCl_3$ at room temperature).

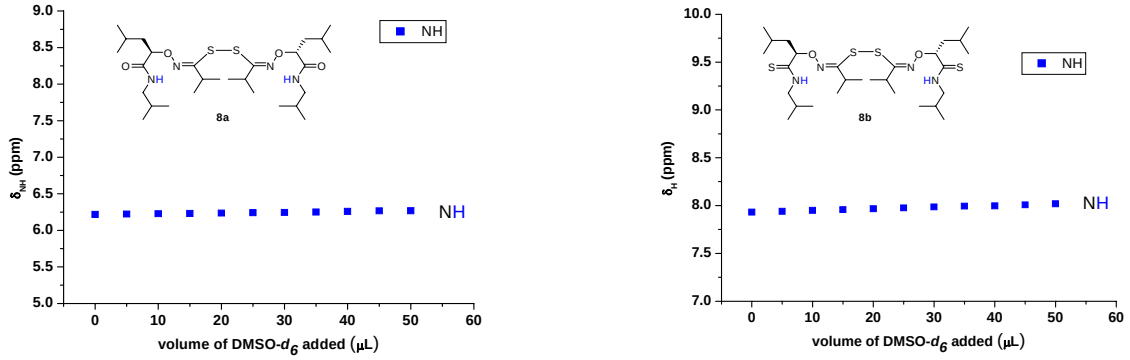


Figure S2. Amide proton chemical shift as a function of the amount of DMSO-d_6 added in a 5 mM solution of compounds **8a** and **8b** (0.5 mL in $CDCl_3$ at room temperature).

CD spectra:

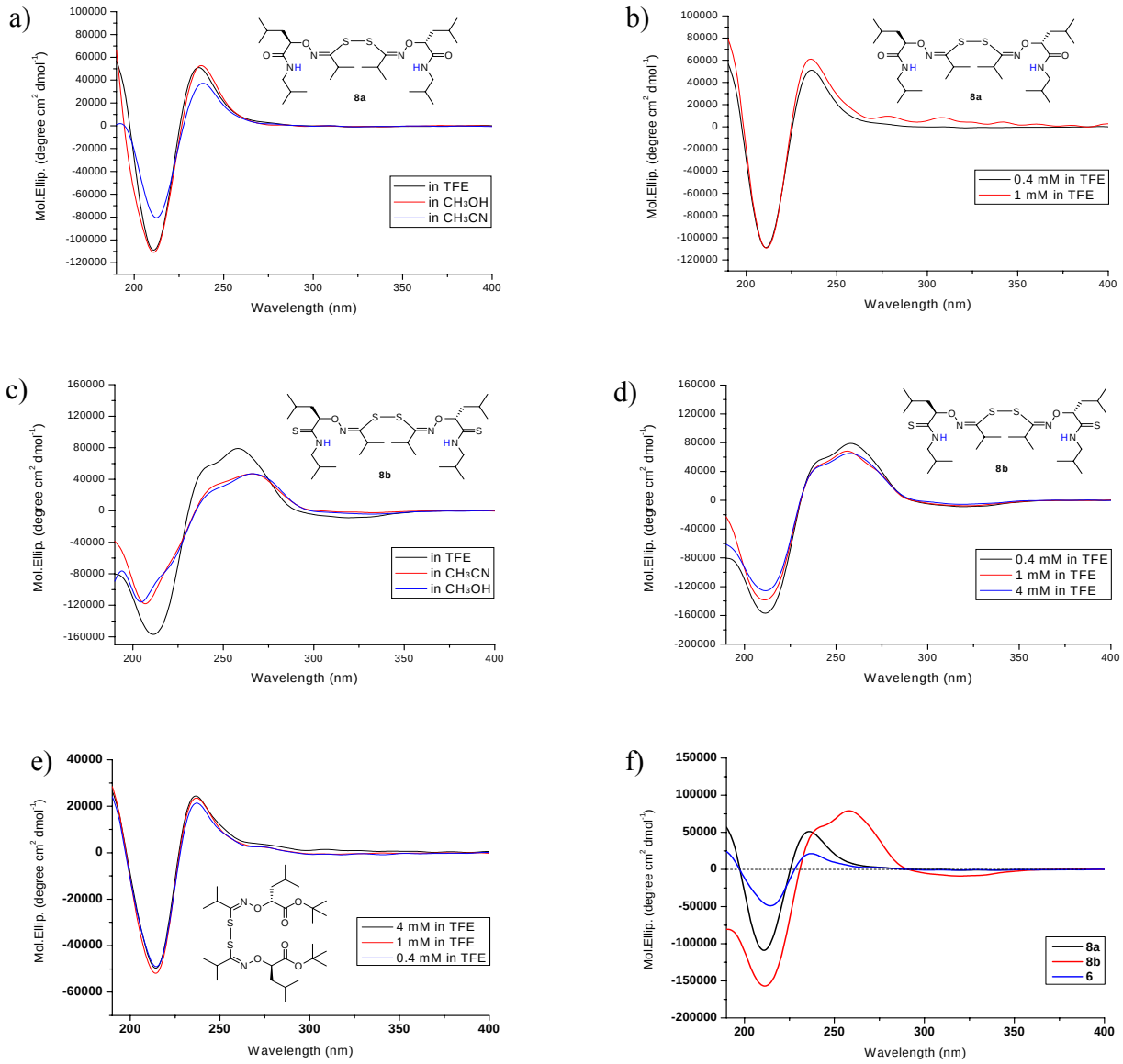


Figure S3. CD spectra of **6**, **8a** and **8b** at 190−400 nm. (a) CD spectra of **8a** in different solvents (0.4 mM); (b) CD spectra of **8a** at different concentrations in trifluoroethanol; (c) CD spectra of **8b** in different solvents (0.4 mM); (d) CD spectra of **8b** at different concentrations in trifluoroethanol; (e) CD spectra of **6** at different concentrations in trifluoroethanol; (f) CD spectra of **6**, **8a** and **8b** at 0.4 mM in trifluoroethanol.

X-Ray crystal structure of compound 8b

The crystal of compound **8b** is a macle. The twin crystal has another component of BASF=0.13276 with the same *a* direction and the counter developing of *b*, *c* axes. Although the crystal has 90.00° of either of α, β, γ angles of the cell, it prefers a monoclinic space group P 2_1 rather than orthorhombic P 2_1 2_1 2. There are two unique molecules in the asymmetric unit. Some data are listed below. Only the data of molecule 1 is reported in the text.

Molecule 1

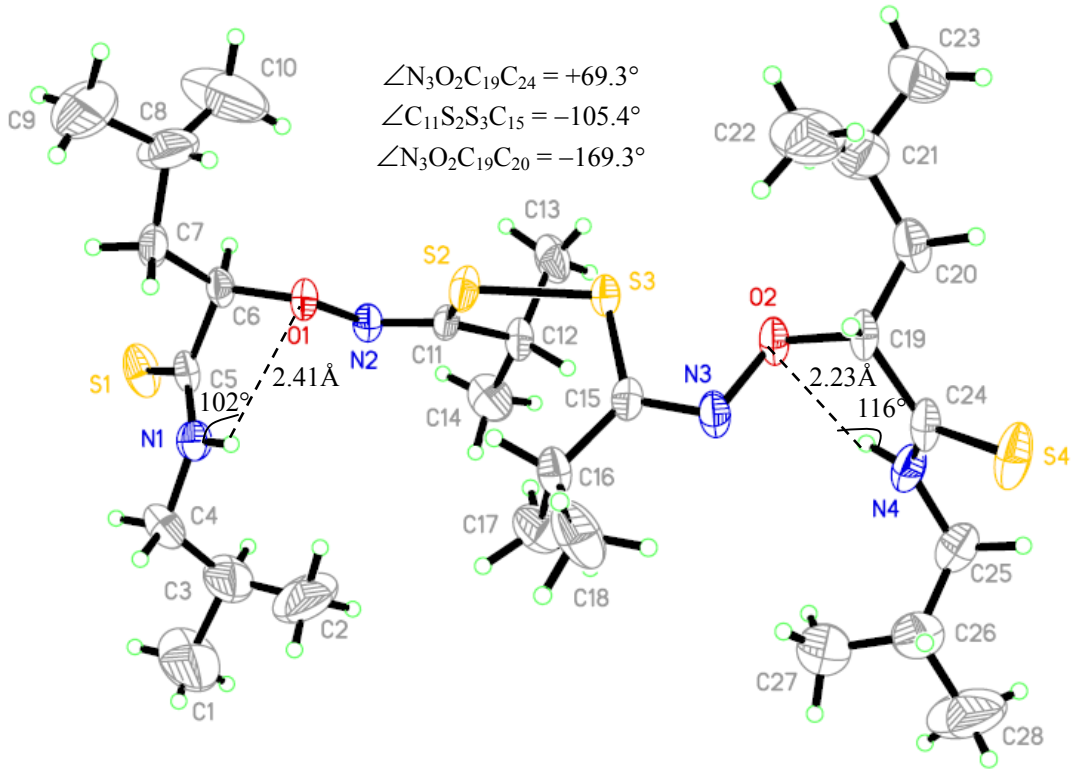


Table S1. Selected Dihedral Angles as well as the Distances and Angles of Intramolecular Hydrogen Bonds of Molecule 1.

$\angle C_{11}S_2S_3C_{15}$	−105.4°	$D_{N4H...O2}$	2.23Å
$\angle N_3O_2C_{19}C_{24}$	+69.3°	$\angle N_4H\ldots O_2$	116°
$\angle N_2O_1C_6C_5$	+66.7°	$D_{N1H...O1}$	2.41Å
$\angle N_3O_2C_{19}C_{20}$	−169.3°	$\angle N_1H\ldots O_1$	102°
$\angle N_2O_1C_6C_7$	−171.0°		
$\angle N_2C_{11}C_{15}N_3$	+164.8°		
$\angle S_1C_5C_{24}S_4$	−157.4°		

Molecule 2

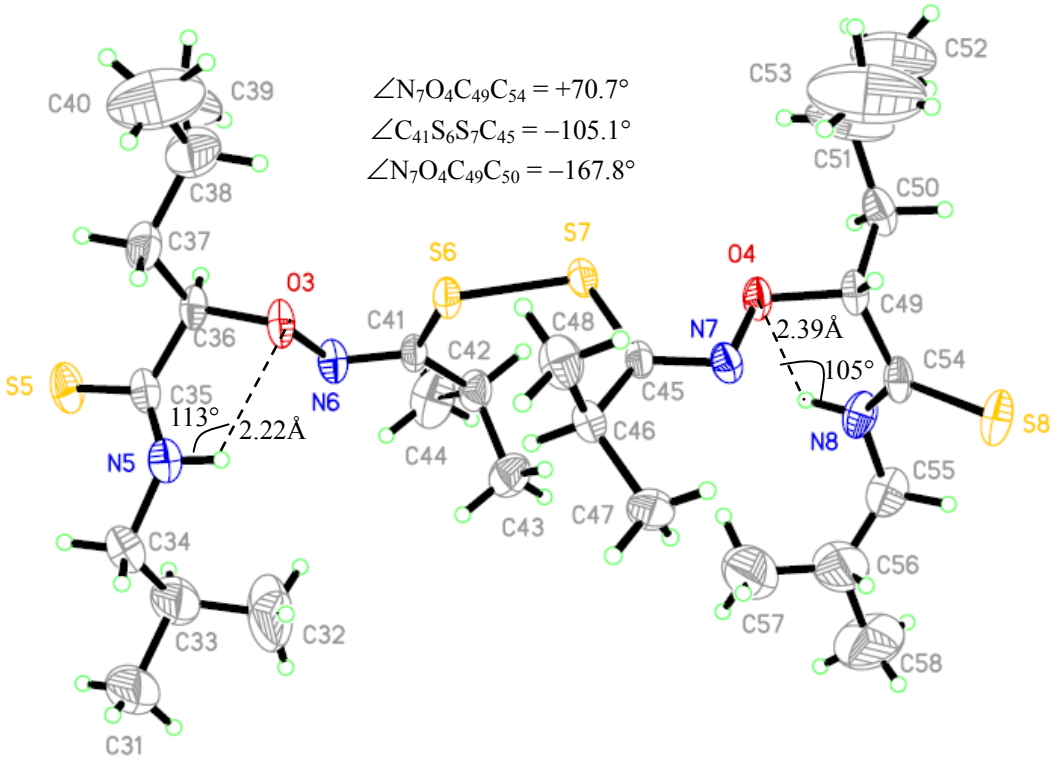


Table S2. Selected Dihedral Angles as well as the Distances and Angles of Intramolecular Hydrogen Bonds of Molecule 2.

$\angle C_{41}S_6S_7C_{45}$	–105.1°	$D_{N8H\ldots O4}$	2.39Å
$\angle N_7O_4C_{49}C_{54}$	+70.7°	$\angle N_8H\ldots O_4$	105°
$\angle N_6O_3C_{36}C_{35}$	+69.5°	$D_{N5H\ldots O3}$	2.22Å
$\angle N_7O_4C_{49}C_{50}$	–167.8°	$\angle N_5H\ldots O_3$	113°
$\angle N_6O_3C_{36}C_{37}$	–167.8°		
$\angle N_6C_{41}C_{45}N_7$	+163.0°		
$\angle S_5C_{35}C_{54}S_8$	–149.3°		

Table S3. Crystal data and structure refinement for **8b**.

Identification code	60222a (**8b**)
Empirical formula	C28 H54 N4 O2 S4
Formula weight	606.99
Temperature	297(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 10.210(2) A alpha = 90 deg.
	b = 18.615(4) A beta = 90 deg.
	c = 19.763(4) A gamma = 90 deg.
Volume	3756.2(14) A^3
Z, Calculated density	4, 1.073 Mg/m^3
Absorption coefficient	0.280 mm^-1
F(000)	1320
Crystal size	0.50 x 0.40 x 0.20 mm
Theta range for data collection	1.03 to 26.50 deg.
Index ranges	-12<=h<=12, -23<=k<=23, -24<=l<=19
Reflections collected / unique	21050 / 13276 [R(int) = 0.0373]
Completeness to 2theta = 26.50	93.4%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9462 and 0.8728
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13276 / 188 / 725
Goodness-of-fit on F^2	0.839
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.1171
R indices (all data)	R1 = 0.1330, wR2 = 0.1440
Absolute structure parameter	-0.13(7)
Largest diff. peak and hole	0.326 and -0.149 e.A^-3

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **8b**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	-1359(1)	4247(1)	2877(1)	112(1)
S(2)	865(1)	3169(1)	5706(1)	80(1)
S(3)	813(1)	3228(1)	6739(1)	78(1)
S(4)	3439(1)	4006(1)	9624(1)	124(1)
O(1)	288(1)	3353(1)	4436(1)	66(1)
O(2)	1484(1)	3478(1)	7978(1)	76(1)
N(1)	794(2)	4463(1)	3576(1)	76(1)
N(2)	-711(2)	3707(1)	4805(1)	68(1)
N(3)	2376(2)	3905(1)	7577(1)	81(1)
N(4)	1413(2)	4504(1)	8941(1)	92(1)
C(1)	607(7)	6441(2)	3370(2)	309(3)
C(2)	990(5)	5773(2)	4382(1)	249(3)
C(3)	450(5)	5739(1)	3715(1)	173(2)
C(4)	960(3)	5174(1)	3313(1)	101(1)
C(5)	-184(2)	4051(1)	3417(1)	68(1)
C(6)	-119(2)	3316(1)	3741(1)	72(1)
C(7)	886(3)	2821(1)	3390(1)	87(1)
C(8)	934(3)	2036(2)	3568(1)	186(2)
C(9)	1693(5)	1634(2)	3087(2)	327(2)
C(10)	-161(4)	1739(2)	3877(2)	311(2)
C(11)	-517(2)	3670(1)	5437(1)	60(1)
C(12)	-1524(2)	3977(1)	5924(1)	81(1)
C(13)	-2478(3)	3422(1)	6143(1)	116(1)
C(14)	-2261(3)	4627(1)	5616(1)	127(1)
C(15)	2083(2)	3843(1)	6949(1)	67(1)
C(16)	2805(3)	4294(1)	6456(1)	90(1)
C(17)	1968(3)	4931(1)	6267(1)	124(1)
C(18)	4105(3)	4519(2)	6694(1)	152(1)
C(19)	2119(2)	3322(1)	8615(1)	82(1)
C(20)	1250(3)	2759(1)	8948(1)	104(1)
C(21)	1021(3)	2086(2)	8574(1)	152(1)
C(22)	2149(4)	1812(2)	8227(2)	200(2)
C(23)	356(4)	1559(2)	8987(2)	215(2)
C(24)	2256(2)	3996(1)	9047(1)	85(1)
C(25)	1372(3)	5163(1)	9297(1)	107(1)

C(26)	2174(5)	5719(2)	9014(1)	180(2)
C(27)	1972(5)	5902(2)	8340(1)	217(2)
C(28)	2055(6)	6398(2)	9377(2)	308(2)
S(5)	8499(1)	4578(1)	7867(1)	106(1)
S(6)	5839(1)	5279(1)	10780(1)	81(1)
S(7)	5844(1)	5286(1)	11812(1)	85(1)
S(8)	3622(1)	4022(1)	14588(1)	102(1)
O(3)	6656(1)	5139(1)	9550(1)	82(1)
O(4)	5288(1)	4997(1)	13067(1)	71(1)
N(5)	6346(2)	4192(1)	8545(1)	82(1)
N(6)	7443(2)	4645(1)	9930(1)	81(1)
N(7)	4257(2)	4679(1)	12675(1)	70(1)
N(8)	5775(2)	3815(1)	13863(1)	87(1)
C(31)	6546(5)	2240(2)	8040(2)	218(2)
C(32)	6506(6)	2729(2)	9171(1)	318(4)
C(33)	6804(5)	2904(1)	8464(1)	182(2)
C(34)	6180(3)	3528(1)	8154(1)	104(1)
C(35)	7311(2)	4641(1)	8469(1)	79(1)
C(36)	7314(2)	5281(1)	8924(1)	76(1)
C(37)	6599(3)	5926(1)	8617(1)	103(1)
C(38)	6676(4)	6614(2)	9075(2)	165(1)
C(39)	7972(4)	6906(2)	9052(2)	242(2)
C(40)	5784(5)	7153(2)	8855(2)	284(3)
C(41)	7117(2)	4667(1)	10548(1)	66(1)
C(42)	7769(2)	4163(1)	11029(1)	88(1)
C(43)	6934(3)	3528(1)	11177(1)	111(1)
C(44)	9083(3)	3929(2)	10757(1)	144(1)
C(45)	4448(2)	4773(1)	12052(1)	60(1)
C(46)	3453(2)	4511(1)	11552(1)	72(1)
C(47)	2630(3)	3900(1)	11858(1)	105(1)
C(48)	2580(2)	5147(1)	11324(1)	101(1)
C(49)	4857(2)	5000(1)	13758(1)	71(1)
C(50)	5839(2)	5492(1)	14132(1)	95(1)
C(51)	5845(2)	6268(2)	13947(2)	227(2)
C(52)	6722(4)	6642(2)	14449(2)	250(2)
C(53)	4571(4)	6607(3)	13903(3)	361(3)
C(54)	4837(2)	4235(1)	14045(1)	72(1)
C(55)	5943(3)	3073(1)	14066(1)	111(1)
C(56)	5624(5)	2548(1)	13604(1)	197(2)
C(57)	5645(6)	2620(2)	12882(2)	254(3)
C(58)	5842(5)	1789(2)	13823(2)	244(3)

Table S5. Bond lengths [A] and angles [deg] for **8b**.

