SUPPORTING INFORMATION

Cinchona alkaloid catalyzed enantioselective sulfa-Michael/aldol cascade reaction of isoindigos: construction of chial bispirooxindole tetrahydrothiophenes with vicinal quaternary spirocenters

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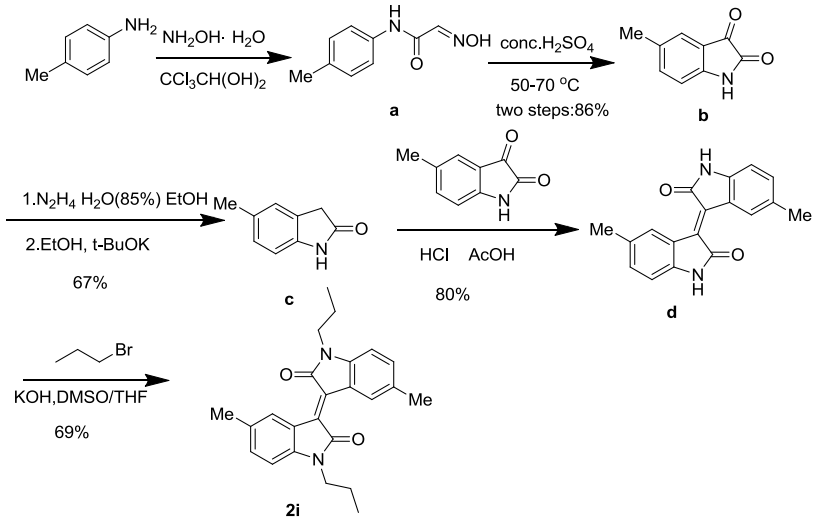
1. General Information

Commercial grade solvent was dried and purified by standard procedures as specified in Purification of Laboratory Chemicals, 4th Ed (Armarego, W. L. F.; Perrin, D. D. Butterworth Heinemann: 1997). NMR spectra are recorded with tetramethylsilane as the internal standard. ^{1}H NMR spectra are recorded at 300 MHz, and ^{13}C NMR spectra were recorded at 75 MHz (Bruker Avance). ^{1}H NMR chemical shifts (δ) were reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm, $(CD_3)_2SO$ at 2.50 ppm). ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.00 ppm, $(CD_3)_2SO$ at 39.52 ppm). Data are given as: s (singlet), d (doublet), t (triplet), q (quartet), dd (double of doublet) or m (multiplets), coupling constants (Hz) and integration. Flash column chromatography was carried out using silica gel eluting with ethyl acetate and petroleum ether. High resolution mass spectra were obtained with the Q-TOF-Premier mass spectrometer. Reactions were monitored by TLC and visualized with ultraviolet light. Enantiomeric excess was determined by HPLC analysis on chiralpak AD-H, or IC columns. Optical rotations are reported as follows: $[\alpha]_D^{25}$ (C in g/100 mL, $CHCl_3$).

2. Preparation and Spectral Data of Substrates



To a solution of chloral hydrate (9.55 g, 57.89 mmol) in deionized water (150 mL), Na_2SO_4 (100 g, 684.19 mmol), 4-methylaniline (5.64 g, 52.63 mmol), H_2SO_4 (40 mL, 1 M) and hydroxylamine hydrochloride (10.97 g, 157.89 mmol) was added. The mixture was heated to 130 °C and refluxed for 30 min. The mixture was then cooled to 80 °C and filtered to collect the product. The product was washed with deionized water and dried under reduced pressure to afford **a** as a

yellowish solid, which was directly used for the next step without further purification.

To a concentrated H_2SO_4 (100 mL) in 250 mL round-bottom flask kept at 50 ^oC, compound **a** was added portionwise with stirring. The mixture was heated to 70 ^oC for 1 h before pouring into ice water. The precipitate was collected by filtration and the filtrate was extract with ethyl acetate (EA). The precipitate and the extraction were combined and subject to column chromatography (silica gel; eluent: PE:EA = 8:1) to afforded **b** as an orange solid (7.3 g，86%).

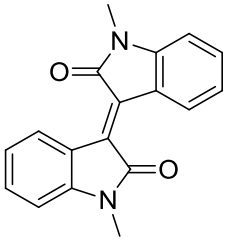
To a solution of **b** (1.85 g, 11.48 mmol) in ethanol (50 mL), hydrazine hydrate (85%, 0.5 mL) was added under nitrogen. After the mixture was refluxed for 30 min, a yellow participate was formed and collected by filtration. The yellow precipitate was then dissolved in anhydrous ethanol (50 mL), and t-BuOK (4.03 g, 35.90 mmol) was added. The mixture was refluxed under nitrogen for 2 h before pouring into water. The mixture was acidified with dilute HCl to pH = 2 and extracted with EA. The combined organic phase was washed with water, brine, dried with Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography (silica gel; eluent: PE:EA = 5:1) to provide **c** as a light-yellow solid (1.13 g, 67%).

To a suspension of **b** (1.04 g, 6.48 mmol) and **c** (0.95 g, 6.48 mmol) in AcOH (75 mL) was added conc. HCl solution (0.4 mL). The mixture was refluxed for 24 h. The mixture was allowed to cool and filtered. The solid material was washed with water, ethanol and ether. After drying under vacuum, deep red 5,5’-dimethylisoindigo **d** (1.51 g, 80%) was obtained.

To a solution of 5,5’-dimethylisoindigo **d** (95 mg, 0.33 mmol) and freshly powered KOH (1.68 g, 12.1 mmol) in dimethyl sulfoxide (DMSO) (20 mL), 1-Bromopropane (102 mg, 0.83 mmol) in THF (20 mL) was added under nitrogen. The mixture was stirred for 24 h at 25 ^oC before pouring into water. The residues were dissolved in $CHCl_3$ (100 mL) and washed with water (3 ×50 mL). The combined organic phase was washed with brine and dired (Na_2SO_4) and concentrated under reduced pressure. The residue was purified by silica gel chromatography with eluting (PE: CH_2Cl_2 = 5:1) to give **2i** as a deep-red solid. (85 mg, 69 %).

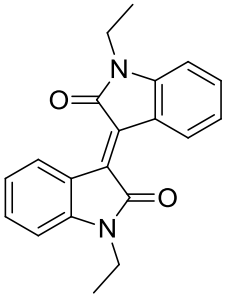
The other *N*-alkyl isoindigos were prepared according to the above procedure.

(*E*)-1,1'-dimethyl-[3,3'-biindolinylidene]-2,2'-dione (2a)



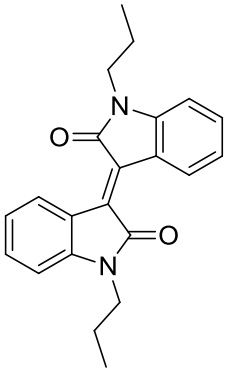
^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.21 (d, *J*=8 Hz, 2H), 7.36 (t, *J*=8 Hz, 2H), 7.06 (t, *J*=8 Hz, 2H), 6.77 (d, *J*=8 Hz, 2H), 3.27 (s, 6H)

(*E*)-1,1'-diethyl-[3,3'-biindolinylidene]-2,2'-dione (2b)



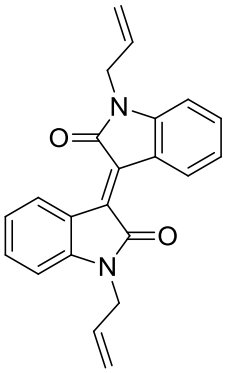
^{1}H NMR (300 MHz, DMSO) δ (ppm): 9.12 (d, *J*=8 Hz, 2H), 7.43 (td, J_1=8 Hz, J_2=1 Hz, 2H), 7.00-7.09 (m, 4H), 3.80 (q, *J*=7 Hz, 4H), 1.19 (t, *J*=7 Hz, 6H)

(*E*)-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione(2c)



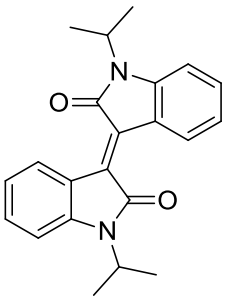
^{1}H NMR (300 MHz, DMSO) δ (ppm): 9.10 (d, *J*=8 Hz, 2H), 7.42 (t, *J*=7 Hz, 2H), 7.00-7.08 (m, 4H), 3.72 (t, *J*=7 Hz, 4H), 1.58-1.70 (m, 4H), 0.90 (t, *J*=7 Hz, 6H);

(*E*)-1,1'-diallyl-[3,3'-biindolinylidene]-2,2'-dione (2d)



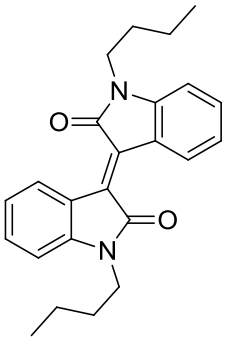
^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.20 (d, *J*=8 Hz, 2H), 7.33 (t, *J*=8 Hz, 2H), 7.06 (t, *J*=8 Hz, 2H), 6.78 (d, *J*=8 Hz, 2H), 5.82-5.95 (m, 2H), 5.22-5.30 (m, 4H), 4.42-4.44 (m, 4H);

(*E*)-1,1'-diisopropyl-[3,3'-biindolinylidene]-2,2'-dione (2e)



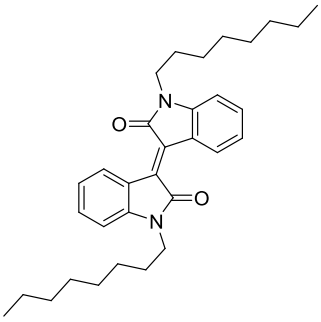
Red solid, mp:269-270℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.12 (dd, J_1=8 Hz, J_2=1 Hz, 2H), 7.31 (td, J_1=8 Hz, J_2=1 Hz, 2H), 7.02 (td, J_1=8 Hz, J_2=1 Hz, 2H), 6.94 (d, J=8 Hz, 2H), 4.64-4.73 (m, 2H), 1.54 (d, J=7 Hz, 12H).

(*E*)-1,1'-dibutyl-[3,3'-biindolinylidene]-2,2'-dione (2f)



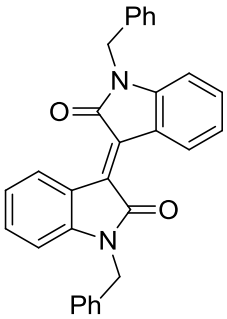
^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.18 (d, J=8 Hz, 2H), 7.32-7.37 (m, 2H), 7.04 (t, J=8 Hz, 2H), 6.78 (d, J=8 Hz, 2H), 3.77 (t, J=7 Hz, 4H), 1.60-1.74 (m, 4H), 1.39-1.46 (m, 4H), 0.96 (t, J=7 Hz, 6H);

(*E*)-1,1'-dioctyl-[3,3'-biindolinylidene]-2,2'-dione (2g)



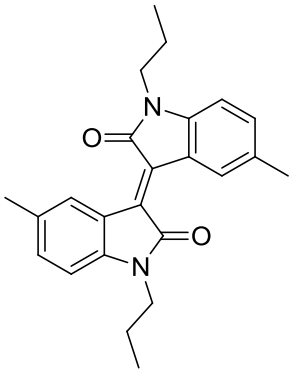
^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.18 (d, J=8 Hz, 2H), 7.35 (t, J=8 Hz, 2H), 7.04 (t, J=8 Hz, 2H), 6.80 (d, J=8 Hz, 2H), 3.77 (t, J=7 Hz, 4H), 1.65-1.75 (m, 4H), 1.26-1.35 (m, 20H), 0.87 (t, J=6 Hz, 6H),

(*E*)-1,1'-dibenzyl-[3,3'-biindolinylidene]-2,2'-dione (2h)



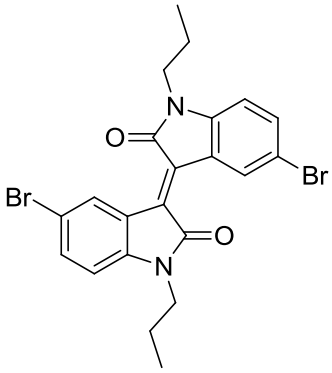
^{1}H NMR (300 MHz, DMSO) δ (ppm): 9.15 (d, J=7 Hz, 2H), 7.28-7.40 (m, 12H), 7.05 (t, J=8 Hz, 2H), 7.00 (t, J=8 Hz, 2H), 5.03 (s, 4H);

(*E*)-5,5'-dimethyl-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2i)



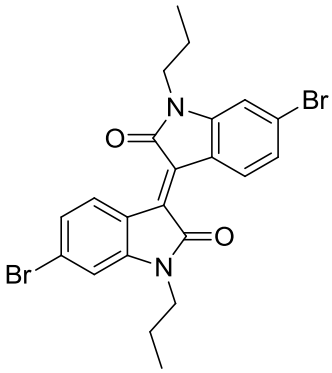
Red solid, mp:284-285℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.99 (s, 2H), 7.15 (d, *J*=8 Hz, 2H), 6.68 (d, *J*=8 Hz, 2H), 3.73 (t, *J*=7 Hz, 4H), 2.38 (s, 6H), 1.70-1.77 (m, 4H), 0.99 (t, *J*=7 Hz, 6H).