S(1)-C(5)	1.646(2)	C(10)-H(10A)	0.9599
S(2)-C(11)	1.773(2)	C(10)-H(10B)	0.9599
S(2)-S(3)	2.0461(8)	C(10)-H(10C)	0.9599
S(3)-C(15)	1.779(2)	C(11)-C(12)	1.521(3)
S(4)-C(24)	1.662(2)	C(12)-C(13)	1.485(3)
O(1)-N(2)	1.417(2)	C(12)-C(14)	1.550(3)
O(1)-C(6)	1.4356(19)	C(12)-H(12)	0.9800
O(2)-N(3)	1.446(2)	C(13)-H(13A)	0.9599
O(2)-C(19)	1.446(2)	C(13)-H(13B)	0.9599
N(1)-C(5)	1.298(3)	C(13)-H(13C)	0.9599
N(1)-C(4)	1.432(3)	C(14)-H(14A)	0.9599
N(1)-H(1X)	0.869(10)	C(14)-H(14B)	0.9599
N(2)-C(11)	1.267(2)	C(14)-H(14C)	0.9599
N(3)-C(15)	1.282(2)	C(15)-C(16)	1.482(3)
N(4)-C(24)	1.296(3)	C(16)-C(18)	1.469(4)
N(4)-C(25)	1.416(3)	C(16)-C(17)	1.509(3)
N(4)-H(4X)	0.813(8)	C(16)-H(16)	0.9800
C(1)-C(3)	1.483(4)	C(17)-H(17A)	0.9599
C(1)-H(1A)	0.9599	C(17)-H(17B)	0.9599
C(1)-H(1B)	0.9599	C(17)-H(17C)	0.9599
C(1)-H(1C)	0.9599	C(18)-H(18A)	0.9599
C(2)-C(3)	1.430(4)	C(18)-H(18B)	0.9599
C(2)-H(2A)	0.9599	C(18)-H(18C)	0.9599
C(2)-H(2B)	0.9599	C(19)-C(20)	1.522(3)
C(2)-H(2C)	0.9599	C(19)-C(24)	1.524(3)
C(3)-C(4)	1.416(4)	C(19)-H(19)	0.9800
C(3)-H(3)	0.9800	C(20)-C(21)	1.474(4)
C(4)-H(4A)	0.9700	C(20)-H(20A)	0.9700
C(4)-H(4B)	0.9700	C(20)-H(20B)	0.9700
C(5)-C(6)	1.512(3)	C(21)-C(22)	1.434(4)
C(6)-C(7)	1.544(3)	C(21)-C(23)	1.446(4)
C(6)-H(6)	0.9800	C(21)-H(21)	0.9800
C(7)-C(8)	1.503(3)	C(22)-H(22A)	0.9599
C(7)-H(7A)	0.9700	C(22)-H(22B)	0.9599
C(7)-H(7B)	0.9700	C(22)-H(22C)	0.9599
C(8)-C(10)	1.389(5)	C(23)-H(23A)	0.9599
C(8)-C(9)	1.437(4)	C(23)-H(23B)	0.9599
C(8)-H(8)	0.9800	C(23)-H(23C)	0.9599
C(9)-H(9A)	0.9599	C(25)-C(26)	1.433(4)
C(9)-H(9B)	0.9599	C(25)-H(25A)	0.9700
C(9)-H(9C)	0.9599	C(25)-H(25B)	0.9700

C(26)-C(27)	1.390(3)	C(37)-H(37B)	0.9700
C(26)-C(28)	1.458(4)	C(38)-C(40)	1.424(5)
C(26)-H(26)	0.9800	C(38)-C(39)	1.431(6)
C(27)-H(27A)	0.9599	C(38)-H(38)	0.9800
C(27)-H(27B)	0.9599	C(39)-H(39A)	0.9599
C(27)-H(27C)	0.9599	C(39)-H(39B)	0.9599
C(28)-H(28A)	0.9599	C(39)-H(39C)	0.9599
C(28)-H(28B)	0.9599	C(40)-H(40A)	0.9599
C(28)-H(28C)	0.9599	C(40)-H(40B)	0.9599
S(5)-C(35)	1.704(2)	C(40)-H(40C)	0.9599
S(6)-C(41)	1.792(2)	C(41)-C(42)	1.493(3)
S(6)-S(7)	2.0395(8)	C(42)-C(43)	1.487(3)
S(7)-C(45)	1.779(2)	C(42)-C(44)	1.509(4)
S(8)-C(54)	1.688(2)	C(42)-H(42)	0.9800
O(3)-C(36)	1.432(2)	C(43)-H(43A)	0.9599
O(3)-N(6)	1.434(2)	C(43)-H(43B)	0.9599
O(4)-N(7)	1.434(2)	C(43)-H(43C)	0.9599
O(4)-C(49)	1.435(2)	C(44)-H(44A)	0.9599
N(5)-C(35)	1.300(3)	C(44)-H(44B)	0.9599
N(5)-C(34)	1.468(3)	C(44)-H(44C)	0.9599
N(5)-H(5X)	0.864(11)	C(45)-C(46)	1.498(3)
N(6)-C(41)	1.266(2)	C(46)-C(47)	1.537(3)
N(7)-C(45)	1.260(2)	C(46)-C(48)	1.551(3)
N(8)-C(54)	1.288(3)	C(46)-H(46)	0.9800
N(8)-C(55)	1.447(3)	C(47)-H(47A)	0.9599
N(8)-H(8X)	0.881(11)	C(47)-H(47B)	0.9599
C(31)-C(33)	1.517(4)	C(47)-H(47C)	0.9599
C(31)-H(31A)	0.9599	C(48)-H(48A)	0.9599
C(31)-H(31B)	0.9599	C(48)-H(48B)	0.9599
C(31)-H(31C)	0.9599	C(48)-H(48C)	0.9599
C(32)-C(33)	1.466(4)	C(49)-C(54)	1.532(3)
C(32)-H(32A)	0.9599	C(49)-C(50)	1.545(3)
C(32)-H(32B)	0.9599	C(49)-H(49)	0.9800
C(32)-H(32C)	0.9599	C(50)-C(51)	1.490(4)
C(33)-C(34)	1.459(4)	C(50)-H(50A)	0.9700
C(33)-H(33)	0.9800	C(50)-H(50B)	0.9700
C(34)-H(34A)	0.9700	C(51)-C(53)	1.449(5)
C(34)-H(34B)	0.9700	C(51)-C(52)	1.506(4)
C(35)-C(36)	1.491(3)	C(51)-H(51)	0.9800
C(36)-C(37)	1.532(3)	C(52)-H(52A)	0.9599
C(36)-H(36)	0.9800	C(52)-H(52B)	0.9599
C(37)-C(38)	1.571(4)	C(52)-H(52C)	0.9599
C(37)-H(37A)	0.9700	C(53)-H(53A)	0.9599

C(53)-H(53B)	0.9599
C(53)-H(53C)	0.9599
C(55)-C(56)	1.376(4)
C(55)-H(55A)	0.9700
C(55)-H(55B)	0.9700
C(56)-C(57)	1.433(4)
C(56)-C(58)	1.495(4)
C(56)-H(56)	0.9800
C(57)-H(57A)	0.9599
C(57)-H(57B)	0.9599
C(57)-H(57C)	0.9599
C(58)-H(58A)	0.9599
C(58)-H(58B)	0.9599
C(58)-H(58C)	0.9599

C(11)-S(2)-S(3)	104.49(6)
C(15)-S(3)-S(2)	104.35(7)
N(2)-O(1)-C(6)	107.87(13)
N(3)-O(2)-C(19)	107.79(14)
C(5)-N(1)-C(4)	123.38(18)
C(5)-N(1)-H(1X)	123.7(9)
C(4)-N(1)-H(1X)	110.9(10)
C(11)-N(2)-O(1)	111.72(15)
C(15)-N(3)-O(2)	109.50(16)
C(24)-N(4)-C(25)	124.85(19)
C(24)-N(4)-H(4X)	111.8(7)
C(25)-N(4)-H(4X)	123.3(7)
C(3)-C(1)-H(1A)	109.5
C(3)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(3)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-C(2)	114.0(3)
C(4)-C(3)-C(1)	110.9(3)
C(2)-C(3)-C(1)	110.0(3)
C(4)-C(3)-H(3)	107.2
C(2)-C(3)-H(3)	107.2
C(1)-C(3)-H(3)	107.2
C(3)-C(4)-N(1)	116.1(2)
C(3)-C(4)-H(4A)	108.3
N(1)-C(4)-H(4A)	108.3
C(3)-C(4)-H(4B)	108.3
N(1)-C(4)-H(4B)	108.3
H(4A)-C(4)-H(4B)	107.4
N(1)-C(5)-C(6)	113.48(17)
N(1)-C(5)-S(1)	125.89(16)
C(6)-C(5)-S(1)	120.50(15)
O(1)-C(6)-C(5)	112.00(15)
O(1)-C(6)-C(7)	105.46(16)
C(5)-C(6)-C(7)	112.21(16)
O(1)-C(6)-H(6)	109.0
C(5)-C(6)-H(6)	109.0
C(7)-C(6)-H(6)	109.0
C(8)-C(7)-C(6)	119.72(19)
C(8)-C(7)-H(7A)	107.4
C(6)-C(7)-H(7A)	107.4
C(8)-C(7)-H(7B)	107.4
C(6)-C(7)-H(7B)	107.4
H(7A)-C(7)-H(7B)	106.9
C(10)-C(8)-C(9)	121.2(3)
C(10)-C(8)-C(7)	117.6(3)
C(9)-C(8)-C(7)	111.7(2)
C(10)-C(8)-H(8)	100.3
C(9)-C(8)-H(8)	100.3
C(7)-C(8)-H(8)	100.3
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(2)-C(11)-C(12)	119.87(18)
N(2)-C(11)-S(2)	116.67(15)

C(12)-C(11)-S(2)	123.14(13)	O(2)-C(19)-H(19)	109.5
C(13)-C(12)-C(11)	111.48(18)	C(20)-C(19)-H(19)	109.5
C(13)-C(12)-C(14)	109.8(2)	C(24)-C(19)-H(19)	109.5
C(11)-C(12)-C(14)	111.91(17)	C(21)-C(20)-C(19)	117.4(2)
C(13)-C(12)-H(12)	107.8	C(21)-C(20)-H(20A)	108.0
C(11)-C(12)-H(12)	107.8	C(19)-C(20)-H(20A)	108.0
C(14)-C(12)-H(12)	107.8	C(21)-C(20)-H(20B)	108.0
C(12)-C(13)-H(13A)	109.5	C(19)-C(20)-H(20B)	108.0
C(12)-C(13)-H(13B)	109.5	H(20A)-C(20)-H(20B)	107.2
H(13A)-C(13)-H(13B)	109.5	C(22)-C(21)-C(23)	113.9(3)
C(12)-C(13)-H(13C)	109.5	C(22)-C(21)-C(20)	114.5(3)
H(13A)-C(13)-H(13C)	109.5	C(23)-C(21)-C(20)	111.6(2)
H(13B)-C(13)-H(13C)	109.5	C(22)-C(21)-H(21)	105.2
C(12)-C(14)-H(14A)	109.5	C(23)-C(21)-H(21)	105.2
C(12)-C(14)-H(14B)	109.5	C(20)-C(21)-H(21)	105.2
H(14A)-C(14)-H(14B)	109.5	C(21)-C(22)-H(22A)	109.5
C(12)-C(14)-H(14C)	109.5	C(21)-C(22)-H(22B)	109.5
H(14A)-C(14)-H(14C)	109.5	H(22A)-C(22)-H(22B)	109.5
H(14B)-C(14)-H(14C)	109.5	C(21)-C(22)-H(22C)	109.5
N(3)-C(15)-C(16)	117.91(19)	H(22A)-C(22)-H(22C)	109.5
N(3)-C(15)-S(3)	117.00(15)	H(22B)-C(22)-H(22C)	109.5
C(16)-C(15)-S(3)	125.07(14)	C(21)-C(23)-H(23A)	109.5
C(18)-C(16)-C(15)	113.64(19)	C(21)-C(23)-H(23B)	109.5
C(18)-C(16)-C(17)	111.5(2)	H(23A)-C(23)-H(23B)	109.5
C(15)-C(16)-C(17)	109.0(2)	C(21)-C(23)-H(23C)	109.5
C(18)-C(16)-H(16)	107.5	H(23A)-C(23)-H(23C)	109.5
C(15)-C(16)-H(16)	107.5	H(23B)-C(23)-H(23C)	109.5
C(17)-C(16)-H(16)	107.5	N(4)-C(24)-C(19)	116.71(18)
C(16)-C(17)-H(17A)	109.5	N(4)-C(24)-S(4)	125.88(18)
C(16)-C(17)-H(17B)	109.5	C(19)-C(24)-S(4)	117.39(17)
H(17A)-C(17)-H(17B)	109.5	N(4)-C(25)-C(26)	114.5(2)
C(16)-C(17)-H(17C)	109.5	N(4)-C(25)-H(25A)	108.6
H(17A)-C(17)-H(17C)	109.5	C(26)-C(25)-H(25A)	108.6
H(17B)-C(17)-H(17C)	109.5	N(4)-C(25)-H(25B)	108.6
C(16)-C(18)-H(18A)	109.5	C(26)-C(25)-H(25B)	108.6
C(16)-C(18)-H(18B)	109.5	H(25A)-C(25)-H(25B)	107.6
H(18A)-C(18)-H(18B)	109.5	C(27)-C(26)-C(25)	117.8(3)
C(16)-C(18)-H(18C)	109.5	C(27)-C(26)-C(28)	104.3(3)
H(18A)-C(18)-H(18C)	109.5	C(25)-C(26)-C(28)	112.7(3)
H(18B)-C(18)-H(18C)	109.5	C(27)-C(26)-H(26)	107.2
O(2)-C(19)-C(20)	104.71(17)	C(25)-C(26)-H(26)	107.2
O(2)-C(19)-C(24)	111.24(17)	C(28)-C(26)-H(26)	107.2
C(20)-C(19)-C(24)	112.19(17)	C(26)-C(27)-H(27A)	109.5

C(26)-C(27)-H(27B)	109.5	N(5)-C(34)-H(34A)	108.9
H(27A)-C(27)-H(27B)	109.5	C(33)-C(34)-H(34B)	108.9
C(26)-C(27)-H(27C)	109.5	N(5)-C(34)-H(34B)	108.9
H(27A)-C(27)-H(27C)	109.5	H(34A)-C(34)-H(34B)	107.7
H(27B)-C(27)-H(27C)	109.5	N(5)-C(35)-C(36)	116.44(19)
C(26)-C(28)-H(28A)	109.5	N(5)-C(35)-S(5)	125.14(17)
C(26)-C(28)-H(28B)	109.5	C(36)-C(35)-S(5)	118.31(17)
H(28A)-C(28)-H(28B)	109.5	O(3)-C(36)-C(35)	111.85(17)
C(26)-C(28)-H(28C)	109.5	O(3)-C(36)-C(37)	105.25(18)
H(28A)-C(28)-H(28C)	109.5	C(35)-C(36)-C(37)	112.73(17)
H(28B)-C(28)-H(28C)	109.5	O(3)-C(36)-H(36)	109.0
C(41)-S(6)-S(7)	104.96(6)	C(35)-C(36)-H(36)	109.0
C(45)-S(7)-S(6)	105.16(6)	C(37)-C(36)-H(36)	109.0
C(36)-O(3)-N(6)	107.92(15)	C(36)-C(37)-C(38)	112.8(2)
N(7)-O(4)-C(49)	106.93(14)	C(36)-C(37)-H(37A)	109.0
C(35)-N(5)-C(34)	124.64(19)	C(38)-C(37)-H(37A)	109.0
C(35)-N(5)-H(5X)	112.0(16)	C(36)-C(37)-H(37B)	109.0
C(34)-N(5)-H(5X)	115.8(18)	C(38)-C(37)-H(37B)	109.0
C(41)-N(6)-O(3)	109.66(17)	H(37A)-C(37)-H(37B)	107.8
C(45)-N(7)-O(4)	110.87(16)	C(40)-C(38)-C(39)	108.4(3)
C(54)-N(8)-C(55)	126.2(2)	C(40)-C(38)-C(37)	111.5(3)
C(54)-N(8)-H(8X)	119.7(11)	C(39)-C(38)-C(37)	109.7(3)
C(55)-N(8)-H(8X)	112.0(11)	C(40)-C(38)-H(38)	109.1
C(33)-C(31)-H(31A)	109.5	C(39)-C(38)-H(38)	109.1
C(33)-C(31)-H(31B)	109.5	C(37)-C(38)-H(38)	109.1
H(31A)-C(31)-H(31B)	109.5	C(38)-C(39)-H(39A)	109.5
C(33)-C(31)-H(31C)	109.5	C(38)-C(39)-H(39B)	109.5
H(31A)-C(31)-H(31C)	109.5	H(39A)-C(39)-H(39B)	109.5
H(31B)-C(31)-H(31C)	109.5	C(38)-C(39)-H(39C)	109.5
C(33)-C(32)-H(32A)	109.5	H(39A)-C(39)-H(39C)	109.5
C(33)-C(32)-H(32B)	109.5	H(39B)-C(39)-H(39C)	109.5
H(32A)-C(32)-H(32B)	109.5	C(38)-C(40)-H(40A)	109.5
C(33)-C(32)-H(32C)	109.5	C(38)-C(40)-H(40B)	109.5
H(32A)-C(32)-H(32C)	109.5	H(40A)-C(40)-H(40B)	109.5
H(32B)-C(32)-H(32C)	109.5	C(38)-C(40)-H(40C)	109.5
C(34)-C(33)-C(32)	119.1(3)	H(40A)-C(40)-H(40C)	109.5
C(34)-C(33)-C(31)	109.9(3)	H(40B)-C(40)-H(40C)	109.5
C(32)-C(33)-C(31)	108.0(3)	N(6)-C(41)-C(42)	118.45(19)
C(34)-C(33)-H(33)	106.4	N(6)-C(41)-S(6)	117.35(15)
C(32)-C(33)-H(33)	106.4	C(42)-C(41)-S(6)	124.13(14)
C(31)-C(33)-H(33)	106.4	C(43)-C(42)-C(41)	111.7(2)
C(33)-C(34)-N(5)	113.5(2)	C(43)-C(42)-C(44)	110.5(2)
C(33)-C(34)-H(34A)	108.9	C(41)-C(42)-C(44)	110.55(19)