(*E*)-5,5'-dibromo-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2j)



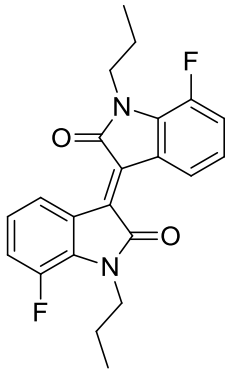
Red solid, mp:233-235℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.40 (d, *J*=2 Hz, 2H), 7.47 (dd, J_1=8 Hz, J_2=2 Hz, 2H), 6.68 (d, *J*=8 Hz, 2H), 3.73 (t, *J*=7 Hz, 4H), 1.66-1.78 (m, 4H), 0.99 (t, *J*=7 Hz, 6H);

(*E*)-6,6'-dibromo-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2k)



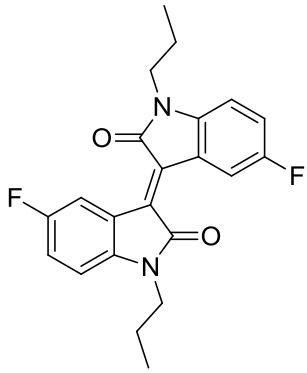
Red solid, mp: 181-182℃;^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.28 (d, *J*=2 Hz, 2H), 7.33 (dd, J_1=8 Hz, J_2=2 Hz, 2H), 6.72 (d, *J*=8 Hz, 2H), 3.74 (t, *J*=7 Hz, 4H), 1.70-1.77 (m, 4H), 1.00 (t, *J*=7 Hz, 6H);

(*E*)-7,7'-difluoro-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2l)



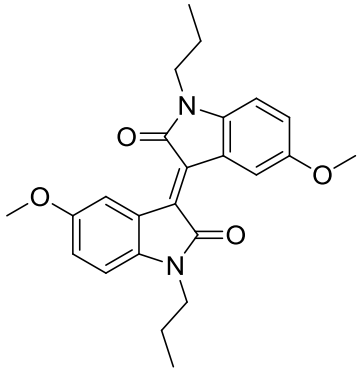
Red solid, mp: 142-143℃;^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.96 (dd, J_1=8 Hz, J_2=1 Hz, 2H), 7.11 (m, 2H), 6.95 (m, 2H), 3.91 (td, J_1=7 Hz, J_2=2 Hz, 4H), 1.75 (m, 4H), 0.98 (t, J=7 Hz, 6H);

(*E*)-5,5'-difluoro-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2m)



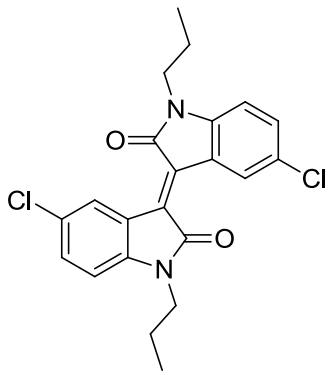
Red solid, mp: 160-161℃;^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.10 (dd, J_1=8 Hz, J_2=1 Hz, 2H), 7.07-7.14 (m, 2H), 6.93-7.00 (m, 2H), 3.72 (t, J=7 Hz 4H), 1.72-1.79 (m, 4H), 0.99 (t, J=7 Hz, 6H);

(*E*)-5,5'-dimethoxy-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2n)



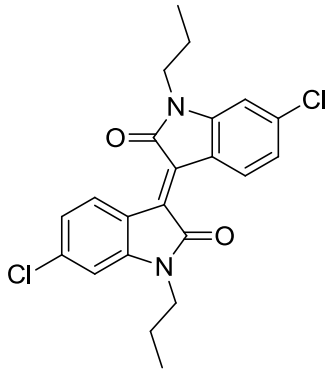
Red solid, mp:273-274℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.97 (d, J= 3 Hz, 2H), 6.90 (dd, J=8 Hz, J_2=3 Hz, 2H), 6.68 (d, J=8 Hz, 2H), 3.85 (s, 6H), 3.70 (t, J=7 Hz, 4H), 1.67-1.75 (m, 4H), 0.98 (t, J=7 Hz, 6H).

(*E*)-5,5'-dichloro-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2o)



Red solid, mp:287-288℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.27 (d, J= 2 Hz, 2H), 7.33 (dd, J=8 Hz, J_2=2 Hz, 2H), 6.70 (d, J=8 Hz, 2H), 3.74 (t, J=7 Hz, 4H), 1.67-1.79 (m, 4H), 0.99 (t, J=7 Hz, 6H).

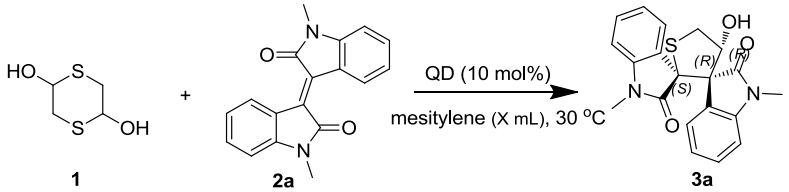
(*E*)-6,6'-dichloro-1,1'-dipropyl-[3,3'-biindolinylidene]-2,2'-dione (2p)



Red solid, mp:282-283℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.16 (d, *J*= 8 Hz, 2H), 6.99 (dd, *J*=8 Hz, J_2=2 Hz, 2H), 6.78 (d, *J*=2 Hz, 2H), 3.72 (t, *J*=7 Hz, 4H), 1.56-1.77 (m, 4H), 1.00 (t, *J*=7 Hz, 6H).

3. Optimization Studies

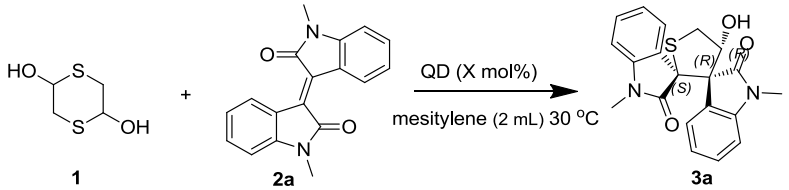
Table S1 Screening of concentrations [a]



entry	X	Time(h)	Yield(%) [b]	dr [c]	ee(%) [d]
1	4	12	75	79/21	81
2	2	6	80	84/16	80
3	1.0	3	78	83/17	80
4	0.5	3	77	89/11	80

[a] Unless otherwise specified, the reaction was performed on a scale of 0.06 mmol **1** and 0.1 mmol **2a** in 1 mL solvent at 30 ℃. [b] Isolated yield. [c] Determined by isolated yields of two diastereomers. [d] Enantiomeric excess of the major diastereoisomer determined by chiral HPLC analysis.

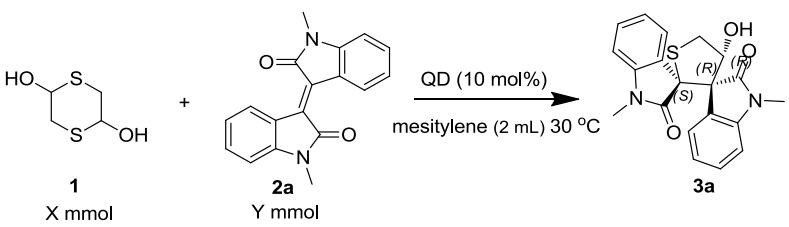
Table S2 Screening of catalyst loadings[a]



entry	X	Time(h)	Yield(%) [b]	dr [c]	ee(%) [d]
1	40	3	78	78/22	80
2	20	3	76	81/19	80
3	10	3	78	80/20	86
4	5	72	72	80/20	78

[a] Unless otherwise specified, the reaction was performed on a scale of 0.06 mmol **1** and 0.1 mmol **2a** in 2 mL solvent at 30 ℃. [b] Isolated yield. [c] Determined by isolated yields of two diastereomers. [d] Enantiomeric excess of the major diastereoisomer determined by chiral HPLC analysis.

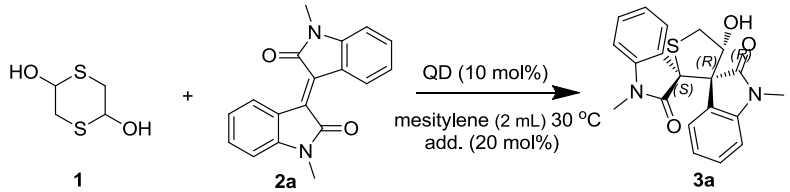
Table S3 Screening of substrate ratios[a]



entry	X	Y	Time(h)	Yield(%) [c]	dr [d]	ee(%) [e]
1	0.05	0.1	48	78	75/25	80
2	0.075	0.1	3	80	80/20	86
3	0.10	0.1	3	78	80/20	87
4	0.15	0.1	3	82	74/26	87

[a] Unless otherwise specified, the reaction was performed with the substrate ratio outlined in the table in 2 mL solvent at 30 ℃. [b] Isolated yield. [c] Determined by isolated yields of two diastereomers.. [d] Enantiomeric excess of the major diastereoisomer determined by chiral HPLC analysis.

Table S4 Screening of additive [a]

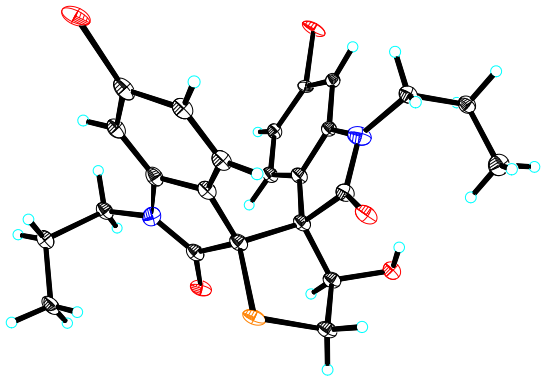


entry	Add.	Time(h)	Yield(%) [b]	dr [c]	ee(%) [d]
1	5A MS(50 mg)	3	82	81/19	87
2	4A MS(50 mg)	3	80	82/18	86
3	3A MS(50 mg)	3	78	82/28	86
4	$MgSO_4$(50 mg)	3	90	82/18	86
5	Et_3N (20mol %)	3	80	75/25	86
6	DABCO (20mol %)	3	67	70/30	82
7	DIPEA (20mol %)	3	86	75/25	86
8	DBU (20mol %)	1	68	68/32	8

[a] Unless otherwise specified, the reaction was performed on a scale of 0.06 mmol **1** and 0.1 mmol **2a** in 2 mL solvent at 30 ℃. [b] Isolated yield. [c] Determined by isolated yields of two diastereomers.[d] Enantiomeric excess of the major diastereoisomer determined by chiral HPLC analysis.

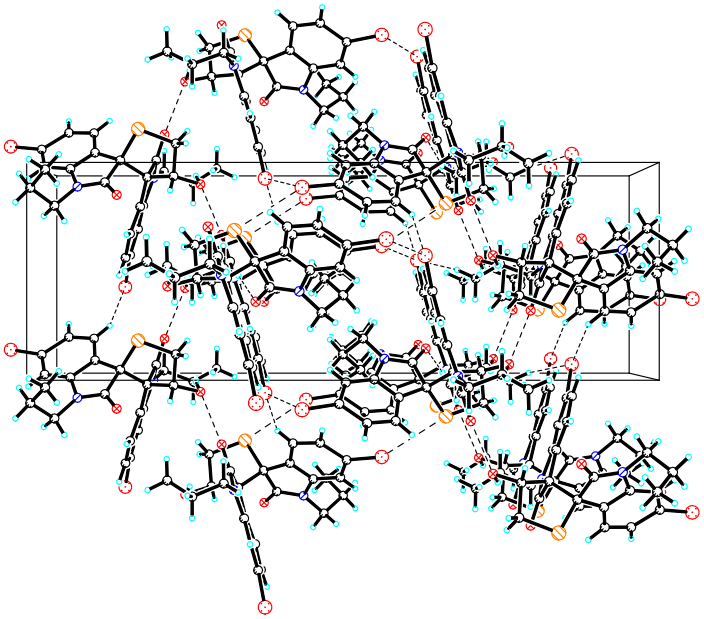
4. Single-Crystal X-ray Crystallography of Products of 3k

Crystal data for 3k: $C_{24}H_{24}Br_2N_2O_3S$, M = 580.33, orthorhombic, a = 9.181(4) Å, b = 9.395(4) Å, c = 27.281(11) Å, α = 90.00 °, β = 90.00 °, γ = 90.00 °, V = 2353.1(17) Å^3, T = 293(2) K, space group $P212121$, Z = 4, μ(MoKα) = 3.563 mm^{-1}, 13144 reflections measured, 4084 independent reflections (R_{int} = 0.1756). The final R_1 values were 0.1472 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.3251 ($I > 2\sigma(I)$). The final R_1 values were 0.1828 (all data). The final $wR(F^2)$ values were 0.3460 (all data). The goodness of fit on F^2 was 1.094. Flack parameter = 0.159(19). The Hooft parameter is 0.140(15) for 1710 Bijvoet pairs.