C(43)-C(42)-H(42)	108.0	C(51)-C(50)-H(50A)	108.0
C(41)-C(42)-H(42)	108.0	C(49)-C(50)-H(50A)	108.0
C(44)-C(42)-H(42)	108.0	C(51)-C(50)-H(50B)	108.0
C(42)-C(43)-H(43A)	109.5	C(49)-C(50)-H(50B)	108.0
C(42)-C(43)-H(43B)	109.5	H(50A)-C(50)-H(50B)	107.2
H(43A)-C(43)-H(43B)	109.5	C(53)-C(51)-C(50)	115.7(3)
C(42)-C(43)-H(43C)	109.5	C(53)-C(51)-C(52)	111.9(3)
H(43A)-C(43)-H(43C)	109.5	C(50)-C(51)-C(52)	106.8(3)
H(43B)-C(43)-H(43C)	109.5	C(53)-C(51)-H(51)	107.4
C(42)-C(44)-H(44A)	109.5	C(50)-C(51)-H(51)	107.4
C(42)-C(44)-H(44B)	109.5	C(52)-C(51)-H(51)	107.4
H(44A)-C(44)-H(44B)	109.5	C(51)-C(52)-H(52A)	109.5
C(42)-C(44)-H(44C)	109.5	C(51)-C(52)-H(52B)	109.5
H(44A)-C(44)-H(44C)	109.5	H(52A)-C(52)-H(52B)	109.5
H(44B)-C(44)-H(44C)	109.5	C(51)-C(52)-H(52C)	109.5
N(7)-C(45)-C(46)	119.54(18)	H(52A)-C(52)-H(52C)	109.5
N(7)-C(45)-S(7)	117.39(15)	H(52B)-C(52)-H(52C)	109.5
C(46)-C(45)-S(7)	122.86(13)	C(51)-C(53)-H(53A)	109.5
C(45)-C(46)-C(47)	110.72(16)	C(51)-C(53)-H(53B)	109.5
C(45)-C(46)-C(48)	109.39(17)	H(53A)-C(53)-H(53B)	109.5
C(47)-C(46)-C(48)	111.39(19)	C(51)-C(53)-H(53C)	109.5
C(45)-C(46)-H(46)	108.4	H(53A)-C(53)-H(53C)	109.5
C(47)-C(46)-H(46)	108.4	H(53B)-C(53)-H(53C)	109.5
C(48)-C(46)-H(46)	108.4	N(8)-C(54)-C(49)	116.87(18)
C(46)-C(47)-H(47A)	109.5	N(8)-C(54)-S(8)	125.47(18)
C(46)-C(47)-H(47B)	109.5	C(49)-C(54)-S(8)	117.63(16)
H(47A)-C(47)-H(47B)	109.5	C(56)-C(55)-N(8)	117.8(2)
C(46)-C(47)-H(47C)	109.5	C(56)-C(55)-H(55A)	107.9
H(47A)-C(47)-H(47C)	109.5	N(8)-C(55)-H(55A)	107.9
H(47B)-C(47)-H(47C)	109.5	C(56)-C(55)-H(55B)	107.9
C(46)-C(48)-H(48A)	109.5	N(8)-C(55)-H(55B)	107.9
C(46)-C(48)-H(48B)	109.5	H(55A)-C(55)-H(55B)	107.2
H(48A)-C(48)-H(48B)	109.5	C(55)-C(56)-C(57)	126.2(3)
C(46)-C(48)-H(48C)	109.5	C(55)-C(56)-C(58)	116.4(3)
H(48A)-C(48)-H(48C)	109.5	C(57)-C(56)-C(58)	111.9(3)
H(48B)-C(48)-H(48C)	109.5	C(55)-C(56)-H(56)	97.8
O(4)-C(49)-C(54)	110.57(16)	C(57)-C(56)-H(56)	97.8
O(4)-C(49)-C(50)	105.07(16)	C(58)-C(56)-H(56)	97.8
C(54)-C(49)-C(50)	112.45(16)	C(56)-C(57)-H(57A)	109.5
O(4)-C(49)-H(49)	109.6	C(56)-C(57)-H(57B)	109.5
C(54)-C(49)-H(49)	109.6	H(57A)-C(57)-H(57B)	109.5
C(50)-C(49)-H(49)	109.6	C(56)-C(57)-H(57C)	109.5
C(51)-C(50)-C(49)	117.3(2)	H(57A)-C(57)-H(57C)	109.5

H(57B)-C(57)-H(57C)	109.5	C(56)-C(58)-H(58C)	109.5
C(56)-C(58)-H(58A)	109.5	H(58A)-C(58)-H(58C)	109.5
C(56)-C(58)-H(58B)	109.5	H(58B)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58B)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters (A^2 x 10^3) for **8b**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	79(1)	191(1)	66(1)	33(1)	-19(1)	-6(1)
S(2)	105(1)	93(1)	44(1)	-9(1)	-8(1)	32(1)
S(3)	104(1)	89(1)	41(1)	3(1)	-8(1)	-3(1)
S(4)	92(1)	215(1)	64(1)	-27(1)	-23(1)	1(1)
O(1)	69(1)	91(1)	39(1)	-1(1)	1(1)	12(1)
O(2)	64(1)	124(1)	41(1)	4(1)	-1(1)	-8(1)
N(1)	75(1)	89(1)	64(1)	3(1)	-6(1)	5(1)
N(2)	69(1)	86(1)	51(1)	-3(1)	6(1)	0(1)
N(3)	79(1)	119(1)	46(1)	5(1)	0(1)	-16(1)
N(4)	85(1)	129(1)	61(1)	-21(1)	-13(1)	-10(1)
C(1)	538(9)	97(2)	290(4)	60(2)	171(5)	88(4)
C(2)	450(8)	86(2)	210(3)	-34(2)	-56(4)	8(3)
C(3)	268(5)	90(2)	159(3)	28(2)	49(3)	22(2)
C(4)	93(2)	103(1)	106(2)	38(1)	26(2)	12(1)
C(5)	57(1)	105(1)	41(1)	8(1)	10(1)	2(1)
C(6)	73(1)	102(1)	40(1)	2(1)	-2(1)	-18(1)
C(7)	98(2)	110(1)	52(1)	-12(1)	17(1)	-8(1)
C(8)	212(3)	87(2)	257(3)	-55(2)	106(3)	-24(2)
C(9)	506(5)	129(2)	345(4)	-65(3)	233(3)	50(3)
C(10)	294(4)	155(3)	485(6)	106(3)	165(4)	6(3)
C(11)	73(1)	67(1)	40(1)	-4(1)	2(1)	7(1)
C(12)	90(2)	105(1)	46(1)	-2(1)	2(1)	12(1)
C(13)	118(2)	143(2)	88(2)	17(2)	46(2)	4(2)
C(14)	124(2)	116(2)	139(2)	22(2)	39(2)	40(2)
C(15)	71(1)	81(1)	48(1)	-1(1)	1(1)	19(1)
C(16)	93(2)	119(2)	59(1)	6(1)	17(1)	2(1)
C(17)	130(2)	118(2)	123(2)	43(2)	-8(2)	4(2)
C(18)	78(2)	247(3)	132(2)	68(2)	13(2)	-22(2)
C(19)	85(2)	123(2)	38(1)	2(1)	-1(1)	4(1)
C(20)	92(2)	153(2)	68(1)	23(1)	-8(1)	-14(2)
C(21)	152(3)	140(2)	165(3)	1(2)	19(2)	-43(2)
C(22)	227(4)	113(2)	259(4)	9(2)	38(3)	48(2)
C(23)	282(4)	184(3)	180(3)	29(3)	6(3)	-91(3)
C(24)	72(1)	142(2)	41(1)	-2(1)	-1(1)	-2(1)
C(25)	92(2)	132(2)	97(2)	-34(1)	-1(2)	-2(2)

C(26)	269(5)	132(2)	139(2)	-23(2)	40(3)	-60(2)
C(27)	359(7)	141(3)	150(2)	5(2)	-1(4)	-49(3)
C(28)	403(6)	210(2)	311(3)	-158(2)	198(4)	-151(3)
S(5)	93(1)	165(1)	61(1)	-13(1)	27(1)	-3(1)
S(6)	112(1)	89(1)	43(1)	2(1)	14(1)	2(1)
S(7)	109(1)	97(1)	48(1)	-11(1)	15(1)	-31(1)
S(8)	78(1)	159(1)	68(1)	30(1)	23(1)	5(1)
O(3)	86(1)	118(1)	41(1)	7(1)	7(1)	27(1)
O(4)	57(1)	114(1)	41(1)	-1(1)	-2(1)	-17(1)
N(5)	79(1)	106(1)	61(1)	3(1)	-3(1)	7(1)
N(6)	86(1)	109(1)	49(1)	4(1)	-4(1)	11(1)
N(7)	70(1)	92(1)	48(1)	-9(1)	-2(1)	-3(1)
N(8)	64(1)	117(1)	79(1)	24(1)	12(1)	11(1)
C(31)	377(7)	115(2)	163(3)	-26(2)	-25(4)	-7(3)
C(32)	642(10)	199(3)	112(2)	32(2)	-28(4)	141(5)
C(33)	314(5)	98(2)	133(2)	-28(2)	7(3)	32(2)
C(34)	108(2)	126(2)	79(2)	-23(1)	-4(2)	6(2)
C(35)	81(2)	105(1)	50(1)	-2(1)	-2(1)	22(1)
C(36)	78(2)	106(1)	45(1)	10(1)	16(1)	12(1)
C(37)	121(2)	117(2)	71(1)	19(1)	-1(2)	23(2)
C(38)	225(3)	105(2)	165(3)	20(2)	0(3)	54(2)
C(39)	232(3)	144(3)	349(5)	-99(3)	-106(3)	39(2)
C(40)	213(3)	147(3)	491(8)	27(4)	0(5)	70(3)
C(41)	75(1)	84(1)	40(1)	4(1)	0(1)	-6(1)
C(42)	91(2)	108(2)	63(1)	13(1)	-16(1)	-6(1)
C(43)	122(2)	104(2)	105(2)	26(1)	-6(2)	3(2)
C(44)	85(2)	217(3)	129(2)	51(2)	-29(2)	26(2)
C(45)	71(1)	71(1)	39(1)	-1(1)	3(1)	2(1)
C(46)	75(1)	87(1)	53(1)	-9(1)	2(1)	7(1)
C(47)	105(2)	107(2)	103(2)	-9(1)	-16(2)	-35(2)
C(48)	96(2)	129(2)	79(2)	0(1)	-22(1)	24(2)
C(49)	58(1)	113(1)	41(1)	-1(1)	4(1)	2(1)
C(50)	73(2)	151(2)	62(1)	-31(1)	3(1)	-15(1)
C(51)	155(3)	132(2)	394(4)	-106(2)	-70(3)	-38(2)
C(52)	209(3)	164(3)	377(5)	-69(3)	-82(3)	-59(3)
C(53)	258(3)	176(3)	649(8)	-66(5)	-173(4)	47(3)
C(54)	59(1)	120(1)	38(1)	4(1)	-8(1)	5(1)
C(55)	97(2)	120(2)	118(2)	29(2)	14(2)	28(2)
C(56)	322(6)	100(2)	170(3)	11(2)	-13(4)	34(3)
C(57)	452(8)	149(3)	160(2)	-10(2)	-12(5)	-14(5)
C(58)	306(6)	107(2)	319(5)	52(2)	20(5)	51(3)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **8b**.

	x	y	z	U(eq)
H(1X)	1291(12)	4393(8)	3927(5)	68(5)
H(4X)	913(9)	4404(5)	8635(4)	17(3)
H(1A)	1505	6591	3399	463
H(1B)	57	6791	3584	463
H(1C)	362	6394	2903	463
H(2A)	1794	6040	4371	373
H(2B)	1159	5295	4542	373
H(2C)	380	6006	4679	373
H(3)	-493	5653	3763	207
H(4A)	1889	5258	3249	121
H(4B)	549	5196	2872	121
H(6)	-986	3092	3718	86
H(7A)	735	2855	2906	104
H(7B)	1749	3019	3475	104
H(8)	1542	2048	3951	223
H(9A)	1899	1171	3273	490
H(9B)	2490	1887	2990	490
H(9C)	1199	1574	2678	490
H(10A)	-881	1740	3564	467
H(10B)	-387	2018	4268	467
H(10C)	28	1255	4011	467
H(12)	-1056	4146	6327	97
H(13A)	-2043	3074	6422	174
H(13B)	-2840	3189	5753	174
H(13C)	-3169	3645	6397	174
H(14A)	-2673	4485	5200	190
H(14B)	-1651	5008	5527	190
H(14C)	-2915	4792	5928	190
H(16)	2933	4006	6046	108
H(17A)	2341	5168	5881	186
H(17B)	1933	5261	6641	186
H(17C)	1099	4771	6160	186
H(18A)	4724	4140	6615	228
H(18B)	4067	4621	7170	228
H(18C)	4373	4942	6454	228
H(19)	2988	3117	8530	98
H(20A)	1635	2636	9382	125
H(20B)	406	2978	9039	125
H(21)	396	2211	8216	183

H(22A)	2466	2167	7915	300
H(22B)	1914	1385	7983	300
H(22C)	2821	1701	8549	300
H(23A)	762	1538	9424	323
H(23B)	412	1096	8774	323
H(23C)	-547	1692	9036	323
H(25A)	1649	5079	9760	128
H(25B)	473	5331	9310	128
H(26)	3087	5562	9056	216
H(27A)	2157	6403	8277	325
H(27B)	1077	5808	8220	325
H(27C)	2541	5621	8058	325
H(28A)	1679	6753	9083	462
H(28B)	2907	6554	9521	462
H(28C)	1502	6333	9765	462
H(5X)	6070(2)	4180(14)	8958(5)	180(12)
H(8X)	6255(13)	3923(9)	13507(5)	93(6)
H(31A)	7133	2234	7660	327
H(31B)	5658	2248	7881	327
H(31C)	6684	1818	8310	327
H(32A)	5633	2884	9277	477
H(32B)	7118	2968	9463	477
H(32C)	6571	2219	9236	477
H(33)	7750	2991	8443	218
H(34A)	5252	3432	8103	125
H(34B)	6544	3598	7706	125
H(36)	8223	5417	9020	91
H(37A)	5686	5801	8547	124
H(37B)	6978	6034	8178	124
H(38)	6467	6482	9543	198
H(39A)	7946	7405	9173	362
H(39B)	8318	6856	8603	362
H(39C)	8522	6651	9365	362
H(40A)	5066	6932	8621	426
H(40B)	6225	7479	8555	426
H(40C)	5458	7412	9240	426
H(42)	7917	4421	11455	105
H(43A)	6716	3289	10761	166
H(43B)	6145	3682	11398	166
H(43C)	7401	3203	11466	166
H(44A)	8962	3677	10338	215
H(44B)	9500	3618	11079	215
H(44C)	9623	4344	10682	215

H(46)	3917	4324	11155	86
H(47A)	2091	4087	12214	157
H(47B)	3201	3537	12037	157
H(47C)	2085	3695	11513	157
H(48A)	3121	5522	11141	152
H(48B)	2101	5329	11706	152
H(48C)	1976	4986	10984	152
H(49)	3977	5208	13785	85
H(50A)	5663	5456	14613	114
H(50B)	6712	5303	14056	114
H(51)	6259	6309	13502	273
H(52A)	6230	7002	14686	375
H(52B)	7438	6864	14214	375
H(52C)	7056	6297	14766	375
H(53A)	4072	6497	14301	541
H(53B)	4117	6431	13511	541
H(53C)	4679	7118	13867	541
H(55A)	6853	3007	14192	134
H(55B)	5420	2994	14469	134
H(56)	4672	2561	13665	237
H(57A)	6103	3051	12761	380
H(57B)	4763	2643	12715	380
H(57C)	6082	2213	12687	380
H(58A)	6279	1530	13468	366
H(58B)	5014	1566	13916	366
H(58C)	6373	1783	14223	366

Table S8. Torsion angles [deg] for **8b**.

C(11)-S(2)-S(3)-C(15)	-105.44(10)
C(6)-O(1)-N(2)-C(11)	170.44(16)
C(19)-O(2)-N(3)-C(15)	157.18(17)
C(2)-C(3)-C(4)-N(1)	58.7(4)
C(1)-C(3)-C(4)-N(1)	-176.4(3)
C(5)-N(1)-C(4)-C(3)	93.8(3)
C(4)-N(1)-C(5)-C(6)	178.08(18)
C(4)-N(1)-C(5)-S(1)	2.3(3)
N(2)-O(1)-C(6)-C(5)	66.69(19)
N(2)-O(1)-C(6)-C(7)	-170.98(15)
N(1)-C(5)-C(6)-O(1)	42.0(2)
S(1)-C(5)-C(6)-O(1)	-141.98(15)
N(1)-C(5)-C(6)-C(7)	-76.4(2)
S(1)-C(5)-C(6)-C(7)	99.63(19)
O(1)-C(6)-C(7)-C(8)	67.6(2)
C(5)-C(6)-C(7)-C(8)	-170.2(2)
C(6)-C(7)-C(8)-C(10)	19.5(4)
C(6)-C(7)-C(8)-C(9)	166.3(3)
O(1)-N(2)-C(11)-C(12)	-176.24(16)
O(1)-N(2)-C(11)-S(2)	-2.6(2)
S(3)-S(2)-C(11)-N(2)	-179.20(14)
S(3)-S(2)-C(11)-C(12)	-5.78(17)
N(2)-C(11)-C(12)-C(13)	92.9(2)
S(2)-C(11)-C(12)-C(13)	-80.3(2)
N(2)-C(11)-C(12)-C(14)	-30.6(3)
S(2)-C(11)-C(12)-C(14)	156.21(16)
O(2)-N(3)-C(15)-C(16)	174.36(17)
O(2)-N(3)-C(15)-S(3)	-4.6(2)
S(2)-S(3)-C(15)-N(3)	-171.03(15)
S(2)-S(3)-C(15)-C(16)	10.1(2)
N(3)-C(15)-C(16)-C(18)	24.9(3)
S(3)-C(15)-C(16)-C(18)	-156.3(2)
N(3)-C(15)-C(16)-C(17)	-100.2(2)
S(3)-C(15)-C(16)-C(17)	78.7(2)
N(3)-O(2)-C(19)-C(20)	-169.31(16)
N(3)-O(2)-C(19)-C(24)	69.3(2)
O(2)-C(19)-C(20)-C(21)	58.1(3)
C(24)-C(19)-C(20)-C(21)	178.8(2)
C(19)-C(20)-C(21)-C(22)	39.7(3)
C(19)-C(20)-C(21)-C(23)	171.0(3)

C(25)-N(4)-C(24)-C(19)	179.1(2)
C(25)-N(4)-C(24)-S(4)	0.9(3)
O(2)-C(19)-C(24)-N(4)	25.8(3)
C(20)-C(19)-C(24)-N(4)	-91.1(2)
O(2)-C(19)-C(24)-S(4)	-155.80(15)
C(20)-C(19)-C(24)-S(4)	87.3(2)
C(24)-N(4)-C(25)-C(26)	88.0(3)
N(4)-C(25)-C(26)-C(27)	55.7(5)
N(4)-C(25)-C(26)-C(28)	177.2(3)
C(41)-S(6)-S(7)-C(45)	-105.10(10)
C(36)-O(3)-N(6)-C(41)	160.87(17)
C(49)-O(4)-N(7)-C(45)	167.88(16)
C(32)-C(33)-C(34)-N(5)	52.9(5)
C(31)-C(33)-C(34)-N(5)	178.2(3)
C(35)-N(5)-C(34)-C(33)	90.1(3)
C(34)-N(5)-C(35)-C(36)	-179.04(19)
C(34)-N(5)-C(35)-S(5)	4.9(3)
N(6)-O(3)-C(36)-C(35)	69.5(2)
N(6)-O(3)-C(36)-C(37)	-167.80(16)
N(5)-C(35)-C(36)-O(3)	27.3(3)
S(5)-C(35)-C(36)-O(3)	-156.36(15)
N(5)-C(35)-C(36)-C(37)	-91.1(2)
S(5)-C(35)-C(36)-C(37)	85.3(2)
O(3)-C(36)-C(37)-C(38)	61.4(3)
C(35)-C(36)-C(37)-C(38)	-176.4(2)
C(36)-C(37)-C(38)-C(40)	-167.5(3)
C(36)-C(37)-C(38)-C(39)	72.4(3)
O(3)-N(6)-C(41)-C(42)	176.77(17)
O(3)-N(6)-C(41)-S(6)	-0.4(2)
S(7)-S(6)-C(41)-N(6)	-170.04(16)
S(7)-S(6)-C(41)-C(42)	12.9(2)
N(6)-C(41)-C(42)-C(43)	-99.7(2)
S(6)-C(41)-C(42)-C(43)	77.3(2)
N(6)-C(41)-C(42)-C(44)	23.7(3)
S(6)-C(41)-C(42)-C(44)	-159.25(19)
O(4)-N(7)-C(45)-C(46)	-177.35(16)
O(4)-N(7)-C(45)-S(7)	-2.5(2)
S(6)-S(7)-C(45)-N(7)	177.82(14)
S(6)-S(7)-C(45)-C(46)	-7.46(18)
N(7)-C(45)-C(46)-C(47)	-23.4(3)
S(7)-C(45)-C(46)-C(47)	161.99(16)
N(7)-C(45)-C(46)-C(48)	99.7(2)
S(7)-C(45)-C(46)-C(48)	-74.9(2)

N(7)-O(4)-C(49)-C(54)	70.70(19)
N(7)-O(4)-C(49)-C(50)	-167.74(15)
O(4)-C(49)-C(50)-C(51)	66.0(3)
C(54)-C(49)-C(50)-C(51)	-173.7(2)
C(49)-C(50)-C(51)-C(53)	46.4(4)
C(49)-C(50)-C(51)-C(52)	171.6(2)
C(55)-N(8)-C(54)-C(49)	-179.4(2)
C(55)-N(8)-C(54)-S(8)	2.7(3)
O(4)-C(49)-C(54)-N(8)	38.4(2)
C(50)-C(49)-C(54)-N(8)	-78.7(2)
O(4)-C(49)-C(54)-S(8)	-143.50(14)
C(50)-C(49)-C(54)-S(8)	99.41(19)
C(54)-N(8)-C(55)-C(56)	103.4(4)
N(8)-C(55)-C(56)-C(57)	26.8(7)
N(8)-C(55)-C(56)-C(58)	178.4(4)

Symmetry transformations used to generate equivalent atoms:

Table S9. Hydrogen-bonds for **8b** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4X)...O(2)	0.813(8)	2.235(10)	2.696(2)	116.3(8)
C(10)-H(10B)...O(1)	0.96	2.60	3.232(4)	123.7
C(12)-H(12)...S(3)	0.98	2.69	3.199(2)	112.8
C(13)-H(13A)...S(3)	0.96	3.00	3.579(3)	120.4
C(16)-H(16)...S(2)	0.98	2.71	3.242(2)	114.6
C(22)-H(22A)...O(2)	0.96	2.64	3.213(4)	118.5
C(25)-H(25A)...S(4)	0.97	2.72	3.084(3)	102.8
N(5)-H(5X)...O(3)	0.864(11)	2.22(2)	2.674(2)	113(2)
N(5)-H(5X)...N(6)	0.864(11)	2.532(17)	3.075(2)	121.7(18)
C(42)-H(42)...S(7)	0.98	2.75	3.259(2)	112.8
C(48)-H(48A)...S(6)	0.96	2.90	3.506(3)	122.0
C(55)-H(55B)...S(8)	0.97	2.66	3.130(3)	110.1
C(16)-H(16)...S(8)#1	0.98	2.97	3.819(2)	146.1
N(1)-H(1X)...S(8)#1	0.869(10)	2.802(11)	3.6082(19)	154.8(10)
N(4)-H(4X)...S(5)#2	0.813(8)	2.912(9)	3.657(2)	153.4(9)
C(1)-H(1B)...S(3)#3	0.96	2.89	3.636(4)	135.4
N(8)-H(8X)...S(1)#4	0.881(11)	2.802(12)	3.607(2)	152.6(11)
C(42)-H(42)...S(1)#4	0.98	2.92	3.763(2)	144.1
C(52)-H(52B)...S(2)#5	0.96	2.99	3.775(4)	140.0

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x-1,y,z #3 -x,y+1/2,-z+1 #4 x+1,y,z+1

#5 -x+1,y+1/2,-z+2

Table S10. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

- 5.5504 (0.0061) x + 6.5692 (0.0180) y + 15.0502 (0.0085) z = 7.8817 (0.0064)

* -0.0089 (0.0006) N1
* 0.0236 (0.0015) C5
* -0.0075 (0.0005) S1
* -0.0072 (0.0005) C6

Rms deviation of fitted atoms = 0.0136

5.3734 (0.0061) x + 15.8283 (0.0076) y + 0.0910 (0.0207) z = 5.5431 (0.0128)

Angle to previous plane (with approximate esd) = 89.00 (0.07)

* 0.0370 (0.0016) C11
* -0.0125 (0.0005) C12
* -0.0141 (0.0006) N2
* -0.0104 (0.0004) S2
* 0.0642 (0.0024) S3

Rms deviation of fitted atoms = 0.0214

- 6.9422 (0.0053) x + 13.5156 (0.0106) y + 2.0296 (0.0238) z = 5.1643 (0.0145)

Angle to previous plane (with approximate esd) = 74.93 (0.04)

* 0.0018 (0.0005) S3
* -0.0061 (0.0017) C15
* 0.0021 (0.0006) C16
* 0.0022 (0.0006) N3
-0.3239 (0.0026) S2

Rms deviation of fitted atoms = 0.0035

- 6.3335 (0.0059) x - 7.4448 (0.0196) y + 13.3348 (0.0113) z = 7.6702 (0.0163)

Angle to previous plane (with approximate esd) = 78.42 (0.07)

* 0.0029 (0.0005) C19

* -0.0096 (0.0018) C24
* 0.0029 (0.0006) S4
* 0.0037 (0.0007) N4

Rms deviation of fitted atoms = 0.0055

5.7518 (0.0062) x - 9.5594 (0.0179) y + 12.7915 (0.0116) z = 10.5811 (0.0184)

Angle to previous plane (with approximate esd) = 72.98 (0.06)

* -0.0082 (0.0007) N5
* 0.0212 (0.0017) C35
* -0.0064 (0.0005) S5
* -0.0066 (0.0005) C36

Rms deviation of fitted atoms = 0.0123

7.0553 (0.0050) x + 13.0184 (0.0114) y + 3.6139 (0.0235) z = 14.8923 (0.0223)

Angle to previous plane (with approximate esd) = 81.46 (0.07)

* 0.0163 (0.0017) C41
* -0.0056 (0.0006) C42
* -0.0061 (0.0007) N6
* -0.0046 (0.0005) S6
  0.3803 (0.0026) S7

Rms deviation of fitted atoms = 0.0094

- 5.3034 (0.0061) x + 15.8492 (0.0070) y + 1.4349 (0.0210) z = 6.9651 (0.0279)

Angle to previous plane (with approximate esd) = 75.53 (0.05)

* 0.0082 (0.0004) S7
* -0.0294 (0.0016) C45
* 0.0100 (0.0005) C46
* 0.0112 (0.0006) N7
  -0.1481 (0.0024) S6

Rms deviation of fitted atoms = 0.0170

5.6898 (0.0062) x + 5.7482 (0.0185) y + 15.2328 (0.0082) z = 26.5916 (0.0101)

Angle to previous plane (with approximate esd) = 88.31 (0.07)

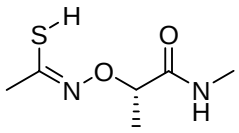
* 0.0034 (0.0005) C49
* -0.0112 (0.0016) C54
* 0.0034 (0.0005) S8
* 0.0044 (0.0006) N8

Rms deviation of fitted atoms = 0.0065

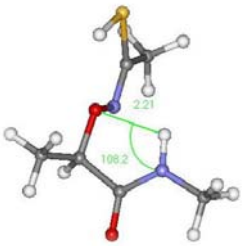
Theoretical Studies on Model Compounds I–IV

All the calculations were conducted by using the Gaussian 98 software package.[1] Structures of model compounds **I** and **II** were fully optimized using B3LYP[2]/6-311+G** method followed by harmonic vibration frequency calculations to ensure that each structure was a minimum. Energies were evaluated by the MP2[3]/6-311+G** calculations on the B3LYP/6-311+G** geometries. Solvent effect was evaluated by the PCM model using the B3LYP/6-311+G** method. The relative free energies of structures were calculated with the MP2/6-311+G** energies plus the enthalpy and entropy corrections along with the solvent energy corrections as shown in eq. 1. Structures of model compounds **III** and **IV** were optimized using B3LYP/6-31G** method by harmonic vibration frequency calculations to ensure that each structure was a minimum. Energies were evaluated by the MP2/6-31G** calculations on the B3LYP/6-31G** geometries. Solvent effect was evaluated by the PCM model using the B3LYP/6-31G** method. The relative free energies of structures were also calculated with the MP2/6-31G** energies plus the enthalpy and entropy corrections along with solvent energy corrections as shown in eq. 1.

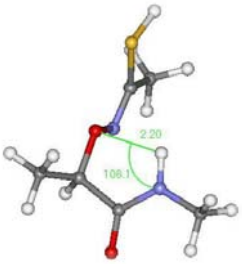
$$\Delta G = \Delta E(MP2) + [\Delta E(B3LYP, solvent) - \Delta E(B3LYP)] + \text{enthalpy correction} - T\Delta S \qquad \text{(eq. 1)}$$



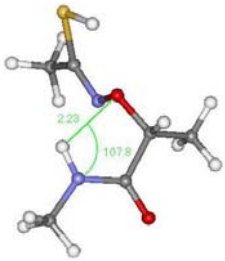
III



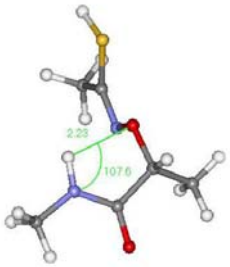
IIIa 0.0 (0.0)



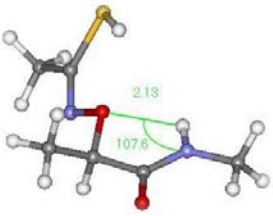
IIIb 0.9 (0.3)



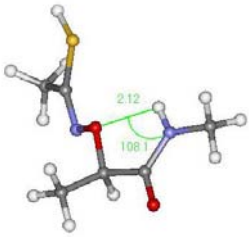
IIIc 0.8 (0.5)



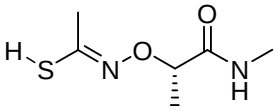
IIId 1.7 (0.7)



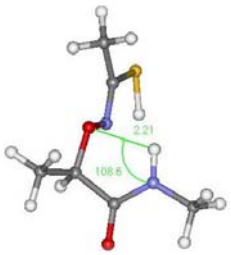
IIIe 0.8 (0.5)



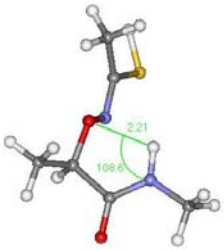
IIIf 1.3 (0.4)



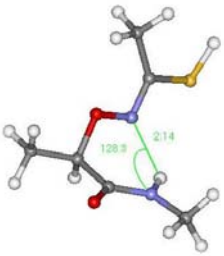
IV



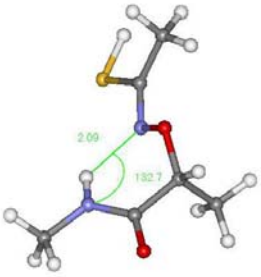
IVa 3.4 (2.8)



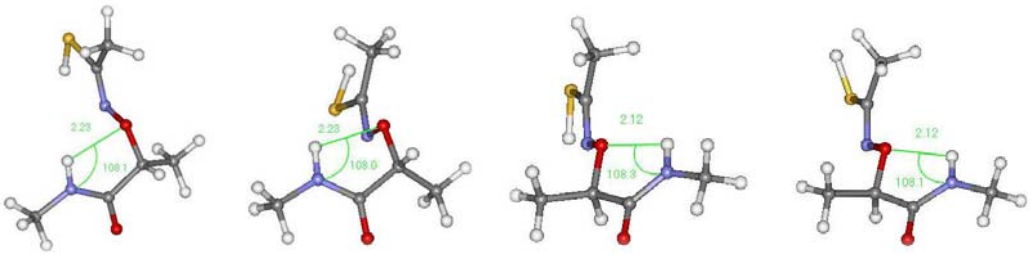
IVb 5.4 (4.2)



IVc 6.0 (5.5)



IVd 6.3 (5.8)



IVe 4.2 (3.7) **IVf** 6.0 (5.0) **IVg** 3.9 (3.1) **IVh** 5.8 (4.4)

Figure S4. B3LYP/6-31G**-Optimized structures of the *Z*-isomer model **III** and *E*-isomer model **IV** with their MP2/6-31G** relative energies (kcal mol^{-1}) in the gas phase and in CH_2Cl_2 (in parentheses). Gray = C, red = O, blue = N, yellow = S, white = H.

References:

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Oritz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98*, revision A.11.3, Gaussian, Inc.: Pittsburgh, PA, 2002.
2. (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785–789.
3. (a) Moller, C.; Plesset, M. S. *Phys. Rev.* **1934,** 46, 618–622. (b) Frisch M. J.; Headgordon M.; Pople, J. A. *Chem. Phys. Lett.* **1990,** 166, 275–280. (c) Frisch, M. J.; Headgordon, M.; Pople J. A. *Chem. Phys. Lett.* **1990,** 166, 281–289.

Table S11. Calculated Energies and Relative Energies of Compounds **I** and **II**

	Gas phase		Solvent (CH_2Cl_2) B3LYP /6-311+G** (hartree)	Enthalpy correction (hartree)	Entropy correction (hartree)	ΔG MP2/6-311+G**	
	B3LPY /6-311+G** (hartree)	MP2 /6-311+G** (hartree)				(Gas phase) (kcal/mol)	(CH_2Cl_2) (kcal/mol)
Ia	-571.560707	-570.4661152	-571.5702187	0.107283	0.068697	0.0	0.0
Ib	-571.540646	-570.4482512	-571.5461839	0.103261	0.064036	7.8	11.7
Ic	-571.539863	-570.4493354	-571.5473399	0.103192	0.064394	8.3	12.2
IIa	-646.734591	-645.4697665	-646.7444046	0.111806	0.069951	7.2	2.7
IIb	-646.740941	-645.4789026	-646.7463531	0.108621	0.067603	0.0	0.0
IIc	-646.738589	-645.4768413	-646.7456439	0.108705	0.067551	1.3	0.4

Table S12. Calculated Energies and Relative Energies of Compounds **III and IV**

	Gas phase		Solvent (CH_2Cl_2) B3LYP /6-31G** (hartree)	Enthalpy correction (hartree)	Entropy correction (hartree)	ΔG MP2/6-31G**	
	B3LPY /6-31G** (hartree)	MP2 /6-31G** (hartree)				(Gas phase) (kcal/mol)	(CH_2Cl_2) (kcal/mol)
IIIa	-893.987053	-891.9606296	-893.9945719	0.198964	0.142400	0.0	0.0
IIIb	-893.985948	-891.9594366	-893.9944757	0.199174	0.142688	0.9	0.3
IIIc	-893.986679	-891.9594899	-893.9947215	0.198949	0.142438	0.8	0.5
IIId	-893.984153	-891.9581573	-893.9932851	0.199109	0.142608	1.7	0.7
IIIe	-893.985405	-891.9595505	-893.9933286	0.198946	0.142505	0.8	0.5
IIIf	-893.985941	-891.9586924	-893.9949667	0.199180	0.142533	1.3	0.4
IVa	-893.981144	-891.9544673	-893.9896404	0.198856	0.141638	3.4	2.8
IVb	-893.978163	-891.951156	-893.9874822	0.198888	0.141468	5.4	4.2
IVc	-893.977188	-891.9497653	-893.9855033	0.198860	0.141171	6.0	5.5
IVd	-893.976176	-891.9490414	-893.9845729	0.198865	0.140890	6.3	5.8
IVe	-893.979549	-891.9534682	-893.9879011	0.198785	0.141991	4.2	3.7
IVf	-893.976674	-891.9503077	-893.9858793	0.198823	0.141706	6.0	5.0
IVg	-893.980974	-891.9534635	-893.9897275	0.198777	0.141447	3.9	3.1
IVh	-893.978193	-891.9505125	-893.9879758	0.198845	0.141501	5.8	4.4

Table S13. Geometries (Cartesian coordinates) of the conformations of compounds **I** and **II** optimized by B3LYP/6-311+G** and those of compounds **III** and **IV** optimized by B3LYP/6-31G**

(1) **Ia**

1	H	0	2.118835	-0.692726	0.893599
2	C	0	2.101183	-0.059188	0.003758
3	N	0	0.911448	0.778430	-0.004979
4	C	0	-0.349444	0.309195	-0.005584
5	S	0	-0.717582	-1.315750	-0.000298
6	C	0	-1.423159	1.374478	0.002320
7	H	0	-2.131526	1.187311	-0.805122
8	H	0	-1.978620	1.321012	0.941079
9	H	0	1.043954	1.778613	-0.009462
10	H	0	-1.018604	2.385972	-0.107471
11	H	0	2.978617	0.588088	-0.004162
12	H	0	2.117034	-0.712190	-0.871794

(2) **Ib**

1	H	0	-2.996042	0.535024	-0.288378
2	C	0	-2.092968	-0.005375	-0.002737
3	N	0	-0.966035	0.910105	-0.005674
4	C	0	0.220088	0.479966	-0.004951
5	S	0	0.613972	-1.303448	0.006303
6	C	0	1.394611	1.422552	0.004589
7	H	0	2.001952	1.277777	0.902512
8	H	0	2.035640	1.256556	-0.866059
9	H	0	1.020946	2.445919	-0.014755
10	H	0	-2.249292	-0.415306	1.002316
11	H	0	-1.953754	-0.846715	-0.694865
12	H	0	1.948856	-1.151684	-0.083298