View of a molecule of 3k with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the hydrogen-bonded motif of 3k.

Hydrogen-bonds are shown as dashed lines.

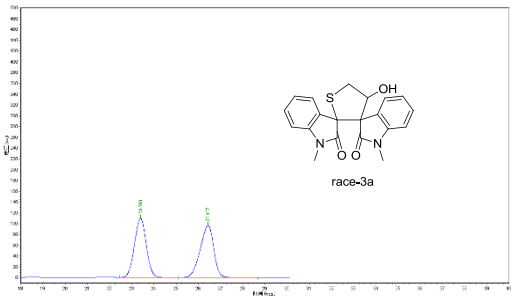
Table 1. Crystal data and structure refinement for 3k.

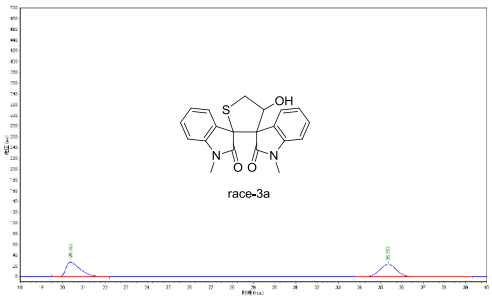
Identification code	3k
Empirical formula	C24 H24 Br2 N2 O3 S
Formula weight	580.33
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 9.181(4) A alpha = 90 deg. b = 9.395(4) A beta = 90 deg. c = 27.281(11) A gamma = 90 deg.
Volume	2353.1(17) A^3
Z, Calculated density	4, 1.638 Mg/m^3

Absorption coefficient	3.563 mm^-1
F(000)	1168
Crystal size	0.22 x 0.21 x 0.20 mm
Theta range for data collection	1.49 to 25.10 deg.
Limiting indices	-10<=h<=10, -11<=k<=10, -32<=l<=32
Reflections collected / unique	13144 / 4084 [R(int) = 0.1756]
Completeness to theta = 25.10	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5360 and 0.5078
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4084 / 834 / 293
Goodness-of-fit on F^2	1.094
Final R indices [I>2sigma(I)]	R1 = 0.1472, wR2 = 0.3251
R indices (all data)	R1 = 0.1828, wR2 = 0.3460
Absolute structure parameter	0.159(19)
Largest diff. peak and hole	1.885 and -2.141 e.A^-3

5. HPLC Spectra

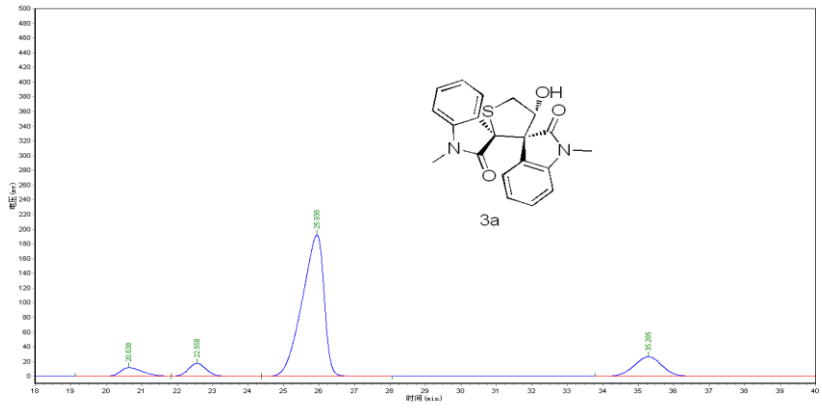
HPLC of 3a





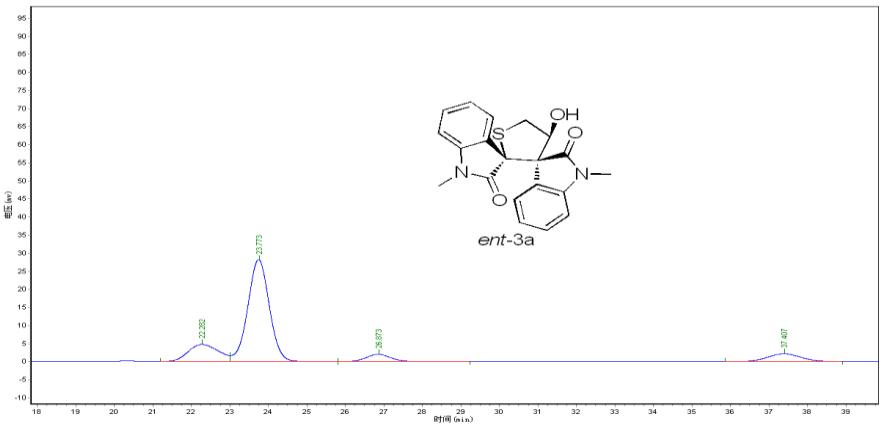
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	23.393	109777.797	4058936.250	49.8843
2	26.437	96290.828	4077772.750	50.1157

Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	20.362	27176.727	1266115.625	49.9552
2	35.353	22978.520	1268387.375	50.0448



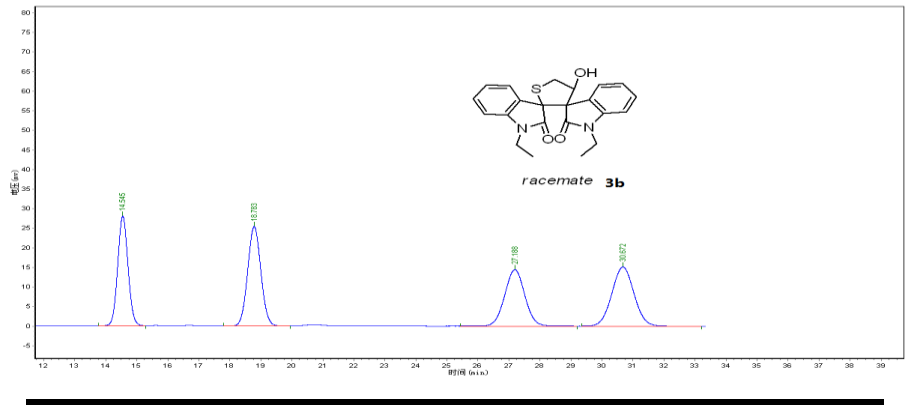
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	20.638	11664.868	511245.688	4.7262
2	22.558	17626.504	618553.688	5.7183
3	25.938	192208.000	8235900.500	76.1374
4	35.285	26478.191	1451454.000	13.4181

HPLC of *ent*-3a

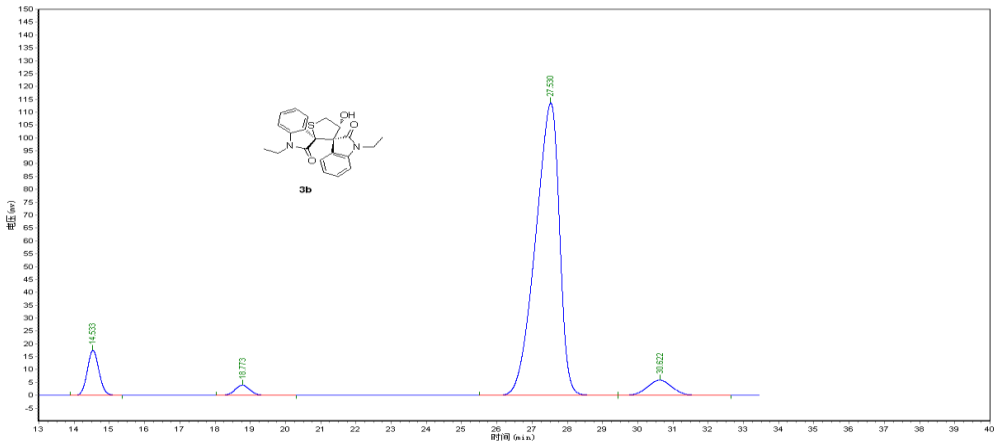


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	22.282	4687.119	257469.359	16.4615
2	23.773	28127.168	1092676.250	69.8612
3	26.873	1976.817	87196.742	5.5750
4	37.407	2121.308	126725.398	8.1023

HPLC of 3b

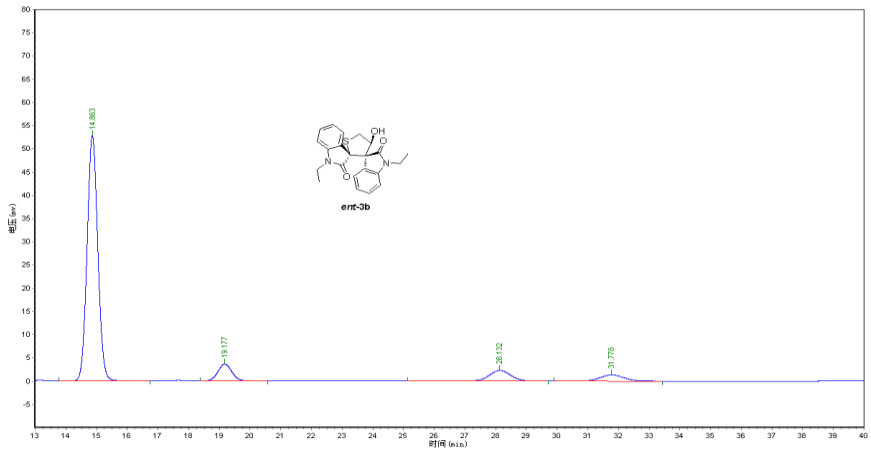


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	14.545	28004.184	646749.750	23.0496
2	18.783	25415.658	754698.438	26.8968
3	27.188	14413.551	650684.500	23.1898
4	30.672	15100.166	753776.500	26.8639



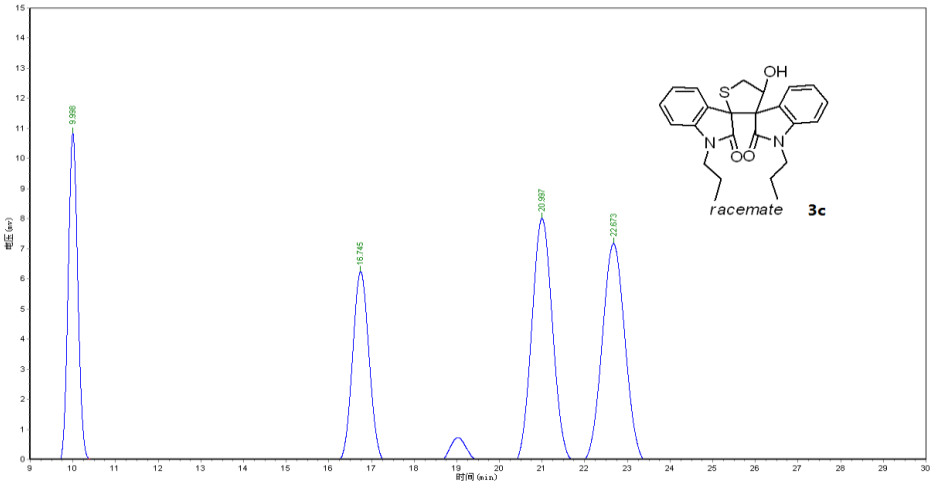
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	14.533	17436.865	401236.375	6.5098
2	18.773	3972.233	118116.000	1.9164
3	27.530	113606.133	5352444.000	86.8403
4	30.622	5925.868	291751.750	4.7335

HPLC of *ent*-3b

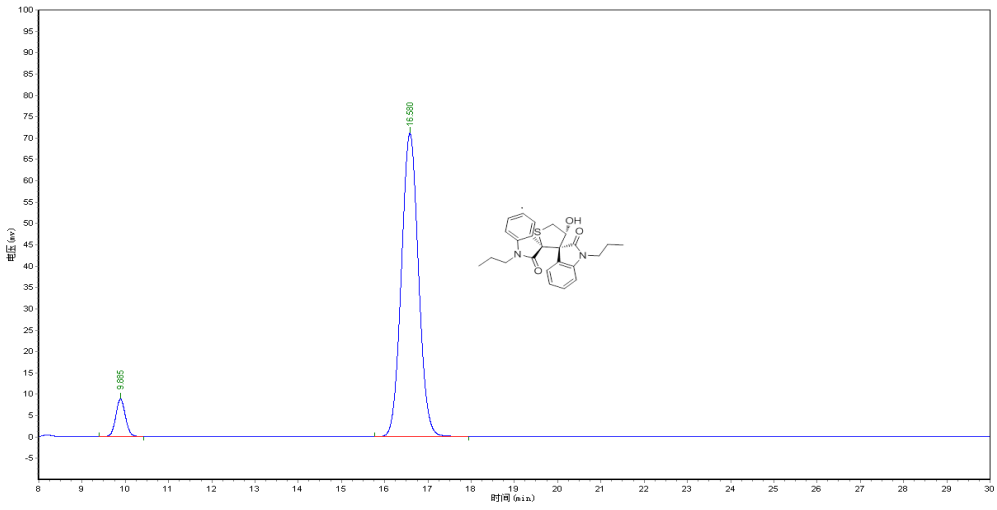


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	14.863	52759.836	1276865.750	81.2043
2	19.177	3643.919	113640.500	7.2271
3	28.132	2274.823	111358.750	7.0820
4	31.778	1332.942	70546.453	4.4865

HPLC of 3c

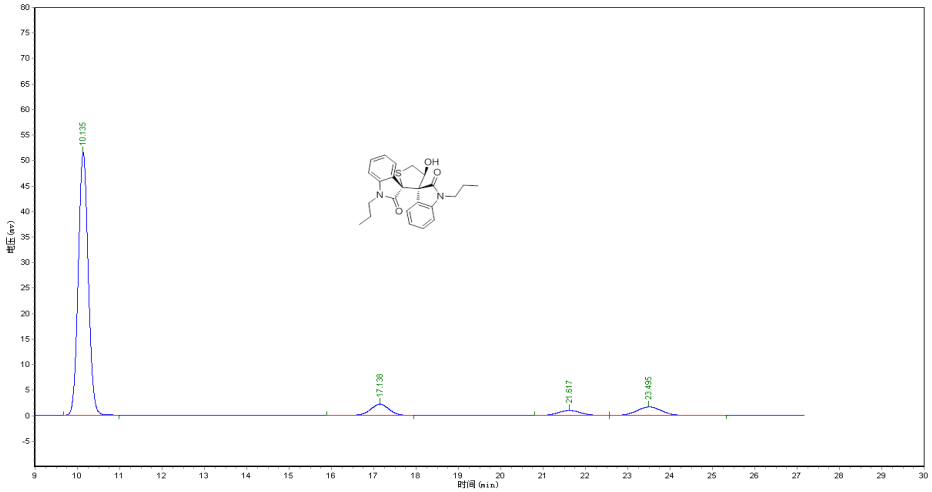


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.998	10918.111	170064.297	18.4362
2	16.745	6391.385	173603.703	18.8199
3	20.997	8283.151	289133.281	31.3441
4	22.673	7458.411	289647.500	31.3998



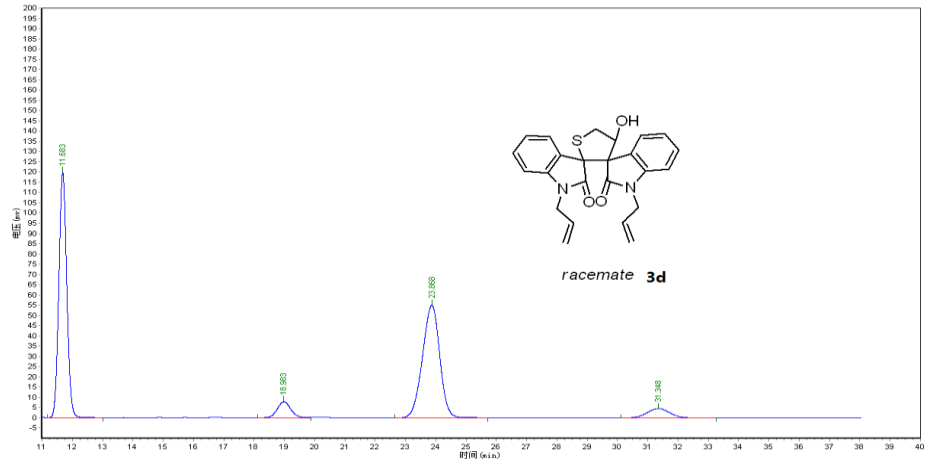
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.885	8757.442	134286.406	6.4600
2	16.580	70978.586	1944439.000	93.5400

HPLC of *ent*-3c



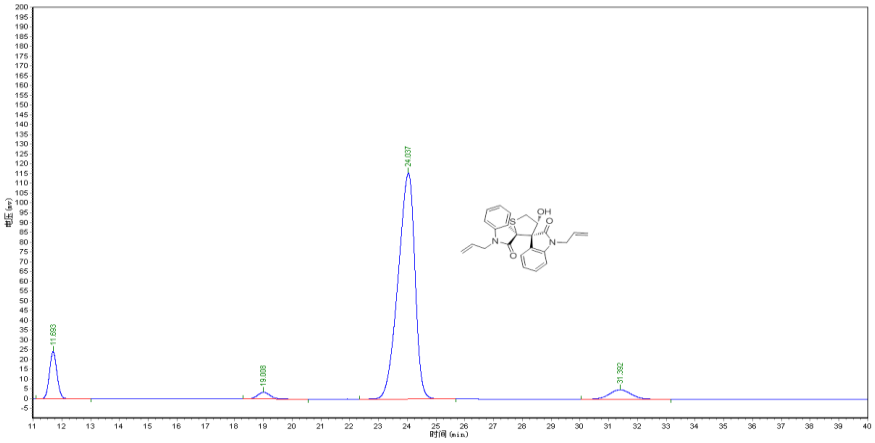
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	10.135	51444.199	838399.063	83.2198
2	17.138	2166.604	65837.852	6.5351
3	21.617	970.164	35525.387	3.5263
4	23.495	1654.137	67688.680	6.7188

HPLC of 3d



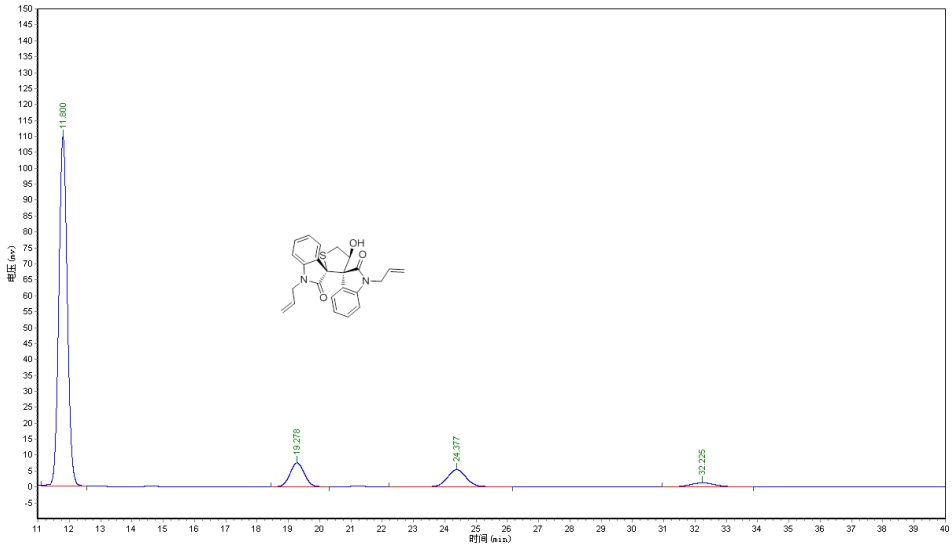
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)

1	11.683	119689.531	2170487.750	45.0283
2	18.983	7838.455	245859.781	5.1005
3	23.868	54998.371	2169290.750	45.0035
4	31.348	4556.082	234635.094	4.8677



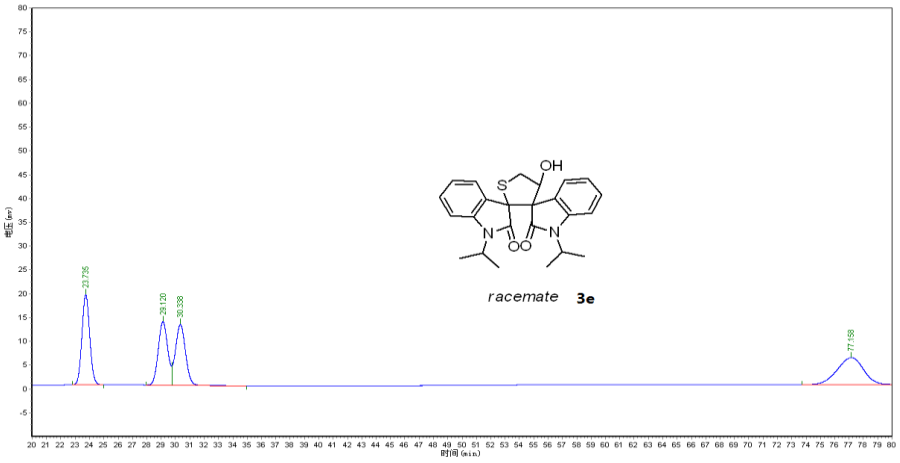
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	11.693	24087.305	440252.688	8.0490
2	19.008	3366.138	102280.297	1.8700
3	24.037	115324.656	4680024.500	85.5633
4	31.392	4810.941	247107.297	4.5178

HPLC of *ent*-3d

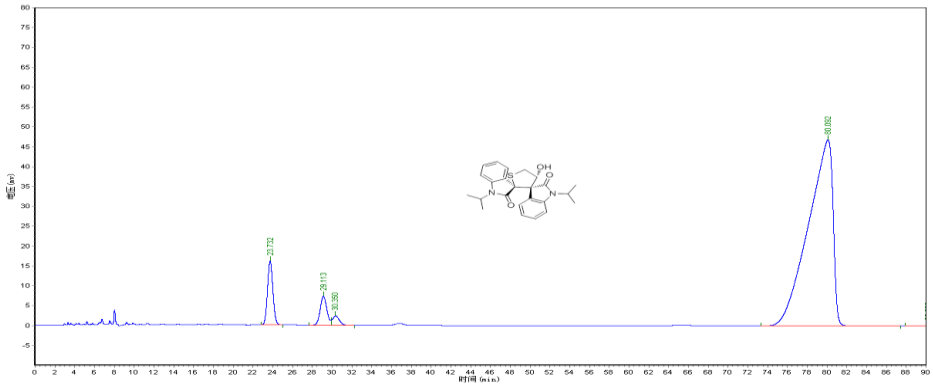


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	11.693	24087.305	440252.688	8.0490
2	19.008	3366.138	102280.297	1.8700
3	24.037	115324.656	4680024.500	85.5633
4	31.392	4810.941	247107.297	4.5178

HPLC of 3e

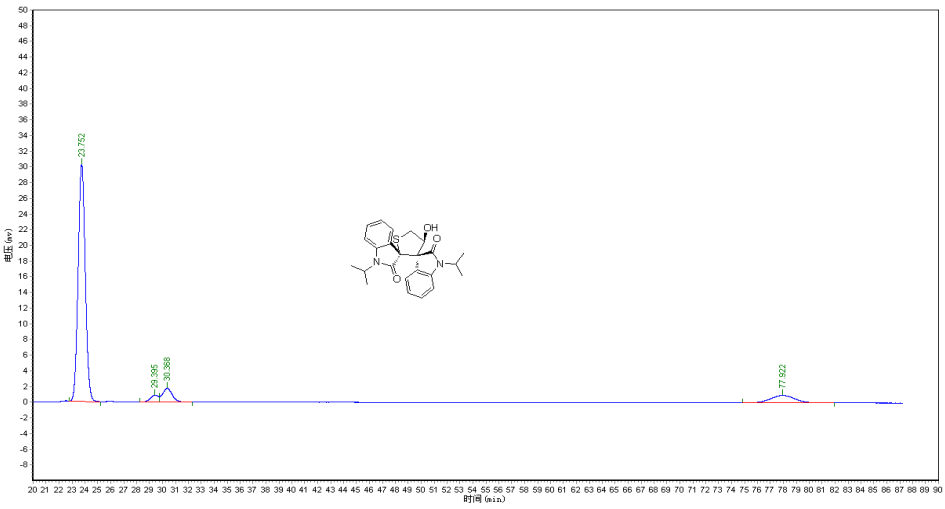


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	23.735	18919.023	713914.063	26.6880
2	29.120	13358.061	620662.875	23.2020
3	30.338	12800.496	621389.000	23.2291
4	77.158	5648.222	719075.750	26.8809



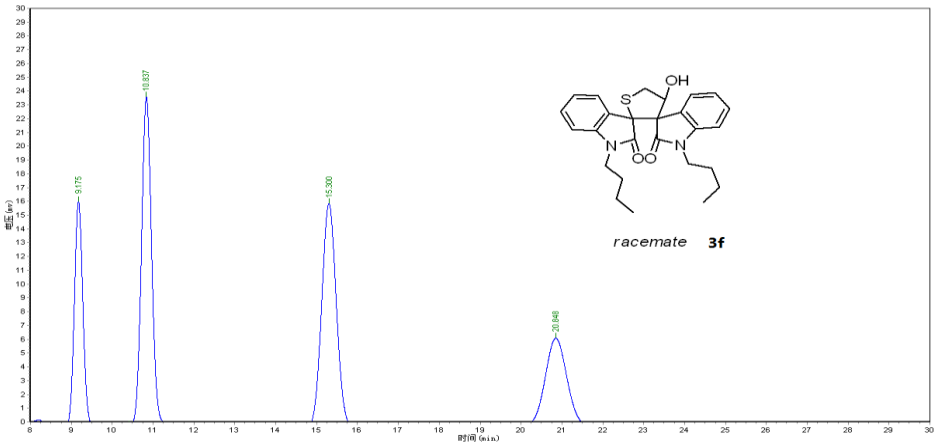
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	23.732	16116.142	609016.313	6.6478
2	29.113	7256.782	343339.906	3.7478
3	30.350	2333.465	111834.133	1.2207
4	80.092	46810.156	8096981.000	88.3837