(3) **Ic**

1	H	0	-3.038986	0.559039	-0.000489
2	C	0	-2.118533	-0.025492	0.000003
3	N	0	-0.985272	0.878270	-0.000037
4	C	0	0.211059	0.474325	-0.000056
5	S	0	0.807621	-1.247556	-0.000037
6	C	0	1.360768	1.447628	0.000030

7	H	0	1.988893	1.305304	0.884023
8	H	0	1.990838	1.303411	-0.882256
9	H	0	0.962330	2.461404	-0.001437
10	H	0	-2.128284	-0.668202	0.890266
11	H	0	-2.127823	-0.668980	-0.889708
12	H	0	-0.391774	-1.857736	0.000587

(4) **IIa**

1	C	0	-2.369849	0.145724	0.482326
2	O	0	-1.552680	-0.302956	-0.614219
3	N	0	-0.404609	-0.927197	-0.162817
4	C	0	0.765533	-0.262616	-0.018107
5	C	0	1.931811	-1.195193	0.228741
6	S	0	0.921268	1.384987	-0.051010
7	H	0	2.700428	-1.009424	-0.522999
8	H	0	2.367489	-0.980743	1.205584
9	H	0	-0.415036	-1.920991	-0.354553
10	H	0	-3.236646	0.605605	0.009060
11	H	0	-2.684117	-0.700699	1.100313
12	H	0	-1.834269	0.885677	1.078550
13	H	0	1.650591	-2.252685	0.195918

(5) **IIb**

1	C	0	2.781340	0.074337	-0.000105
2	O	0	1.423163	-0.362620	0.000296
3	N	0	0.576022	0.754213	0.000016
4	C	0	-0.666214	0.449357	-0.000159
5	C	0	-1.669266	1.566379	-0.000034
6	S	0	-1.346610	-1.195409	0.000054
7	H	0	-2.312108	1.508458	-0.882915
8	H	0	-2.309263	1.510599	0.885083
9	H	0	3.379040	-0.837223	0.000959
10	H	0	2.997844	0.663605	-0.895079
11	H	0	2.997683	0.665605	0.893580
12	H	0	-1.144935	2.521848	-0.001925
13	H	0	-0.155116	-1.825317	-0.001255

(6) **IIc**

1	C	0	-2.768212	0.069229	0.000104
2	O	0	-1.403241	-0.340532	-0.000179
3	N	0	-0.570647	0.783599	-0.000035
4	C	0	0.663703	0.456235	0.000031
5	S	0	1.166462	-1.257988	0.000010
6	C	0	1.695922	1.545689	0.000006
7	H	0	2.334905	1.475656	0.884936
8	H	0	2.334043	1.476362	-0.885609
9	H	0	-3.346851	-0.854372	-0.000372
10	H	0	-2.997543	0.654236	0.895092
11	H	0	-2.997604	0.655208	-0.894227
12	H	0	1.195081	2.514033	0.000618
13	H	0	2.486558	-0.981168	0.000225

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(7) **IIIa**

1	C	0	2.601590	-2.169892	-0.820914
2	N	0	1.738586	-1.038813	-0.539893
3	C	0	2.111520	-0.022208	0.278019
4	C	0	1.071964	1.095168	0.466002
5	C	0	1.531666	2.375260	-0.223443
6	O	0	3.206832	0.073241	0.821890
7	O	0	-0.221704	0.762029	-0.076253
8	N	0	-0.945379	-0.017416	0.850599
9	C	0	-2.135051	-0.287486	0.454355
10	S	0	-2.888264	0.221021	-1.080176
11	C	0	-3.001920	-1.118524	1.357429
12	H	0	0.798941	-1.014814	-0.905899
13	H	0	2.787992	-2.268273	-1.896005
14	H	0	3.548261	-1.993237	-0.309065
15	H	0	2.165273	-3.105339	-0.453005
16	H	0	0.966666	1.252798	1.542776
17	H	0	0.846242	3.197254	-0.002507
18	H	0	2.531183	2.630331	0.133955
19	H	0	1.575503	2.235480	-1.308112
20	H	0	-1.858054	0.990421	-1.481429
21	H	0	-3.327290	-2.033184	0.850592
22	H	0	-2.436327	-1.387367	2.251169
23	H	0	-3.898251	-0.562865	1.651605

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(8) **IIIb**

1	C	0	-2.471170	2.294561	-0.574372
2	N	0	-1.654932	1.109096	-0.400259
3	C	0	-2.078835	0.027309	0.301280
4	O	0	-3.178012	-0.074109	0.836552
5	C	0	-1.092501	-1.150901	0.357359
6	O	0	0.221524	-0.801524	-0.119776
7	N	0	0.991039	-0.253409	0.922200
8	C	0	2.134107	0.137996	0.498387
9	C	0	3.100025	0.725286	1.486957
10	C	0	-1.591603	-2.310595	-0.497771
11	S	0	2.590699	-0.009880	-1.225599
12	H	0	-0.726657	1.068218	-0.794508
13	H	0	-2.658379	2.495075	-1.635203
14	H	0	-3.422373	2.112750	-0.072678
15	H	0	-1.994711	3.175661	-0.129923
16	H	0	-1.010400	-1.448354	1.406171
17	H	0	-0.941579	-3.180611	-0.377439
18	H	0	-2.606725	-2.568903	-0.189457
19	H	0	-1.608220	-2.029560	-1.555216
20	H	0	3.789231	0.588625	-1.076783
21	H	0	3.373384	1.748399	1.207477
22	H	0	2.635382	0.738888	2.474512
23	H	0	4.018872	0.131209	1.533791

(9) **IIIc**

1	C	0	-2.734298	-2.253310	-0.062196
2	N	0	-1.828530	-1.159896	-0.357873
3	C	0	-2.137319	0.134577	-0.085962
4	C	0	-1.057654	1.162843	-0.480690
5	C	0	-1.043158	2.369400	0.447153
6	O	0	-3.214892	0.509512	0.363548
7	O	0	0.245191	0.566433	-0.663649
8	N	0	0.787138	0.171339	0.578935
9	C	0	2.012196	-0.197343	0.490539
10	S	0	3.013902	-0.217145	-0.984819
11	C	0	2.694253	-0.671317	1.742715
12	H	0	-0.888472	-1.355960	-0.665735
13	H	0	-2.352629	-2.884500	0.748864
14	H	0	-3.684581	-1.817080	0.247192

15	H	0	-2.895493	-2.878116	-0.947078
16	H	0	-1.303018	1.486030	-1.499997
17	H	0	-0.352595	3.127733	0.068723
18	H	0	-2.050146	2.785854	0.500184
19	H	0	-0.734857	2.077855	1.452768
20	H	0	2.082188	0.347999	-1.776706
21	H	0	3.563778	-0.045734	1.969068
22	H	0	1.990921	-0.624327	2.575845
23	H	0	3.045690	-1.702190	1.627993

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(10) **IIId**

1	C	0	-2.638068	-2.303516	0.056729
2	N	0	-1.767708	-1.196456	-0.288250
3	C	0	-2.118849	0.099615	-0.081940
4	C	0	-1.071333	1.136067	-0.537820
5	C	0	-1.110466	2.406070	0.299681
6	O	0	-3.204988	0.460904	0.358116
7	O	0	0.251026	0.569818	-0.657858
8	N	0	0.799633	0.300268	0.610890
9	C	0	2.006449	-0.113907	0.508719
10	S	0	2.803001	-0.284058	-1.084619
11	C	0	2.751574	-0.463944	1.764942
12	H	0	-0.830384	-1.374955	-0.615571
13	H	0	-2.225606	-2.898117	0.880277
14	H	0	-3.594769	-1.883302	0.368790
15	H	0	-2.797657	-2.960876	-0.804772
16	H	0	-1.309386	1.375703	-1.581469
17	H	0	-0.439037	3.157052	-0.124737
18	H	0	-2.131167	2.791385	0.309629
19	H	0	-0.808365	2.198783	1.327745
20	H	0	3.965954	-0.741280	-0.578929
21	H	0	3.651358	0.151729	1.868110
22	H	0	2.102426	-0.291376	2.625307
23	H	0	3.060994	-1.514592	1.757121

---

(11) **IIIe**

1	C	0	-3.207294	-2.000707	-0.357030
2	N	0	-2.086489	-1.082009	-0.295977
3	C	0	-2.246793	0.254402	-0.118369

4	C	0	-0.951253	1.083089	-0.132590
5	C	0	-0.968163	2.182689	0.920465
6	O	0	-3.330514	0.814097	0.008444
7	O	0	0.174529	0.198421	0.054416
8	N	0	1.294373	0.691889	-0.641088
9	C	0	2.383043	0.087670	-0.333019
10	S	0	2.573461	-1.212953	0.871756
11	C	0	3.637363	0.494411	-1.053068
12	H	0	-1.140706	-1.422245	-0.386943
13	H	0	-3.138857	-2.761785	0.428067
14	H	0	-4.117506	-1.418144	-0.211332
15	H	0	-3.256950	-2.503473	-1.329386
16	H	0	-0.860335	1.519885	-1.134045
17	H	0	-0.079181	2.810416	0.820014
18	H	0	-1.863689	2.793322	0.793429
19	H	0	-0.983813	1.749912	1.925178
20	H	0	1.317094	-1.125941	1.350056
21	H	0	4.065909	-0.354960	-1.595718
22	H	0	3.402779	1.288304	-1.764187
23	H	0	4.391149	0.853334	-0.344989

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(12) **IIIf**

1	C	0	3.114773	2.037335	-0.313840
2	N	0	2.020660	1.086942	-0.260010
3	C	0	2.222551	-0.250478	-0.152830
4	O	0	3.324449	-0.787976	-0.109032
5	C	0	0.951617	-1.115667	-0.128629
6	O	0	-0.194373	-0.261633	0.065674
7	N	0	-1.326104	-0.811093	-0.554723
8	C	0	-2.378114	-0.130333	-0.291201
9	C	0	-3.681147	-0.564005	-0.898363
10	C	0	1.024154	-2.194071	0.944396
11	S	0	-2.315444	1.306214	0.772801
12	H	0	1.063822	1.409238	-0.266556
13	H	0	3.079915	2.731215	0.533517
14	H	0	4.045354	1.470407	-0.272268
15	H	0	3.090134	2.617597	-1.242953
16	H	0	0.857148	-1.573551	-1.120279
17	H	0	0.153736	-2.851281	0.873960
18	H	0	1.936138	-2.778323	0.809522
19	H	0	1.043956	-1.739976	1.939482

20	H	0	-3.620675	1.611233	0.633430
21	H	0	-4.096971	0.223201	-1.536414
22	H	0	-3.513435	-1.457323	-1.502769
23	H	0	-4.417523	-0.792604	-0.120688

(13) **IVa**

1	C	0	-2.572890	-2.247285	0.821852
2	N	0	-1.790171	-1.049084	0.590772
3	C	0	-2.110271	-0.139382	-0.364290
4	C	0	-1.164938	1.069151	-0.468584
5	C	0	-1.854297	2.329894	0.043578
6	O	0	-3.098914	-0.202372	-1.087741
7	O	0	0.045280	0.912624	0.294917
8	N	0	0.971837	0.130728	-0.446441
9	C	0	2.119505	0.123036	0.125087
10	S	0	3.413373	-0.835802	-0.637067
11	C	0	2.490672	0.837528	1.395640
12	H	0	-0.929394	-0.897968	1.094401
13	H	0	-2.892589	-2.313807	1.867488
14	H	0	-3.453918	-2.190456	0.181424
15	H	0	-2.007080	-3.151562	0.569503
16	H	0	-0.904281	1.175736	-1.525430
17	H	0	-1.224195	3.206528	-0.126372
18	H	0	-2.801864	2.456426	-0.483872
19	H	0	-2.059545	2.247880	1.115417
20	H	0	2.655173	-1.298619	-1.651669
21	H	0	3.572159	0.959751	1.482577
22	H	0	2.005258	1.815366	1.417096
23	H	0	2.137028	0.272377	2.265083

(14) **IVb**

1	C	0	-2.555850	-2.269830	0.806641
2	N	0	-1.779471	-1.066233	0.580865
3	C	0	-2.124069	-0.138601	-0.347750
4	O	0	-3.133320	-0.185970	-1.043377
5	C	0	-1.178245	1.068458	-0.463489
6	O	0	0.035585	0.915788	0.298223
7	N	0	0.970543	0.161923	-0.448985
8	C	0	2.126205	0.152996	0.106302

9	C	0	2.537146	0.869666	1.362996
10	C	0	-1.864424	2.333671	0.041023
11	S	0	3.293803	-0.928214	-0.713393
12	H	0	-0.904264	-0.928855	1.062757
13	H	0	-2.843532	-2.360968	1.859662
14	H	0	-3.455732	-2.197812	0.194667
15	H	0	-1.998262	-3.167420	0.515449
16	H	0	-0.918446	1.166619	-1.521169
17	H	0	-1.235859	3.209012	-0.140872
18	H	0	-2.815100	2.454060	-0.481972
19	H	0	-2.063680	2.261527	1.114757
20	H	0	4.399012	-0.326376	-0.230004
21	H	0	3.504956	1.361764	1.226117
22	H	0	1.787820	1.614763	1.629059
23	H	0	2.642041	0.158573	2.189574

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(15) **IVc**

1	C	0	1.288740	-0.996980	-0.598717
2	C	0	2.120625	0.181038	-0.033211
3	O	0	3.245795	0.009048	0.424502
4	N	0	1.514191	1.394608	-0.128031
5	H	0	0.557640	1.410960	-0.460051
6	C	0	2.115939	2.605990	0.397396
7	H	0	1.568500	2.984125	1.269181
8	H	0	3.135734	2.364875	0.698449
9	H	0	2.141403	3.391194	-0.365569
10	H	0	1.086836	-0.809389	-1.660633
11	C	0	1.997315	-2.324856	-0.407559
12	H	0	1.400596	-3.133401	-0.836730
13	H	0	2.973262	-2.293930	-0.894852
14	H	0	2.164315	-2.519991	0.654010
15	O	0	0.012189	-1.119850	0.073927
16	C	0	-2.035289	-0.232983	0.170301
17	N	0	-0.891205	-0.161212	-0.405328
18	S	0	-3.258393	0.864802	-0.538659
19	H	0	-4.017642	0.961585	0.571360
20	C	0	-2.433633	-1.179451	1.266960
21	H	0	-1.549291	-1.656402	1.688367
22	H	0	-2.972193	-0.648238	2.058042
23	H	0	-3.101826	-1.952136	0.872040

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(16) **IVd**

1	C	0	2.594119	2.311867	-0.250151
2	N	0	1.731294	1.144677	-0.243028
3	C	0	2.228296	-0.112801	-0.143346
4	C	0	1.215009	-1.273287	-0.079163
5	C	0	1.132040	-1.853039	1.332047
6	O	0	3.424599	-0.386697	-0.092325
7	O	0	-0.084072	-1.012026	-0.652887
8	N	0	-0.828735	-0.107811	0.127315
9	C	0	-2.074679	-0.123082	-0.177463
10	S	0	-3.022022	1.159128	0.634225
11	C	0	-2.744632	-1.031365	-1.169723
12	H	0	0.731969	1.258107	-0.133921
13	H	0	2.537121	2.862869	0.696482
14	H	0	3.618487	1.966628	-0.392228
15	H	0	2.321802	2.988966	-1.066120
16	H	0	0.514963	-2.756036	1.335018
17	H	0	2.138445	-2.107133	1.672271
18	H	0	0.697120	-1.128101	2.024520
19	H	0	-4.224684	0.579643	0.450512
20	H	0	-2.937036	-0.492535	-2.103837
21	H	0	-2.098487	-1.882160	-1.384748
22	H	0	-3.705024	-1.386520	-0.784846
23	H	0	1.614640	-2.027815	-0.762233

(17) **IVe**

1	C	0	-2.667985	2.302415	0.207632
2	N	0	-1.874390	1.120332	0.481887
3	C	0	-2.155197	-0.090534	-0.066508
4	C	0	-1.205478	-1.230906	0.354681
5	C	0	-1.050527	-2.283528	-0.734214
6	O	0	-3.127364	-0.318715	-0.778406
7	O	0	0.052769	-0.751748	0.872034
8	N	0	0.827139	-0.192698	-0.181261
9	C	0	2.033134	0.009255	0.202306
10	S	0	3.152816	0.766720	-0.959251
11	C	0	2.608894	-0.311471	1.554413
12	H	0	-1.009766	1.201700	0.994472
13	H	0	-2.112021	3.031456	-0.393653

14	H	0	-3.549170	1.983712	-0.350229
15	H	0	-2.986064	2.785070	1.137940
16	H	0	-1.656041	-1.687952	1.244892
17	H	0	-0.478816	-3.135466	-0.356376
18	H	0	-2.040184	-2.618342	-1.048546
19	H	0	-0.534767	-1.866126	-1.601073
20	H	0	2.246138	0.903856	-1.948117
21	H	0	2.338201	0.468037	2.275095
22	H	0	2.189976	-1.253583	1.913593
23	H	0	3.697932	-0.381006	1.516754

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(18) **IVf**

1	C	0	-2.640207	2.312349	0.259042
2	N	0	-1.858175	1.116437	0.507185
3	C	0	-2.163564	-0.082391	-0.053658
4	C	0	-1.218712	-1.242079	0.322674
5	C	0	-1.074021	-2.254905	-0.804740
6	O	0	-3.155120	-0.290521	-0.744630
7	O	0	0.046541	-0.792159	0.853035
8	N	0	0.823545	-0.211432	-0.177444
9	C	0	2.038597	-0.034263	0.189395
10	S	0	3.010235	0.877039	-1.006973
11	C	0	2.660037	-0.430441	1.500404
12	H	0	-0.978344	1.184889	0.994816
13	H	0	-2.088165	3.035179	-0.353068
14	H	0	-3.540331	2.010470	-0.277427
15	H	0	-2.926142	2.794445	1.199936
16	H	0	-1.668688	-1.727599	1.197711
17	H	0	-0.510284	-3.125980	-0.459792
18	H	0	-2.067505	-2.568105	-1.129062
19	H	0	-0.555184	-1.809738	-1.655925
20	H	0	4.210212	0.463036	-0.553157
21	H	0	2.807716	0.451528	2.133018
22	H	0	2.011301	-1.134136	2.021478
23	H	0	3.639932	-0.889824	1.338920