HPLC of *ent*-3e



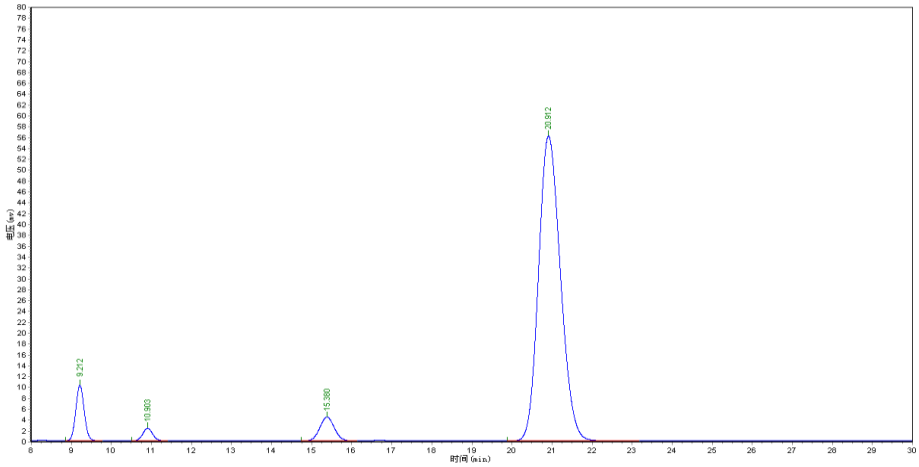
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	23.752	30233.824	1158366.375	82.3087
2	29.395	854.220	37131.332	2.6384
3	30.368	1732.137	89272.664	6.3433
4	77.922	946.784	122572.594	8.7095

HPLC of 3f



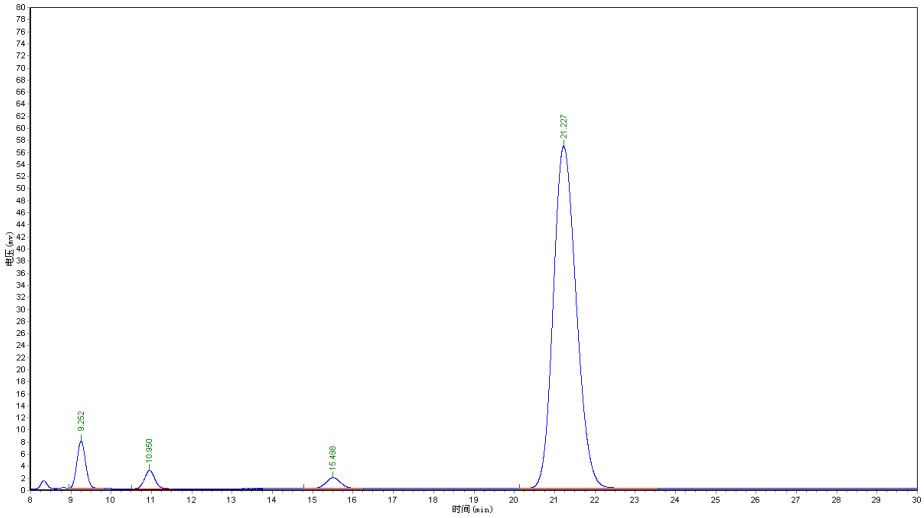
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.175	16354.546	236066.797	17.9923
2	10.837	23821.129	414302.094	31.5769
3	15.300	16342.642	410922.563	31.3193
4	20.848	6468.813	250750.344	19.1115

HPLC of 3f（entry 6）



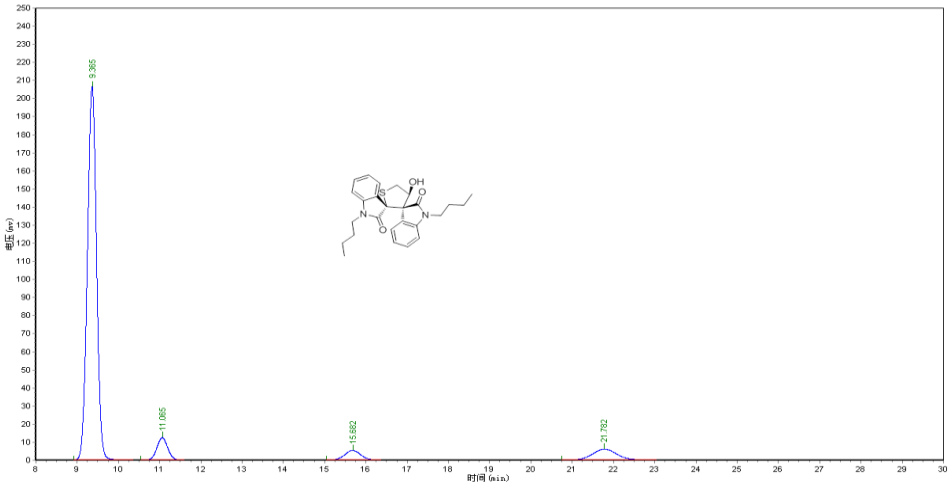
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.212	10184.611	147931.750	6.0959
2	10.903	2291.000	39321.801	1.6204
3	15.380	4345.109	109231.055	4.5011
4	20.912	56121.051	2130253.500	87.7826

HPLC of 3f（entry7）



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.252	7886.436	118847.672	4.8468
2	10.950	3009.131	53042.547	2.1632
3	15.498	1753.653	45128.352	1.8404
4	21.227	56683.957	2235051.000	91.1496

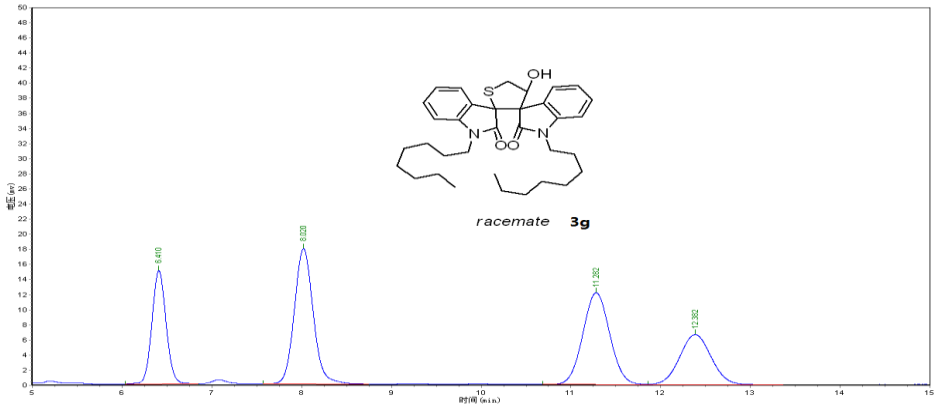
HPLC of *ent*-3f



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.365	206194.328	3175491.000	84.3919
2	11.065	12212.185	218973.797	5.8194
3	15.682	5157.175	135497.203	3.6010

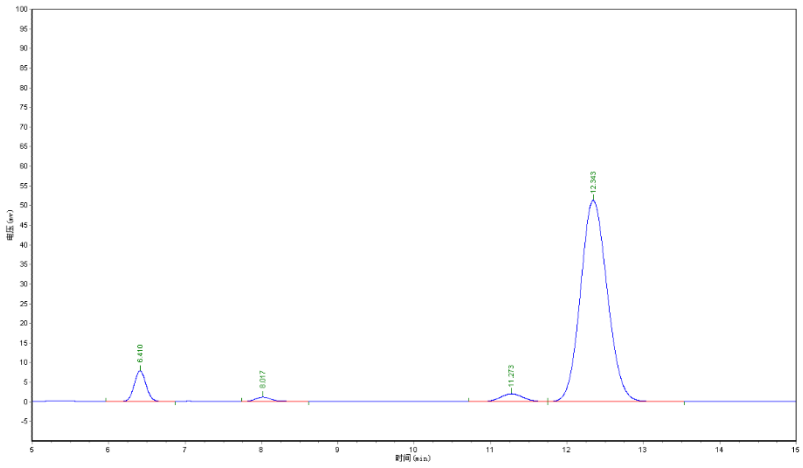
4	21.782	5838.623	232830.406	6.1877

HPLC of 3g



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.410	14970.778	163362.109	19.4946
2	8.020	17872.484	260741.156	31.1152
3	11.282	12146.945	253015.047	30.1932
4	12.382	6618.016	160867.578	19.1969

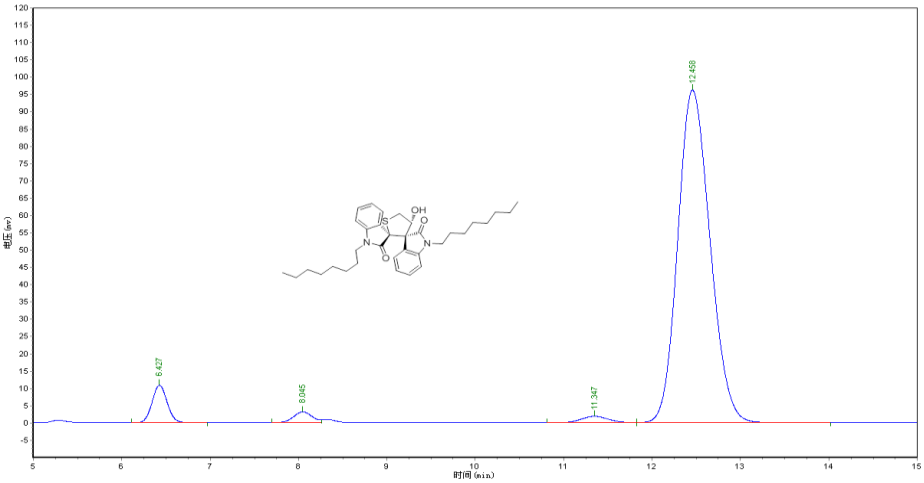
HPLC of 3g（entry8）



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.410	7829.890	84775.398	6.1050
2	8.017	1109.517	16794.600	1.2094
3	11.273	1994.021	41862.691	3.0147
4	12.343	51278.223	1245186.875	

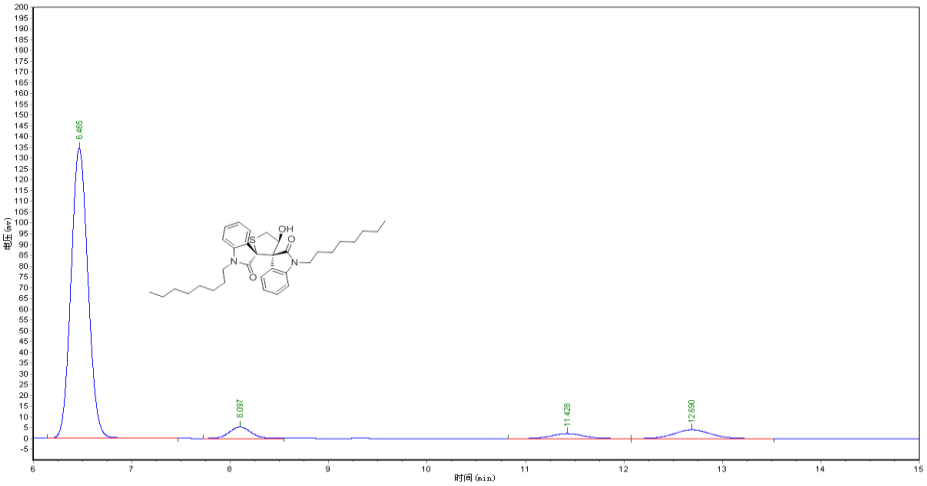
89.6708

HPLC of 3g（entry9）



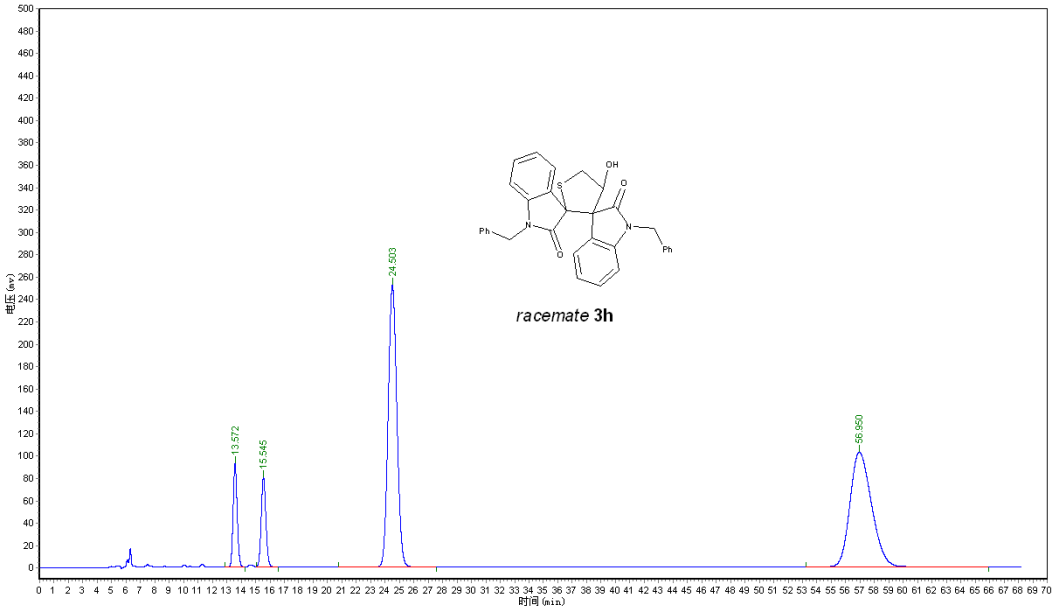
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.427	10767.232	126853.797	4.7886
2	8.045	3059.631	44932.512	1.6962
3	11.347	1831.983	39942.496	1.5078
4	12.458	96186.758	2437340.750	92.0074

HPLC of *ent*-3g

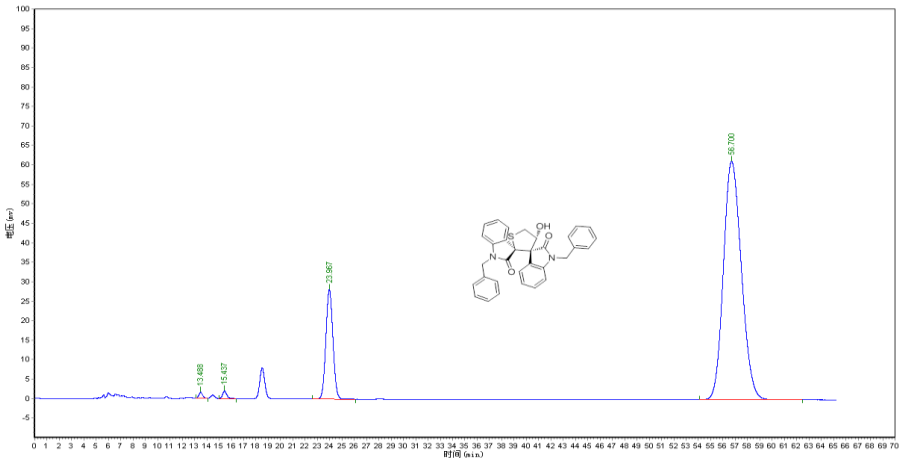


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.465	134569.594	1607247.750	87.2753
2	8.097	5322.147	80661.484	4.3800
3	11.428	2309.685	50658.809	2.7508
4	12.690	3984.293	103015.547	5.5939

HPLC of 3h

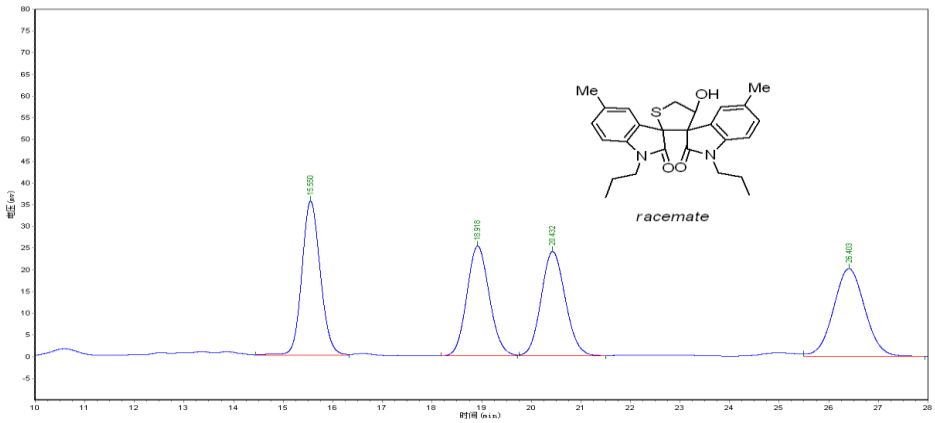


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	13.572	92298.461	1827098.625	7.3517
2	15.545	80315.867	1822047.875	7.3313
3	24.503	251673.563	10596600.000	42.6373
4	56.950	102317.000	10607158.000	42.6798

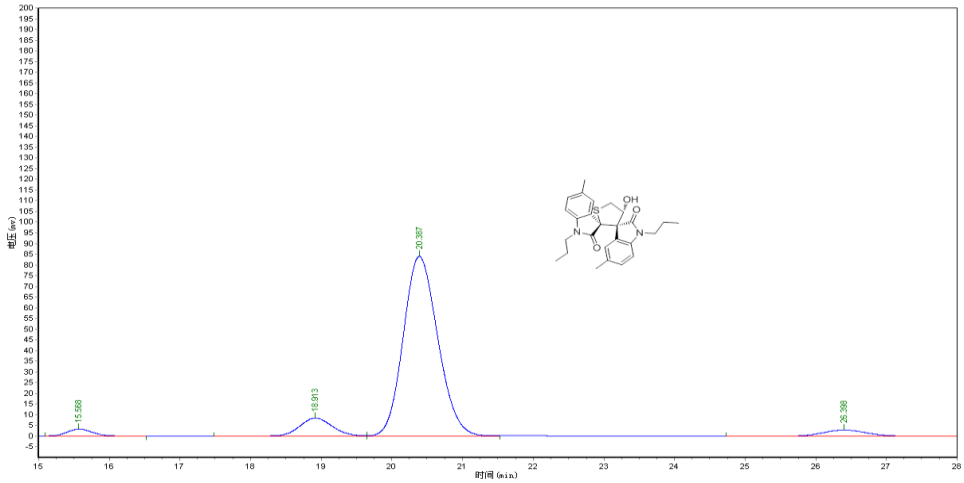


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	13.488	1507.670	32163.295	0.4341
2	15.437	1920.231	45438.551	0.6133
3	23.967	28071.830	1120256.125	15.1212
4	56.700	61175.172	6210668.000	83.8314

HPLC of 3i

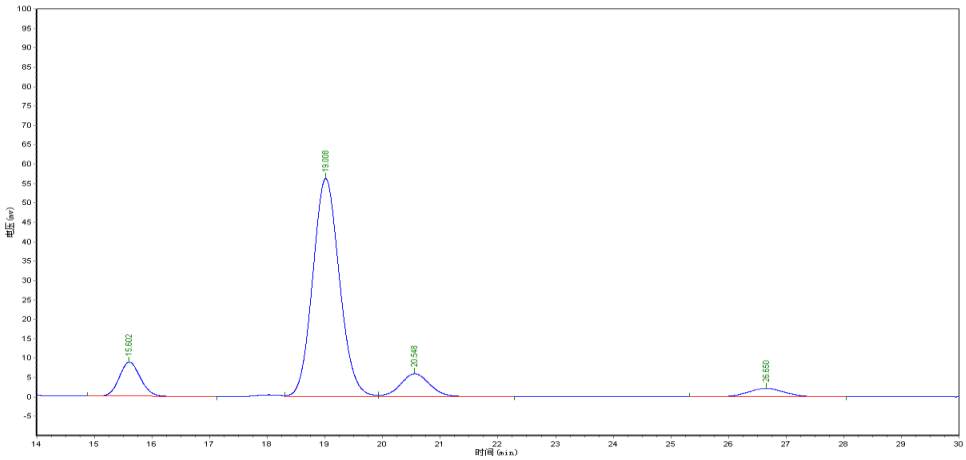


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	15.550	35487.566	917553.938	26.8713
2	18.918	25290.893	799499.125	23.4140
3	20.432	24047.186	816979.500	23.9259
4	26.403	20166.824	880592.625	25.7889



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	15.568	3238.000	80609.102	2.4138
2	18.913	8463.814	275365.656	8.2456
3	20.387	83981.742	2855606.000	85.5088
4	26.398	2926.960	127967.500	3.8319

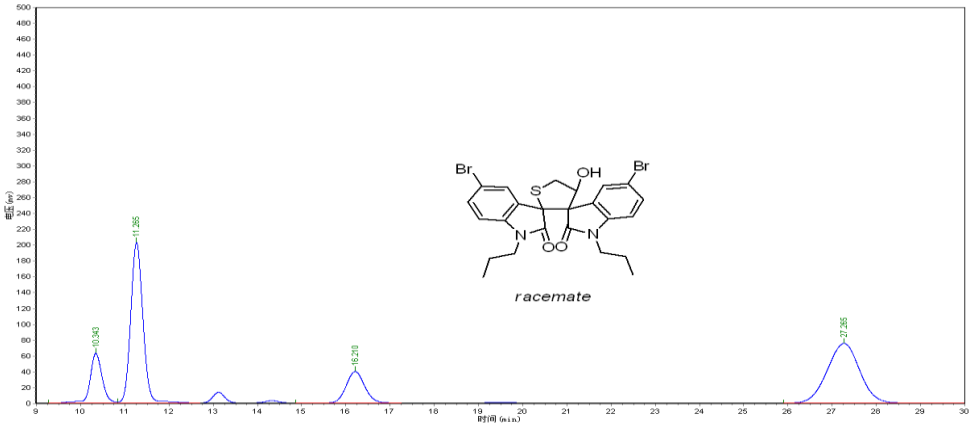
HPLC of *ent*-3i



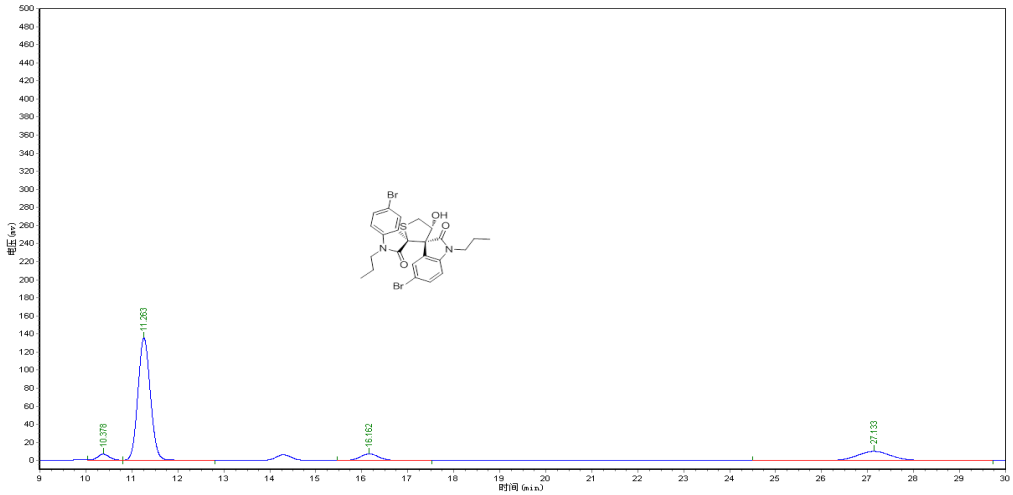
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)

1	15.602	8753.476	221961.141	9.5108
2	19.008	56194.859	1808760.375	77.5036
3	20.548	5888.881	208466.984	8.9326
4	26.650	2138.827	94588.094	4.0530

HPLC of 3j



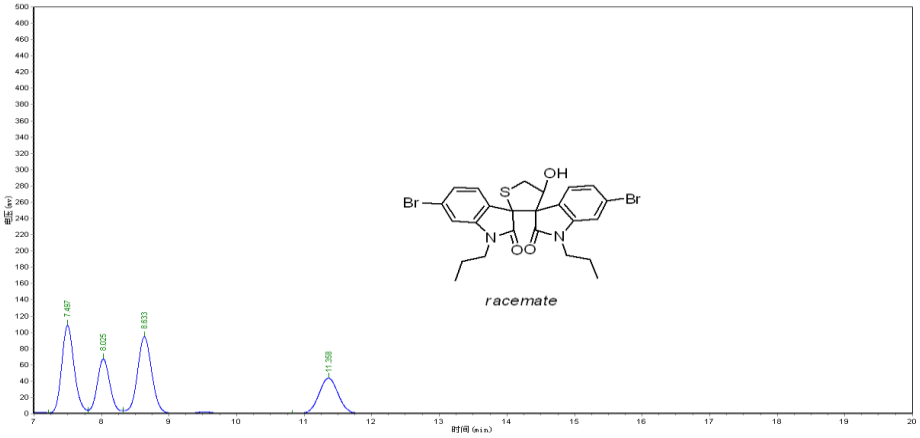
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	10.343	62580.699	1170227.875	11.6085
2	11.265	202249.563	3878350.750	38.4726
3	16.210	39704.207	1161334.750	11.5202
4	27.265	75366.398	3870909.750	38.3987