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(19) **IVg**

1	C	0	-3.523647	-1.870118	-0.248736
2	N	0	-2.320558	-1.062623	-0.192625

3	C	0	-2.351007	0.294519	-0.190795
4	C	0	-0.977647	0.985982	-0.162411
5	C	0	-0.966605	2.181062	0.782102
6	O	0	-3.375034	0.967214	-0.245978
7	O	0	0.026663	0.018243	0.202072
8	N	0	1.263047	0.382973	-0.384892
9	C	0	2.230010	-0.289081	0.121853
10	S	0	3.861192	-0.014824	-0.540985
11	C	0	2.130912	-1.313341	1.218325
12	H	0	-1.412157	-1.497264	-0.126610
13	H	0	-3.615894	-2.508403	0.637197
14	H	0	-4.374161	-1.188668	-0.286822
15	H	0	-3.534692	-2.505696	-1.141310
16	H	0	-0.764796	1.314672	-1.186937
17	H	0	-0.010788	2.705942	0.708717
18	H	0	-1.778369	2.861244	0.518499
19	H	0	-1.110916	1.852119	1.815650
20	H	0	3.475827	0.872991	-1.479882
21	H	0	3.094142	-1.465035	1.709860
22	H	0	1.389004	-0.990573	1.951448
23	H	0	1.801178	-2.274381	0.807785

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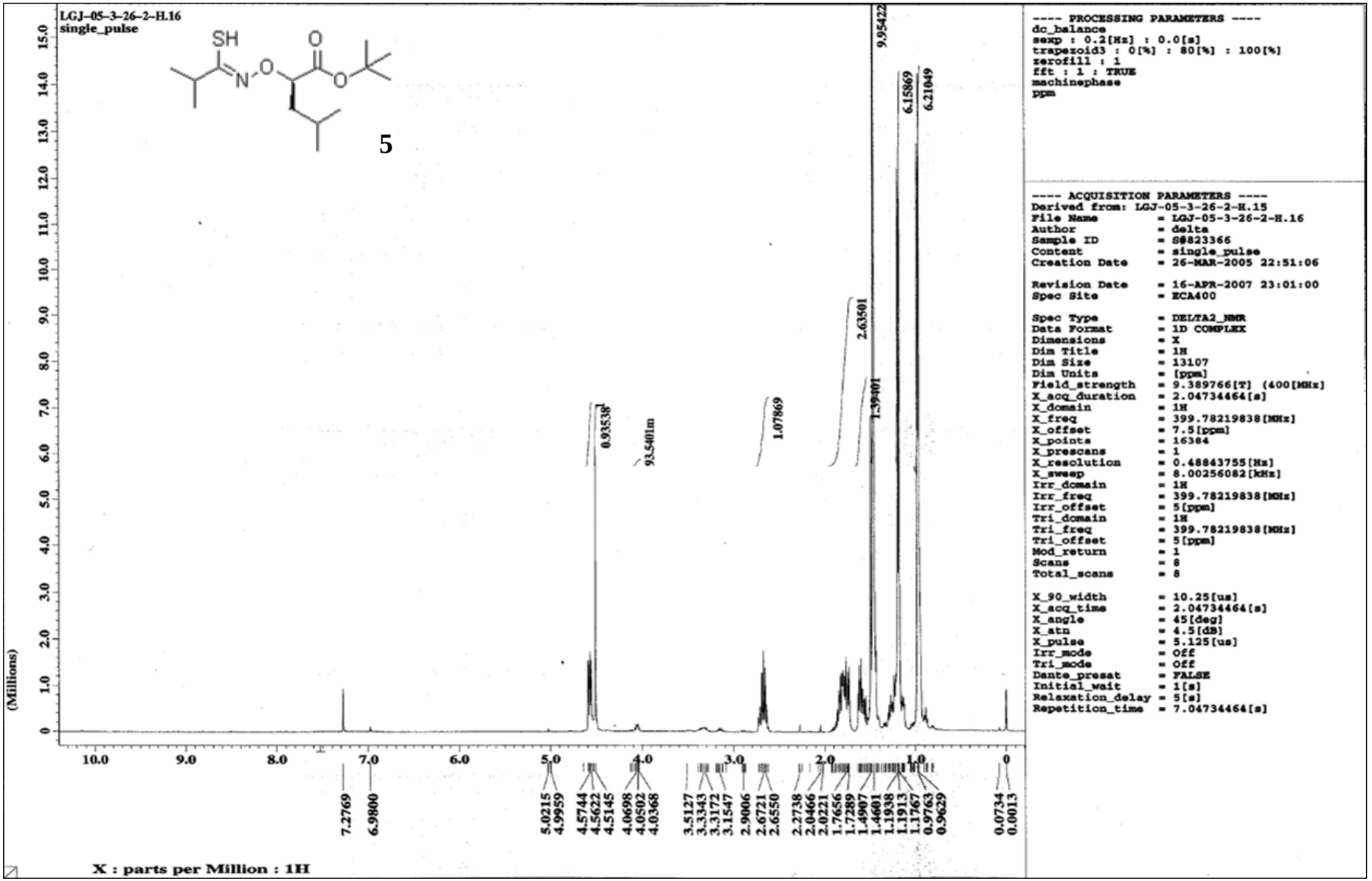
(20) **IVh**

1	C	0	-3.496250	-1.909065	-0.228483
2	N	0	-2.305252	-1.083755	-0.172650
3	C	0	-2.354770	0.272784	-0.197100
4	O	0	-3.387870	0.929374	-0.271636
5	C	0	-0.991570	0.984046	-0.175354
6	O	0	0.022311	0.041281	0.231795
7	N	0	1.249522	0.384077	-0.372539
8	C	0	2.234994	-0.242465	0.157171
9	C	0	2.186996	-1.180931	1.330743
10	C	0	-1.004901	2.207703	0.731098
11	S	0	3.773992	-0.006026	-0.724895
12	H	0	-1.391631	-1.505341	-0.095992
13	H	0	-3.587492	-2.536482	0.665256
14	H	0	-4.355897	-1.240377	-0.283622
15	H	0	-3.490040	-2.556751	-1.112362
16	H	0	-0.768595	1.281756	-1.206855
17	H	0	-0.056172	2.743880	0.648157
18	H	0	-1.824033	2.867292	0.439493

19	H	0	-1.153874	1.909689	1.773370
20	H	0	4.577731	-0.258722	0.327884
21	H	0	3.044162	-1.020099	1.991086
22	H	0	1.264565	-1.027661	1.891130
23	H	0	2.224990	-2.220684	0.987357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SH
O
N
O
O
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1.39401
0.93538
93.540lm
1.07869
(Millions)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2769
6.9800
5.0215
4.9959
4.5744
4.5622
4.5145
4.0698
4.0502
4.0368
3.5127
3.3343
3.3172
3.1547
2.9006
2.6721
2.6550
2.2738
2.0466
2.0221
1.7656
1.7289
1.4907
1.4601
1.1938
1.1913
1.1767
0.9763
0.9629
0.0734
0.0013
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
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File Name = LGJ-05-3-26-2-H.16
Author = delta
Sample ID = S#823366
Content = single_pulse
Creation Date = 26-MAR-2005 22:51:06
Revision Date = 16-APR-2007 23:01:00
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.04734464[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7.5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.48843755[Hz]
X_sweep = 8.00256082[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.04734464[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
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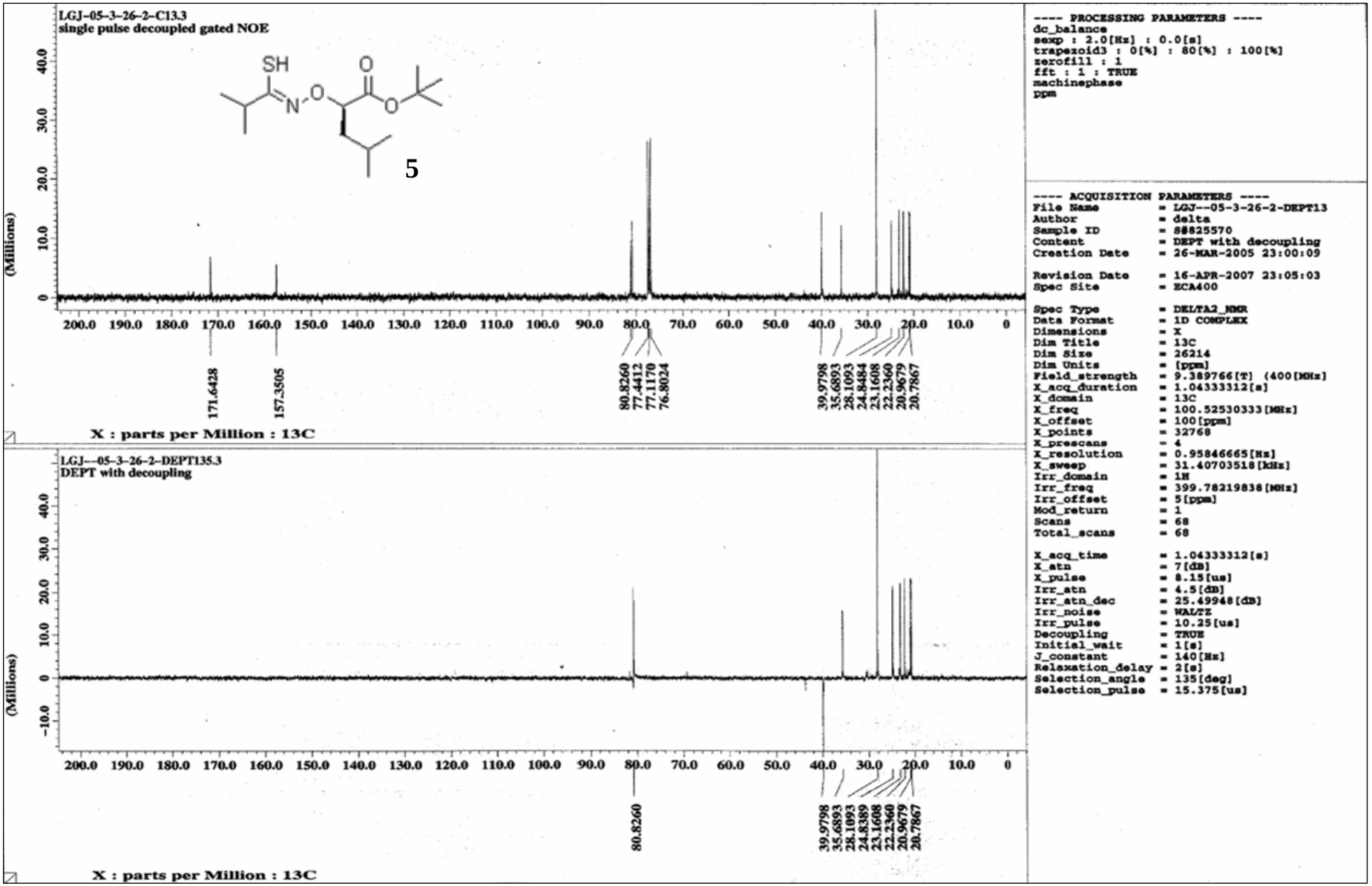
LGJ-05-3-26-2-C13.3
single pulse decoupled gated NOE
SH
O
N
O
O
5
(Millions)
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30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.6428
157.3505
80.8260
77.4412
77.1170
76.8024
39.9798
35.6893
28.1093
24.8484
23.1608
22.2360
20.9679
20.7867
X : parts per Million : 13C
LGJ--05-3-26-2-DEPT135.3
DEPT with decoupling
(Millions)
40.0
30.0
20.0
10.0
0
-10.0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
80.8260
39.9798
35.6893
28.1093
24.8389
23.1608
22.2360
20.9679
20.7867
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
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Author = delta
Sample ID = S#825570
Content = DEPT with decoupling
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Revision Date = 16-APR-2007 23:05:03
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
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X_acq_duration = 1.04333312[s]
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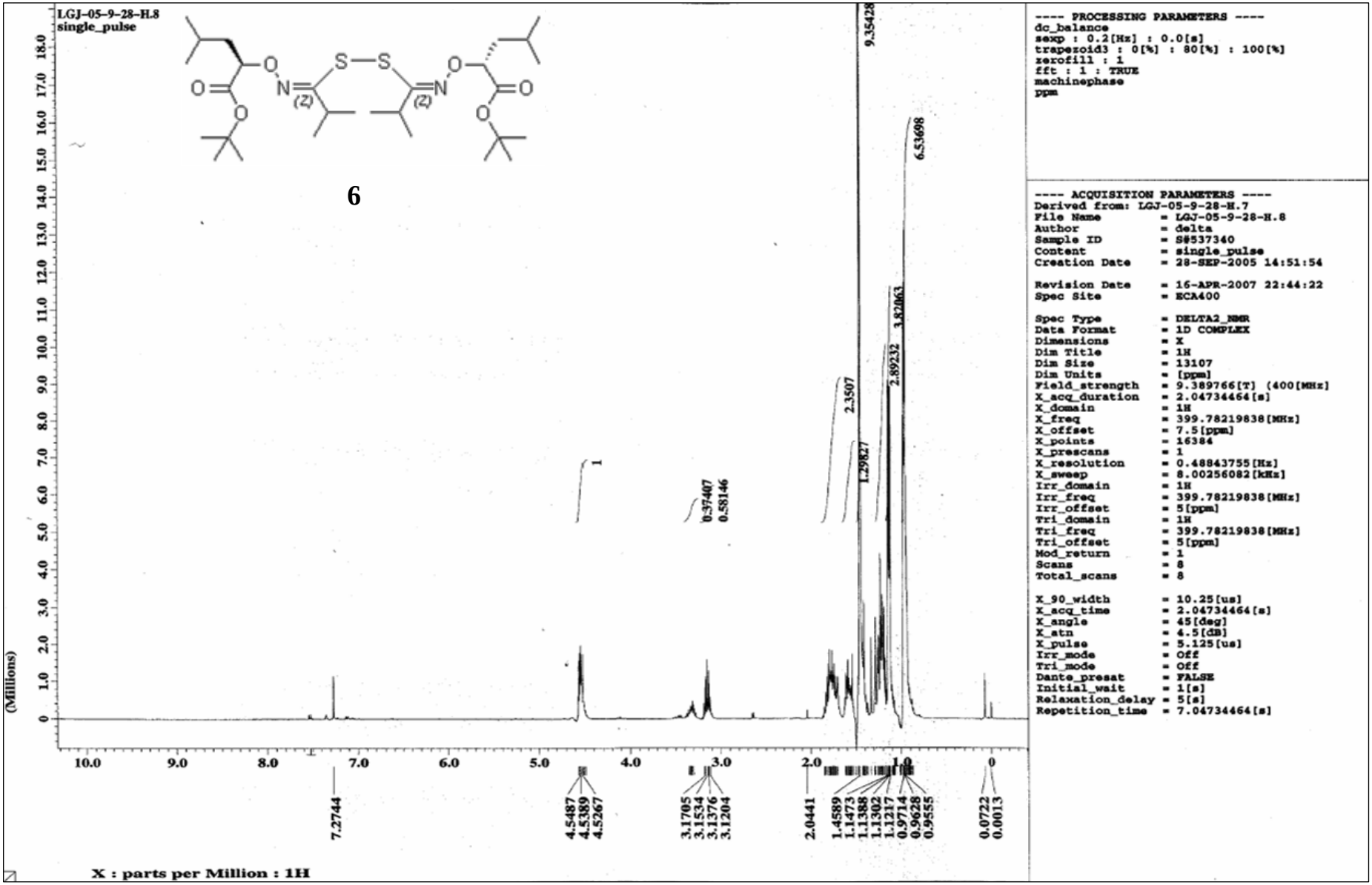
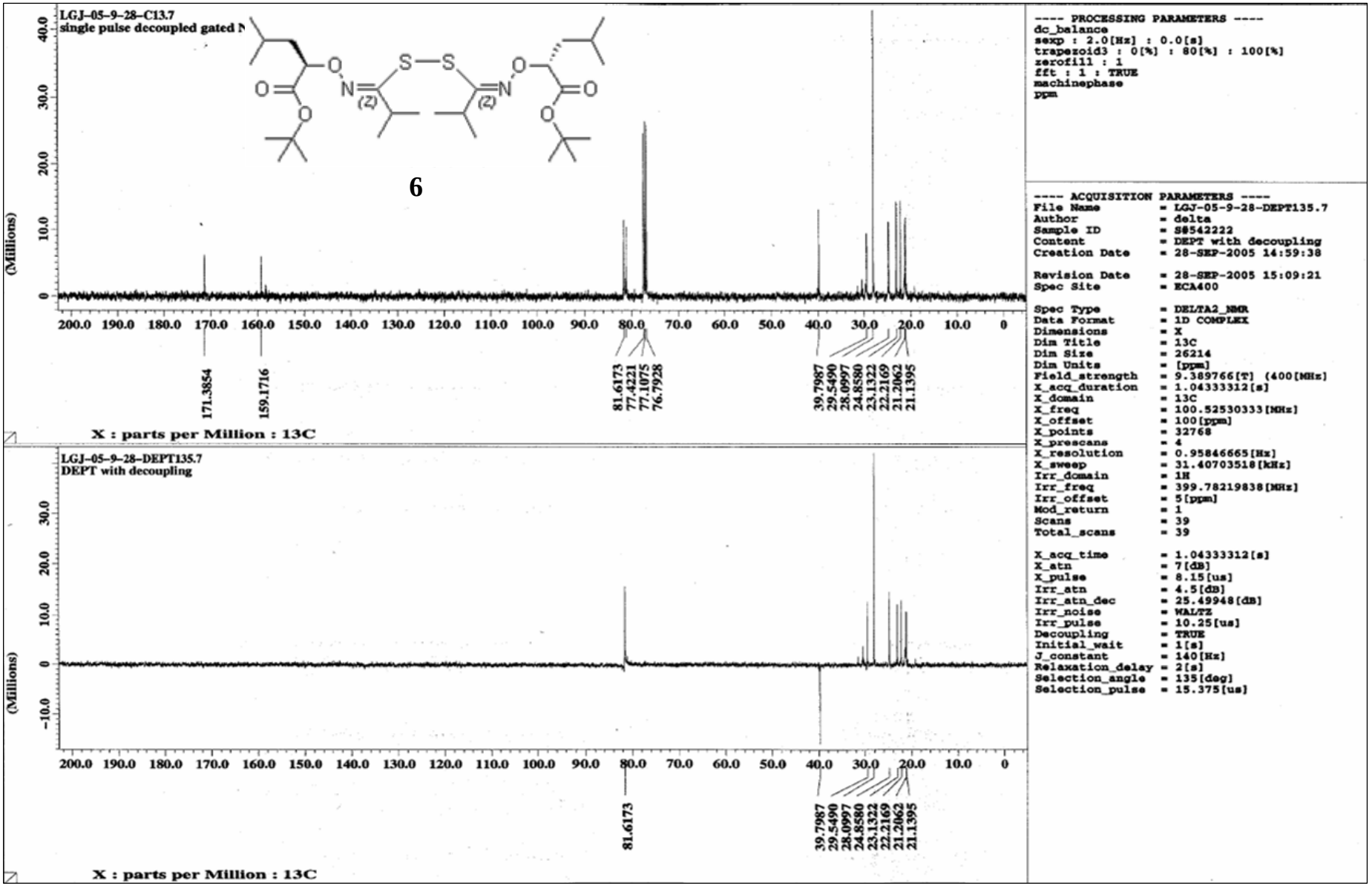
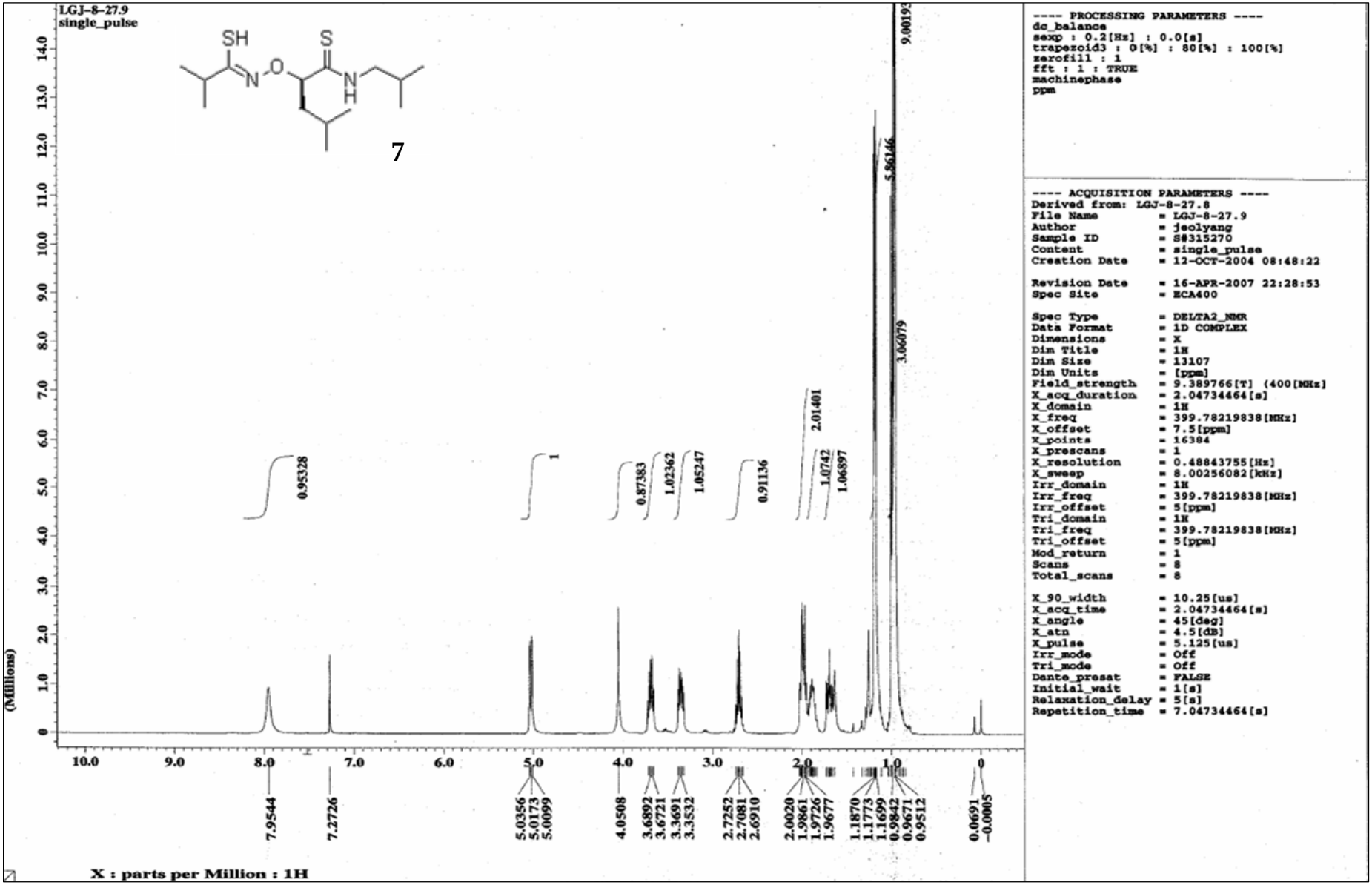
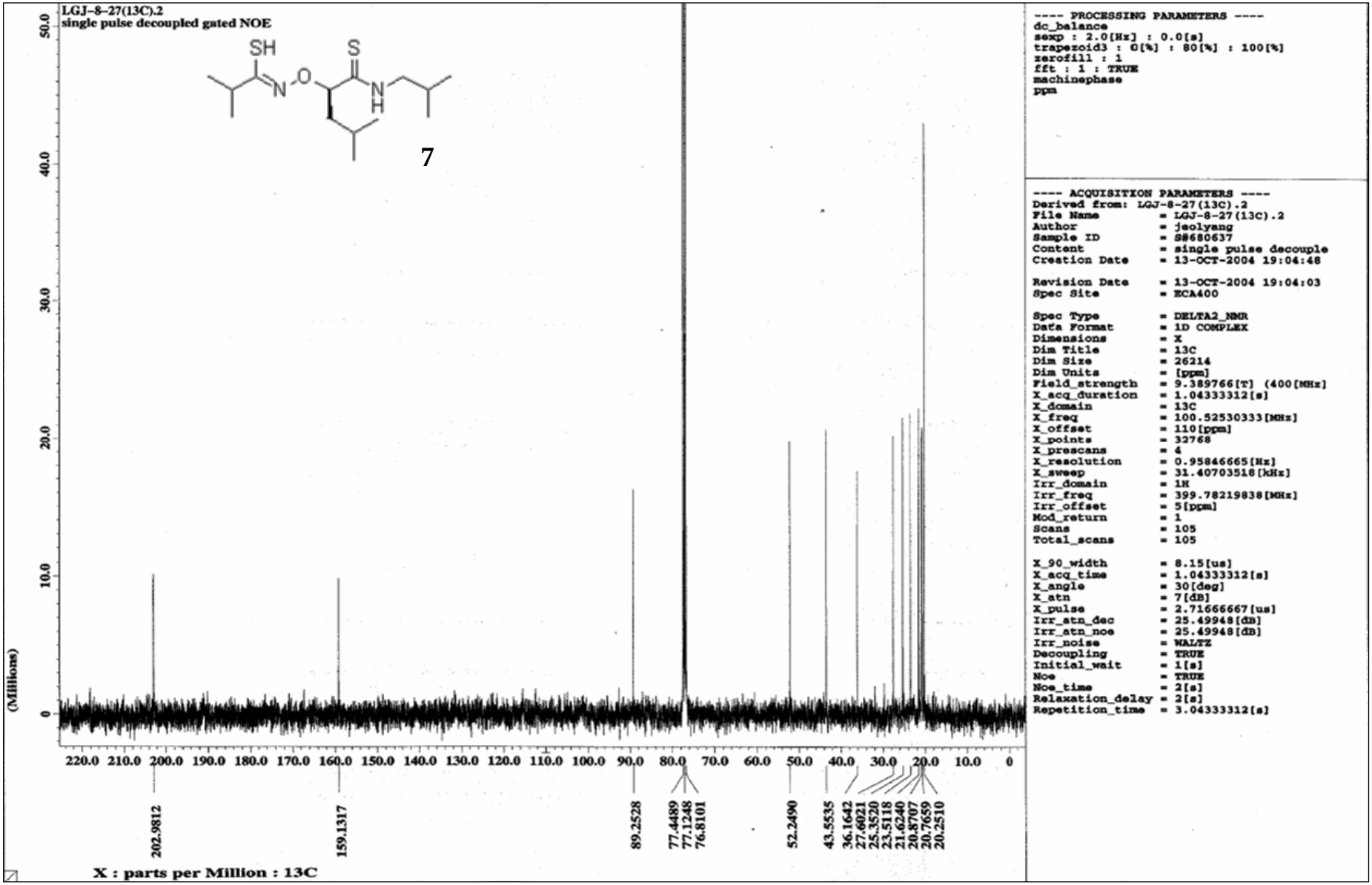
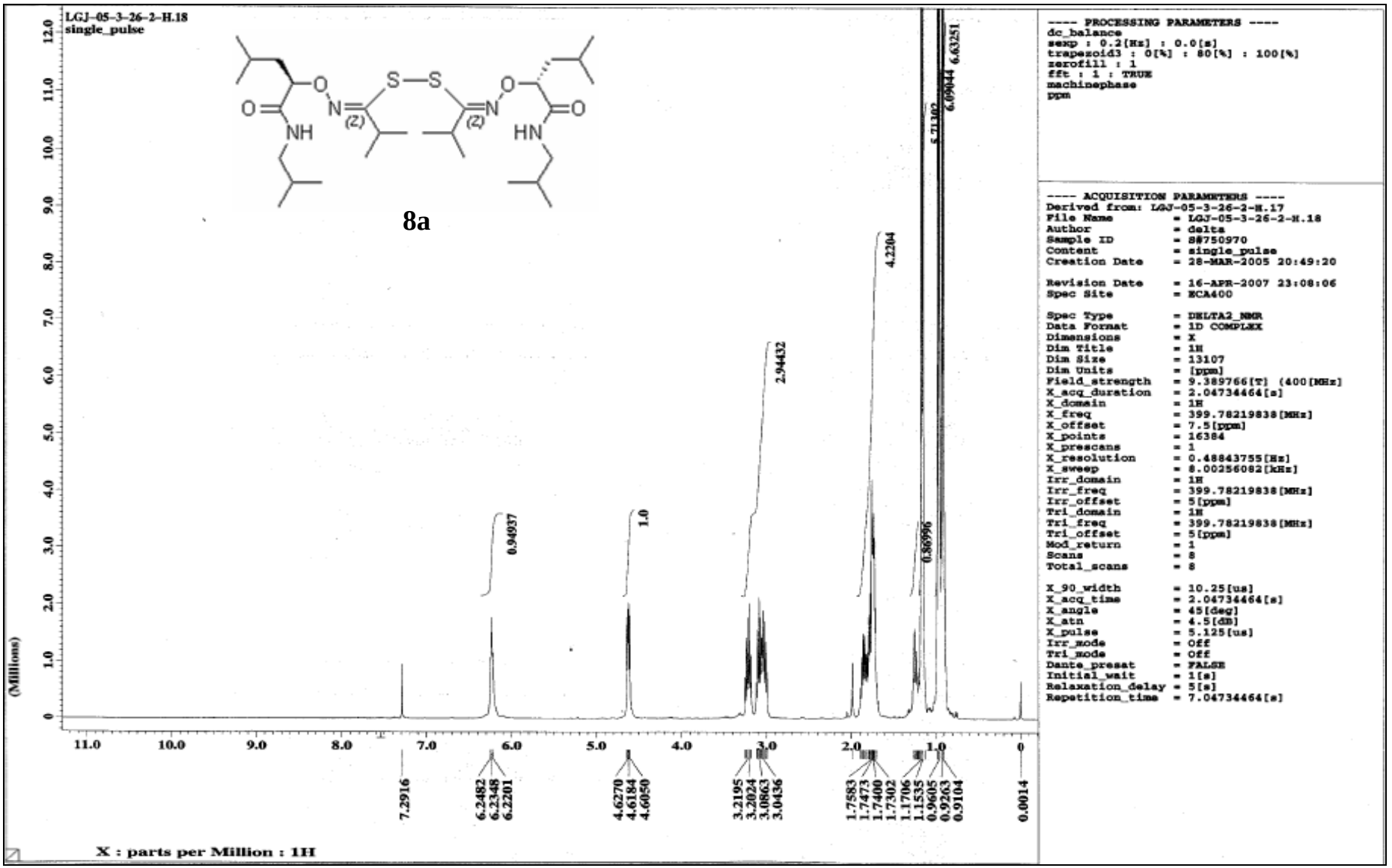
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Mod_return = 1
Scans = 68
Total_scans = 68
X_acq_time = 1.04333312[s]
X_atn = 7[dB]
X_pulse = 8.15[us]
Irr_atn = 4.5[dB]
Irr_atn_dec = 25.49948[dB]
Irr_noise = WALTZ
Irr_pulse = 10.25[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 15.375[us]