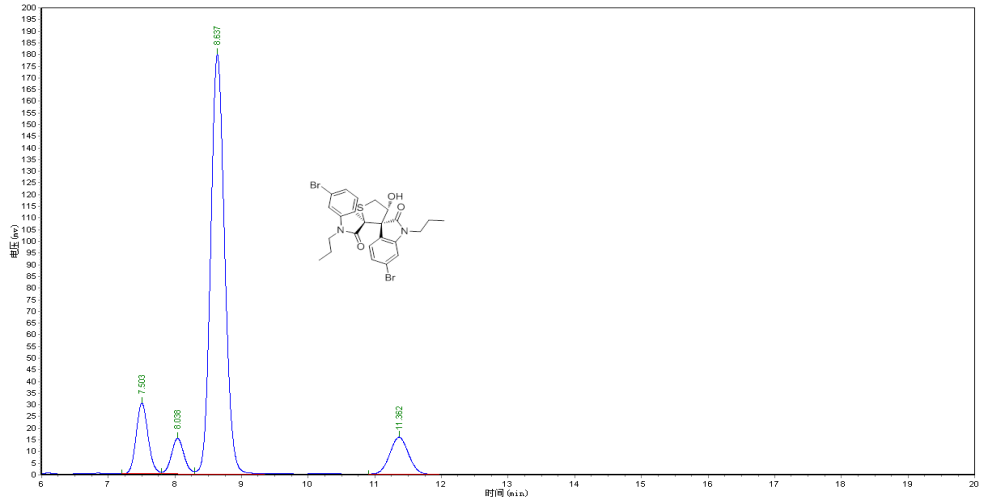
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)

1	10.378	6759.042	122855.336	3.6300
2	11.263	135490.891	2547730.750	75.2776
3	16.162	7192.789	201007.750	5.9392
4	27.133	10059.570	512852.063	15.1532

HPLC of 3k

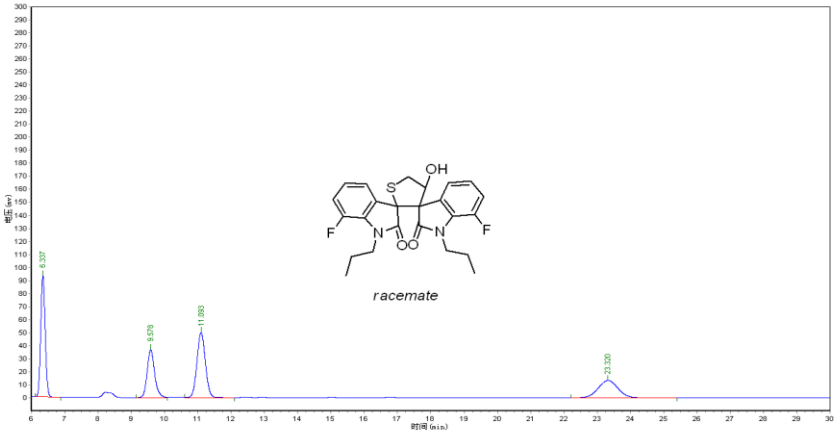


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	7.497	108177.656	1390015.250	30.8556
2	8.025	66838.203	875236.563	19.4285
3	8.633	94033.227	1385637.000	30.7584
4	11.358	43561.902	854015.000	18.9575

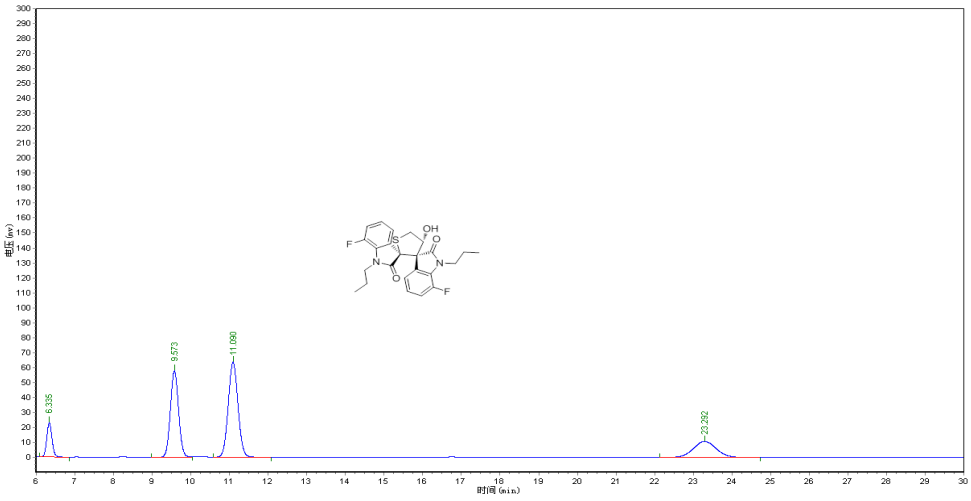


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	7.503	30307.955	374939.531	10.7577
2	8.038	15209.912	199138.984	5.7137
3	8.637	179655.703	2605048.250	74.7437
4	11.362	15756.313	306182.344	8.7849

HPLC of 3l

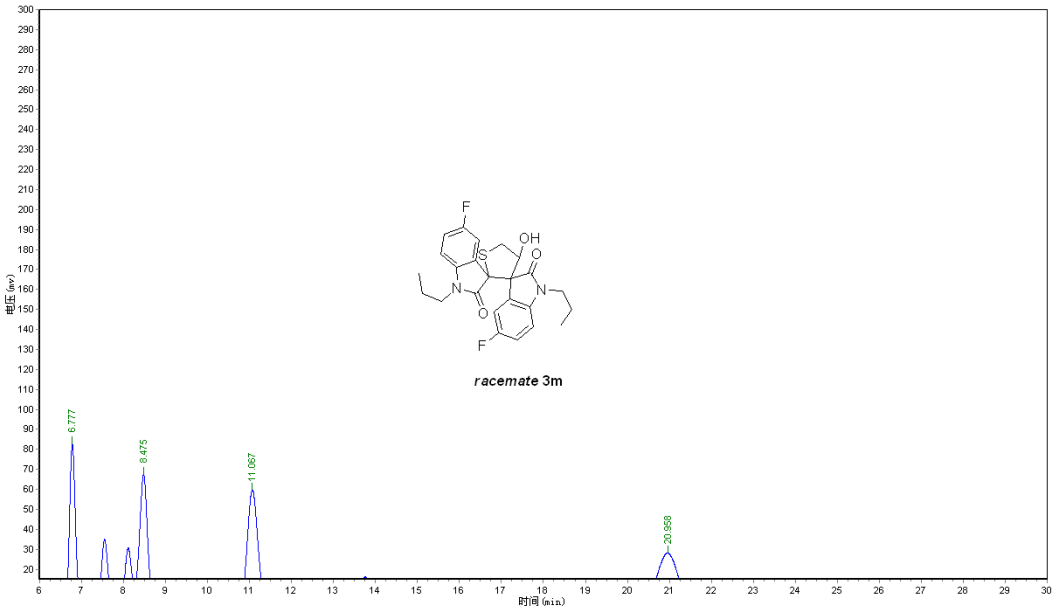


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.337	93209.953	870729.500	30.3308
2	9.578	36691.500	573911.688	19.9915
3	11.093	50006.441	879340.313	30.6307
4	23.320	13234.923	546797.688	19.0470

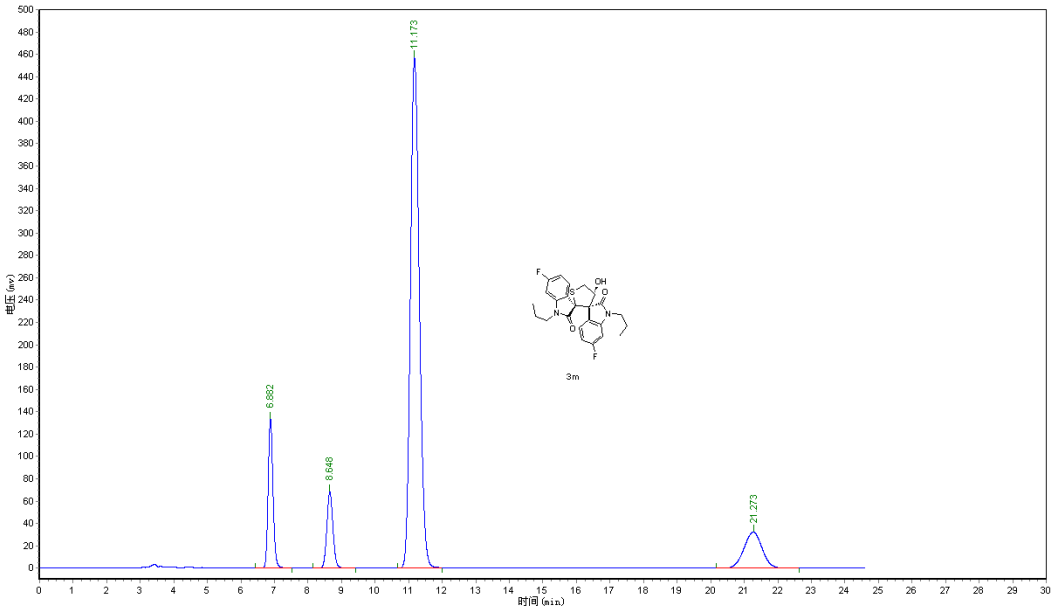


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.335	22872.143	215660.406	8.2255
2	9.573	57669.719	854046.313	32.5740
3	11.090	63437.137	1115562.250	42.5484
4	23.292	10599.099	436595.938	16.6521

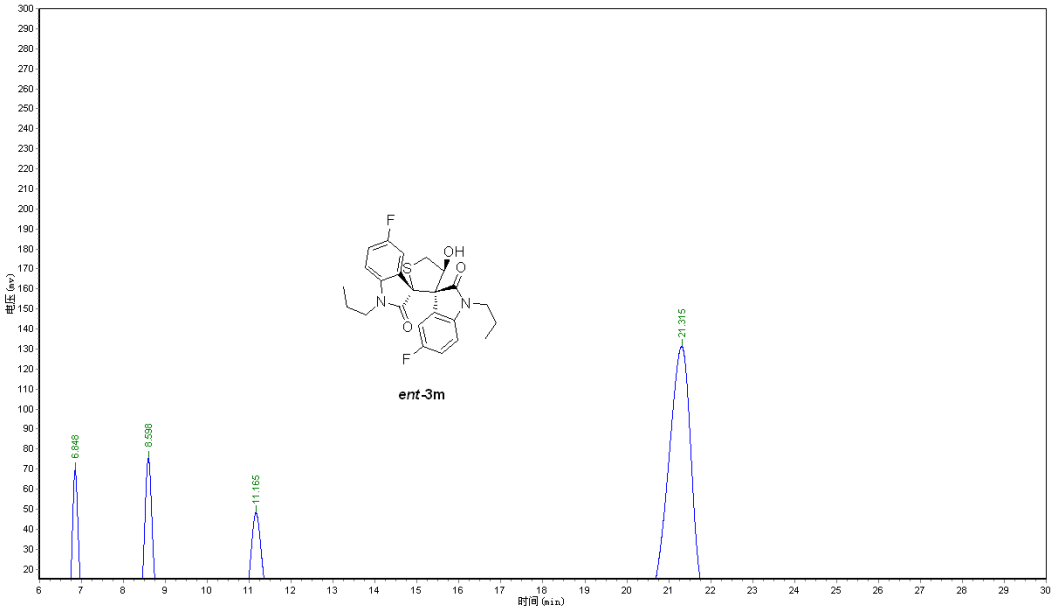
HPLC of 3m



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.777	81174.555	792822.875	20.9706
2	8.475	66077.695	899301.688	23.7870
3	11.067	58985.758	1056304.625	27.9398
4	20.958	27745.822	1032213.875	27.3026