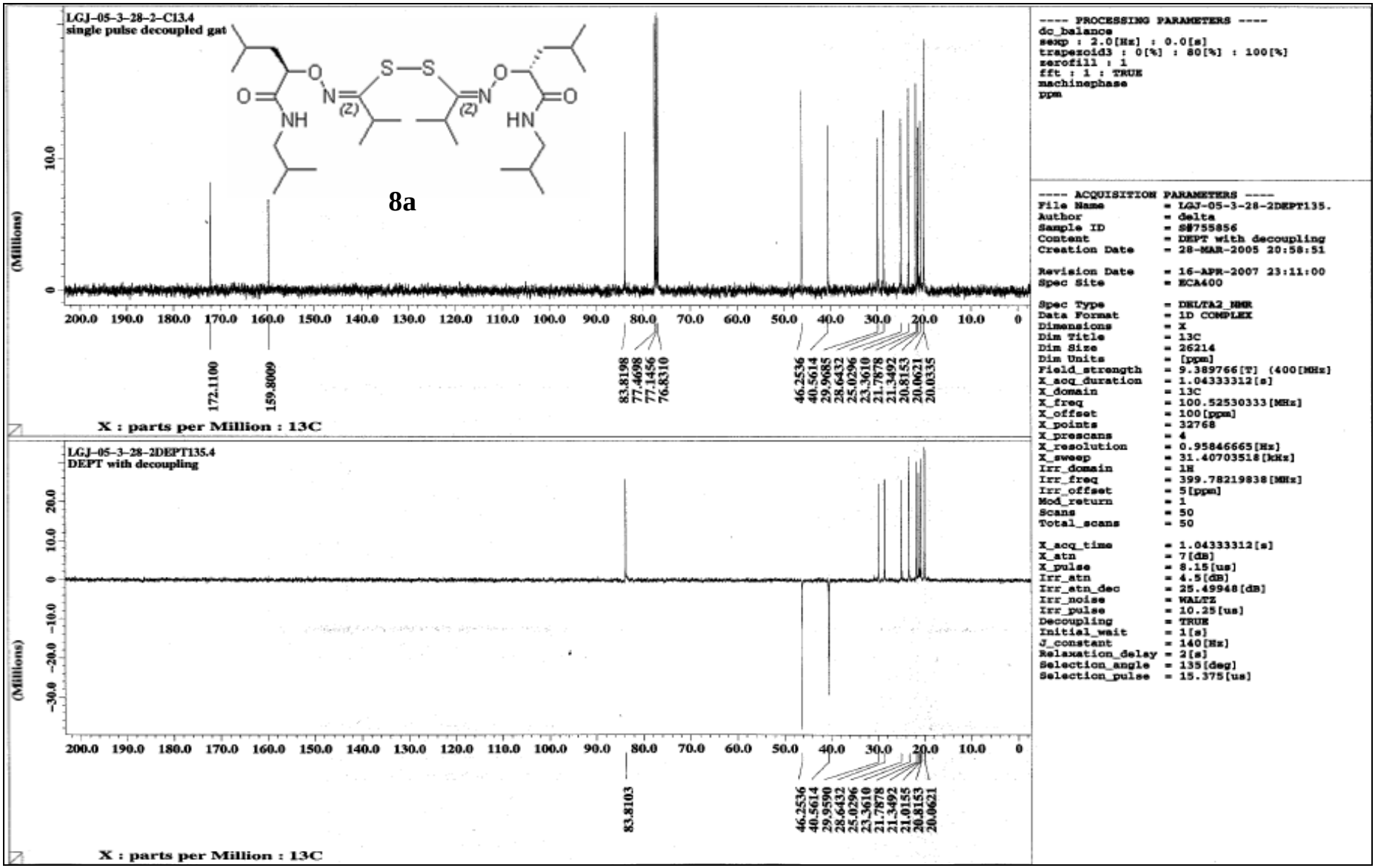

LGJ-05-9-28-H.8
single_pulse
6
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: LGJ-05-9-28-H.7
File Name = LGJ-05-9-28-H.8
Author = delta
Sample ID = S#537340
Content = single_pulse
Creation Date = 28-SEP-2005 14:51:54
Revision Date = 16-APR-2007 22:44:22
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.04734464[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7.5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.48843755[Hz]
X_sweep = 8.00256082[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.04734464[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.04734464[s]
9.35428
6.53698
3.82063
2.89232
2.35071
2.29827
1
0.37407
0.58146
(Millions)
7.2744
4.5487
4.5389
4.5267
3.1705
3.1534
3.1376
3.1204
2.0441
1.4589
1.1473
1.1388
1.1302
1.1217
0.9714
0.9628
0.9555
0.0722
0.0013
X : parts per Million : 1H

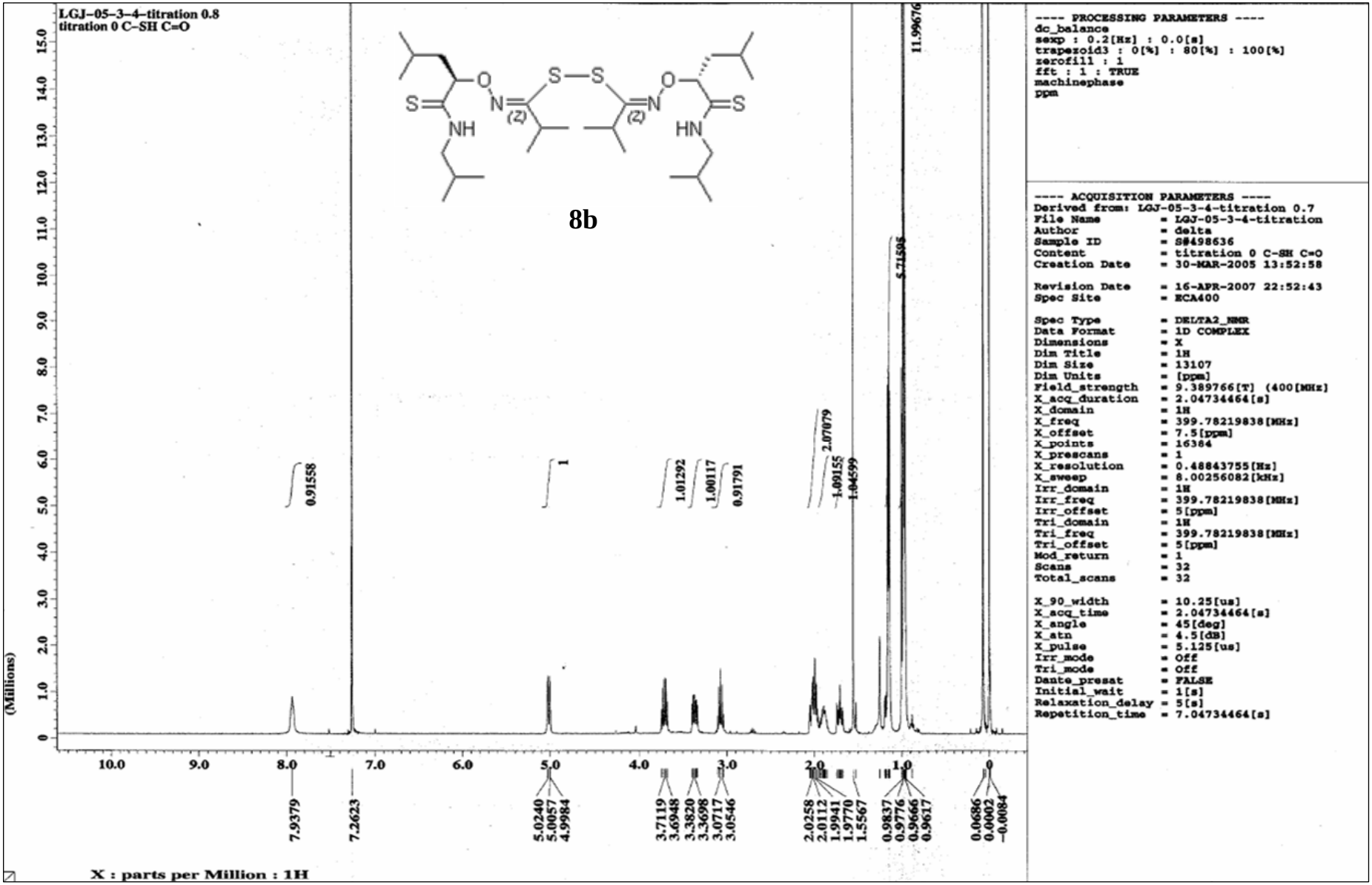

LGJ-05-9-28-C13.7
single pulse decoupled gated
6
(Millions)
171.3854
159.1716
81.6173
77.4221
77.1075
76.7928
39.7987
29.5490
28.0997
24.8580
23.1322
22.2169
21.2062
21.1395
X : parts per Million : 13C
LGJ-05-9-28-DEPT135.7
DEPT with decoupling
(Millions)
81.6173
39.7987
29.5490
28.0997
24.8580
23.1322
22.2169
21.2062
21.1395
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
File Name = LGJ-05-9-28-DEPT135.7
Author = delta
Sample ID = S#542222
Content = DEPT with decoupling
Creation Date = 28-SEP-2005 14:59:38
Revision Date = 28-SEP-2005 15:09:21
Spec Site = ECA400
Spec Type = DEL/TA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Mod_return = 1
Scans = 39
Total_scans = 39
X_acq_time = 1.04333312[s]
X_atn = 7[dB]
X_pulse = 8.15[us]
Irr_atn = 4.5[dB]
Irr_atn_dec = 25.49948[dB]
Irr_noise = WALTZ
Irr_pulse = 10.25[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 15.375[us]

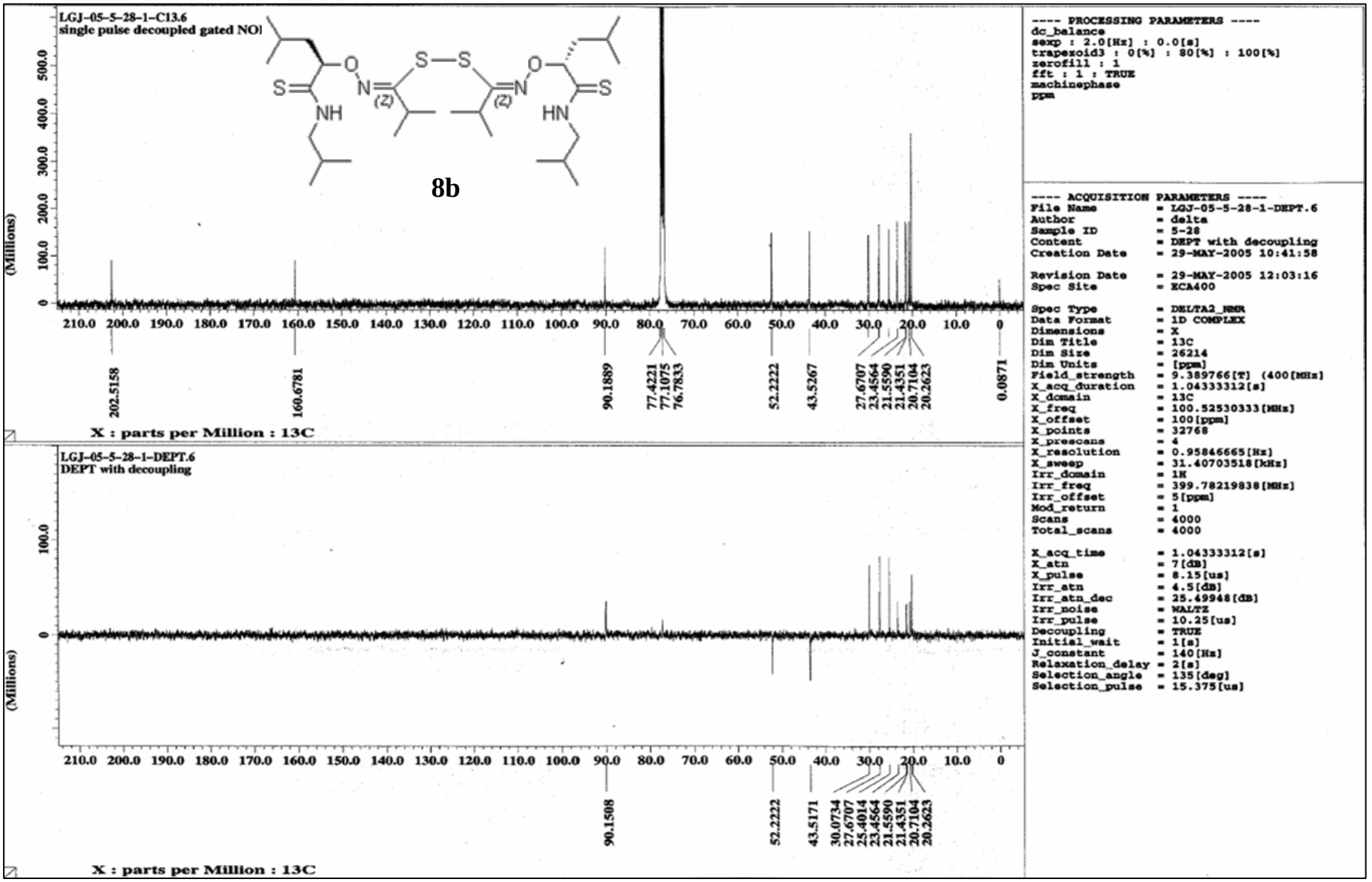

LGJ-8-27.9
single_pulse
SH
S
N
O
N
H
7
(Millions)
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: LGJ-8-27.8
File Name = LGJ-8-27.9
Author = jeolyang
Sample ID = S#315270
Content = single_pulse
Creation Date = 12-OCT-2004 08:48:22
Revision Date = 16-APR-2007 22:28:53
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.04734464[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7.5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.48843755[Hz]
X_sweep = 8.00256082[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.04734464[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.04734464[s]

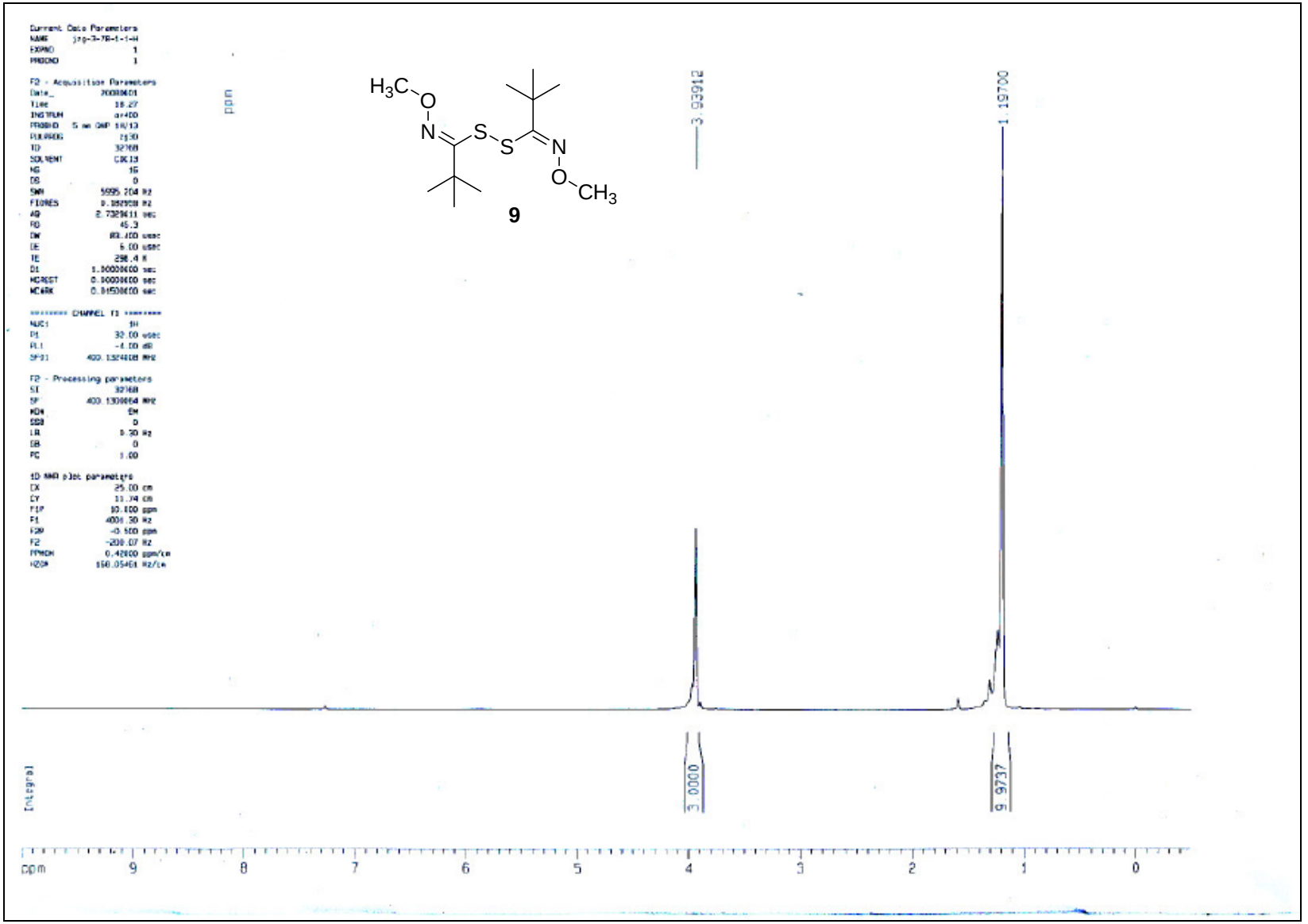

LGJ-8-27(13C).2
single pulse decoupled gated NOE
SH
S
N
O
N
H
7
(Millions)
50.0
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
202.9812
159.1317
89.2528
77.4489
77.1248
76.8101
52.2490
43.5535
36.1642
27.6021
25.3520
23.5118
21.6240
20.8707
20.7659
20.2510
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: LGJ-8-27(13C).2
File Name = LGJ-8-27(13C).2
Author = jeolyang
Sample ID = S#680637
Content = single pulse decouple
Creation Date = 13-OCT-2004 19:04:48
Revision Date = 13-OCT-2004 19:04:03
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 110[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Mod_return = 1
Scans = 105
Total_scans = 105
X_90_width = 8.15[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 7[dB]
X_pulse = 2.71666667[us]
Irr_atn_dec = 25.49948[dB]
Irr_atn_noe = 25.49948[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]

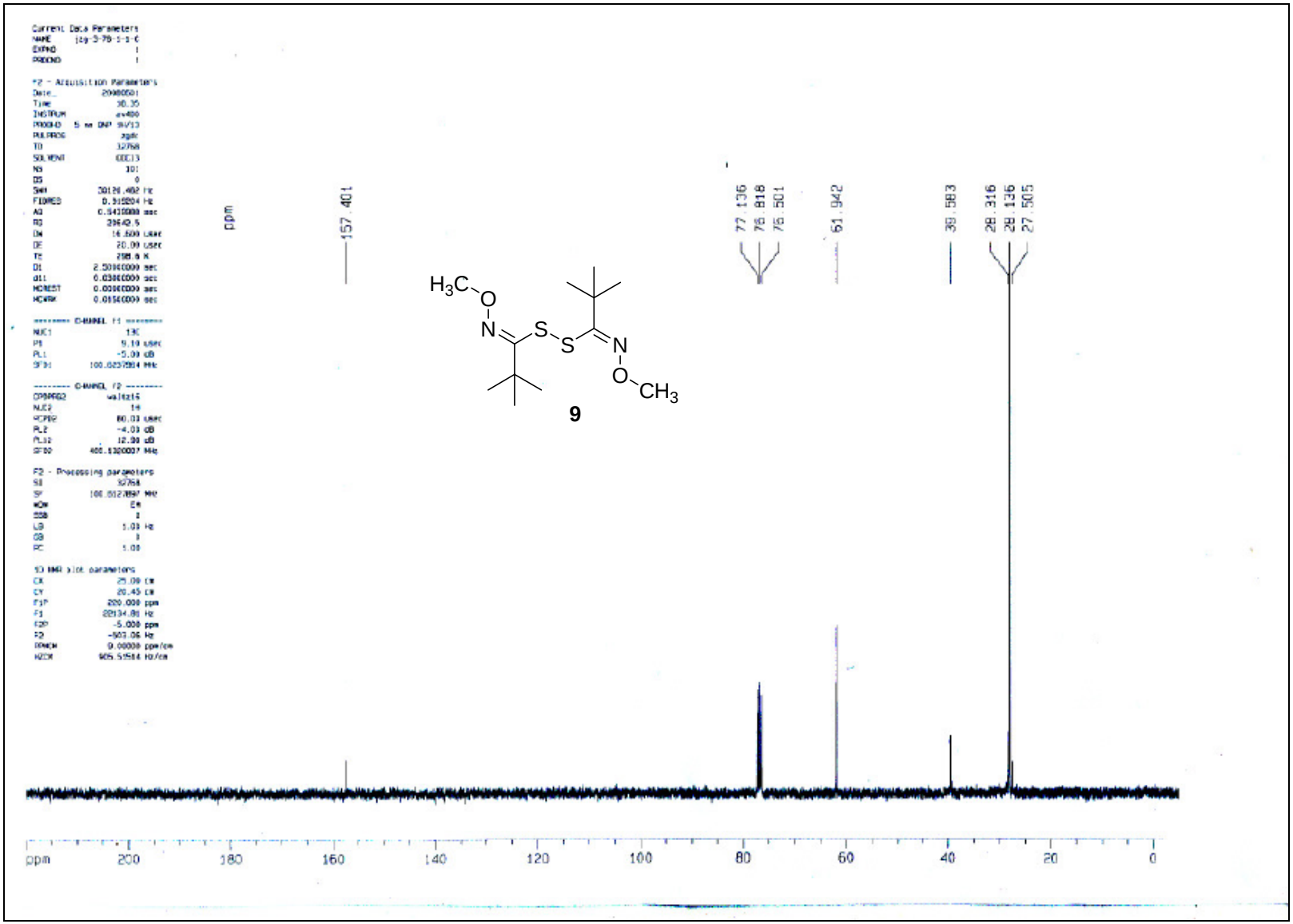

LGJ-05-3-26-2-H.18
single_pulse
8a
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: LGJ-05-3-26-2-H.17
File Name = LGJ-05-3-26-2-H.18
Author = delta
Sample ID = S#750970
Content = single_pulse
Creation Date = 28-MAR-2005 20:49:20
Revision Date = 16-APR-2007 23:08:06
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.04734464[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7.5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.48843755[Hz]
X_sweep = 8.00256082[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.04734464[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.04734464[s]
0.94937
1.0
2.94432
4.2204
0.86996
5.71302
6.09044
6.63251
7.2916
6.2482
6.2348
6.2201
4.6270
4.6184
4.6050
3.2195
3.2024
3.0863
3.0436
1.7583
1.7473
1.7400
1.7302
1.1706
1.1535
0.9605
0.9263
0.9104
0.0014
(Millions)
X : parts per Million : 1H


LGJ-05-3-28-2-C13.4
single pulse decoupled gat
8a
X : parts per Million : 13C
LGJ-05-3-28-2DEPT135.4
DEPT with decoupling
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
File Name = LGJ-05-3-28-2DEPT135.
Author = delta
Sample ID = S#755856
Content = DEPT with decoupling
Creation Date = 28-MAR-2005 20:58:51
Revision Date = 16-APR-2007 23:11:00
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Mod_return = 1
Scans = 50
Total_scans = 50
X_acq_time = 1.04333312[s]
X_atn = 7[dB]
X_pulse = 8.15[us]
Irr_atn = 4.5[dB]
Irr_atn_dec = 25.49948[dB]
Irr_noise = WALTZ
Irr_pulse = 10.25[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 15.375[us]


LGJ-05-3-4-titration 0.8
titration 0 C-SH C=O
8b
X : parts per Million : 1H
(Millions)
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: LGJ-05-3-4-titration 0.7
File Name = LGJ-05-3-4-titration
Author = delta
Sample ID = S#498636
Content = titration 0 C-SH C=O
Creation Date = 30-MAR-2005 13:52:58
Revision Date = 16-APR-2007 22:52:43
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.04734464[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7.5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.48843755[Hz]
X_sweep = 8.00256082[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Mod_return = 1
Scans = 32
Total_scans = 32
X_90_width = 10.25[us]
X_acq_time = 2.04734464[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.04734464[s]


LGJ-05-5-28-1-C13.6
single pulse decoupled gated NOI
8b
(Millions)
500.0
400.0
300.0
200.0
100.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
202.5158
160.6781
90.1889
77.4221
77.1075
76.7833
52.2222
43.5267
27.6707
23.4564
21.5590
21.4351
20.7104
20.2623
0.0871
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
File Name = LGJ-05-5-28-1-DEPT.6
Author = delta
Sample ID = 5-28
Content = DEPT with decoupling
Creation Date = 29-MAY-2005 10:41:58
Revision Date = 29-MAY-2005 12:03:16
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Mod_return = 1
Scans = 4000
Total_scans = 4000
X_acq_time = 1.04333312[s]
X_atn = 7[dB]
X_pulse = 8.15[us]
Irr_atn = 4.5[dB]
Irr_atn_dec = 25.49948[dB]
Irr_noise = WALTZ
Irr_pulse = 10.25[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 15.375[us]
LGJ-05-5-28-1-DEPT.6
DEPT with decoupling
(Millions)
100.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
90.1508
52.2222
43.5171
30.0734
27.6707
25.4014
23.4564
21.5590
21.4351
20.7104
20.2623
X : parts per Million : 13C


Current Data Parameters
NAME jtg-3-78-1-1-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080601
Time 18.27
INSTRUM av400
PROBHD 5 mm DUP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182958 Hz
AQ 2.7329411 sec
RG 45.3
DW 83.400 usec
DE 6.00 usec
TE 298.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.04500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 32.00 usec
PL1 -4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 11.74 cm
F1P 10.000 ppm
F1 4004.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.42800 ppm/cm
HZCM 150.05401 Hz/cm
ppm
3.03912
1.19700
9
Integral
3.0000
9.9737
ppm
9
8
7
6
5
4
3
2
1
0


ppm
157.401
77.136
76.818
76.501
61.942
39.583
28.316
28.136
27.505
9
ppm
200
180
160
140
120
100
80
60
40
20
0