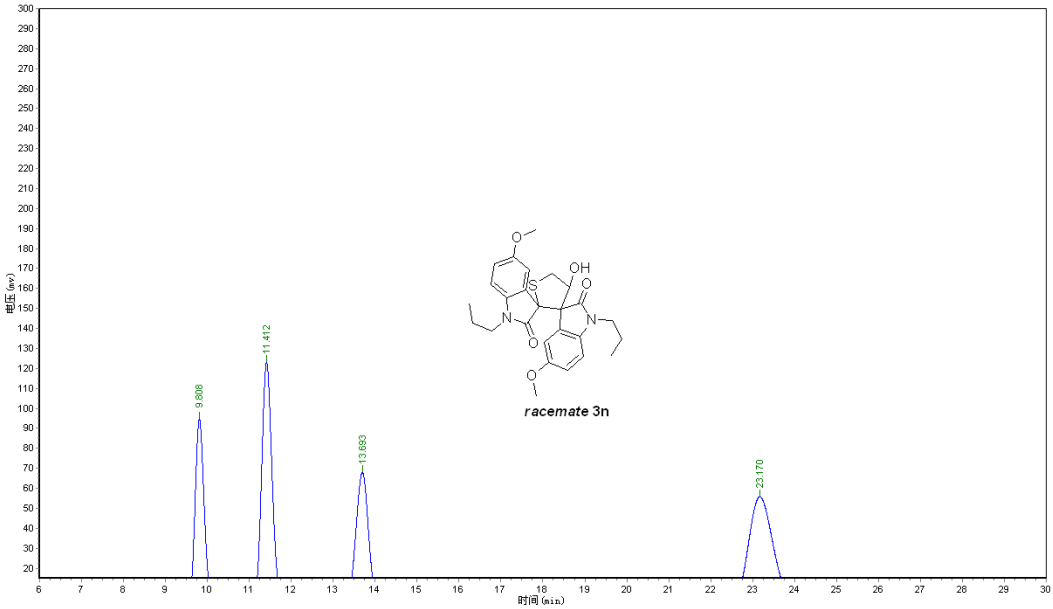
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.882	133073.234	1327281.125	11.2572
2	8.648	67775.313	857053.000	7.2690
3	11.173	456329.031	8399301.000	71.2381
4	21.273	32155.158	1206820.750	10.2356



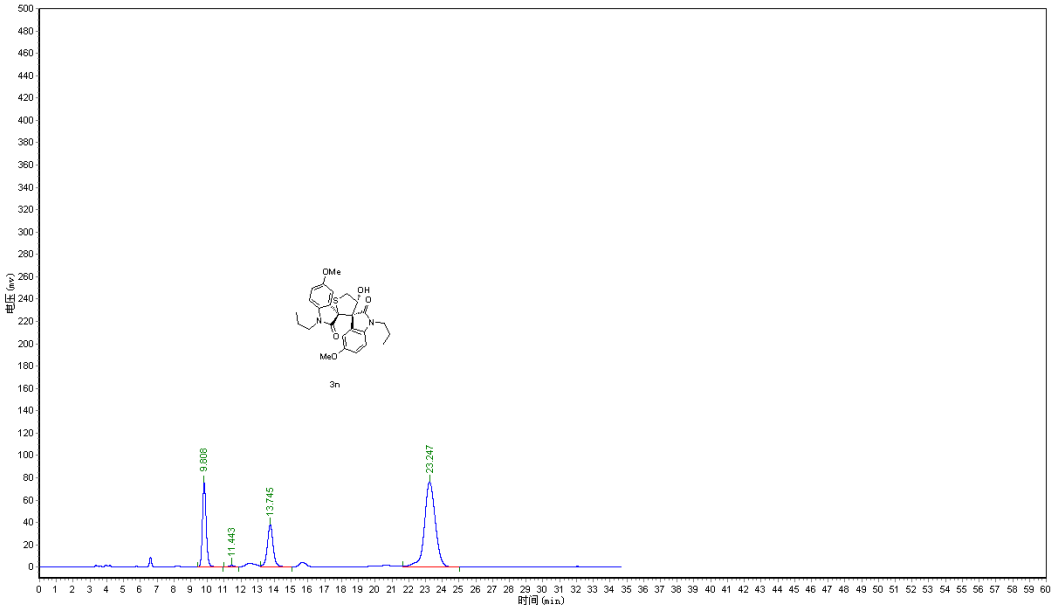
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	6.848	69086.891	677474.125	9.0556
2	8.598	75282.766	938544.688	12.5452
3	11.165	47992.141	862849.625	11.5335

4	21.315	131231.031	5002408.000	66.8657

HPLC of 3n

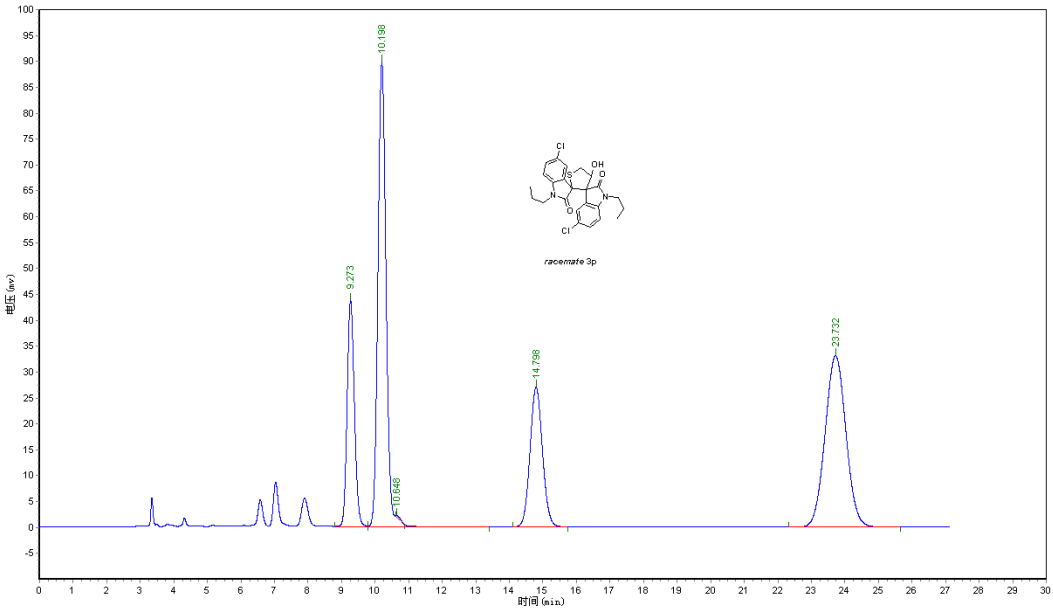


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.808	92788.781	1374358.125	18.6497
2	11.412	122274.430	2126005.250	28.8494
3	13.693	67421.891	1444915.125	19.6072
4	23.170	55664.289	2424040.500	32.8937

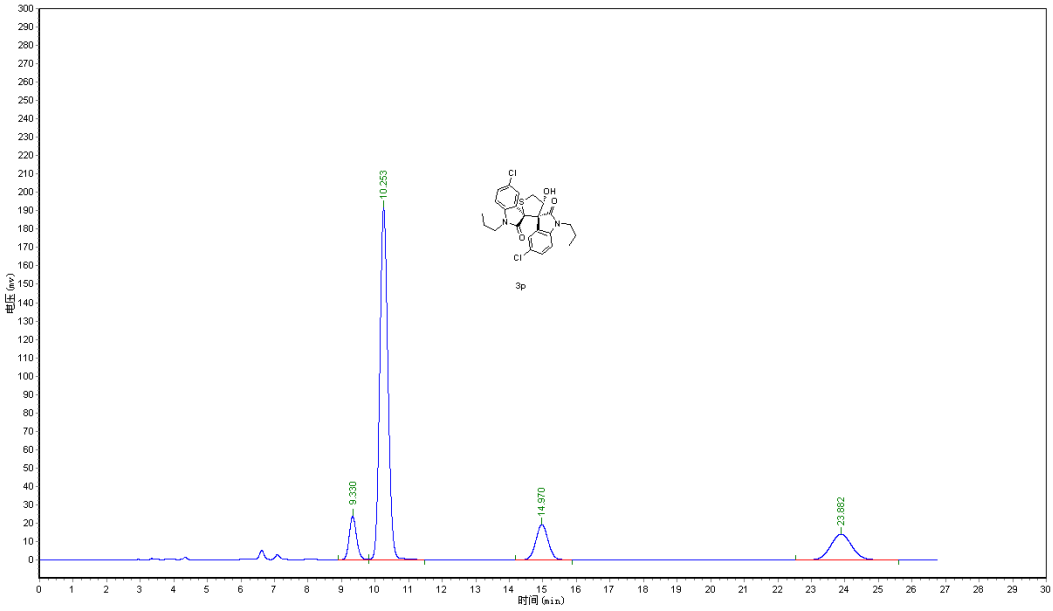


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.808	75052.148	1159748.750	21.1345
2	11.443	1231.233	21346.689	0.3890
3	13.745	37454.383	898470.500	16.3732
4	23.247	76169.508	3407895.000	62.1033

HPLC of 3o

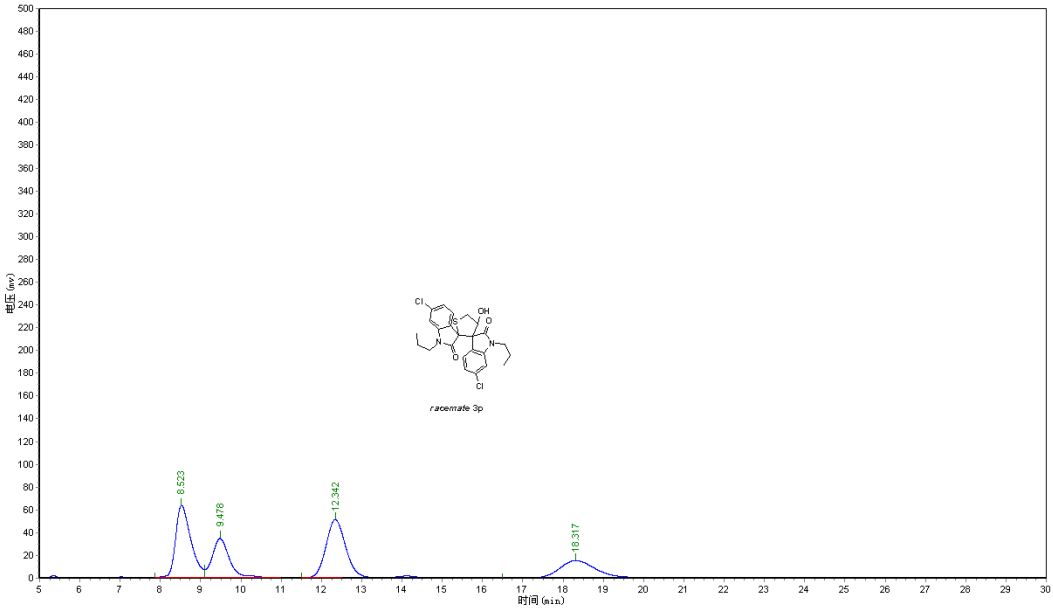


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.273	43647.266	654971.313	15.2544
2	10.198	89590.523	1510184.000	35.1724
3	10.648	288.290	3072.700	0.0716
4	14.798	26918.381	692587.000	16.1305
5	23.732	33118.023	1432843.250	33.3712

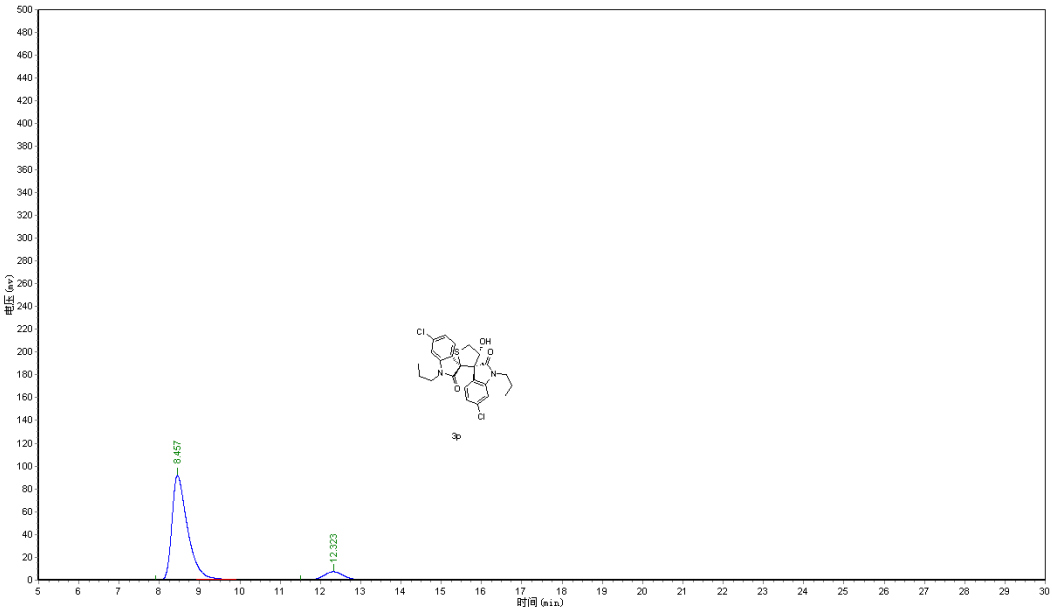


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	9.330	23422.906	356040.813	7.6414
2	10.253	191381.359	3214327.250	68.9866
3	14.970	19134.318	480734.688	10.3176
4	23.882	13976.125	608246.688	13.0543

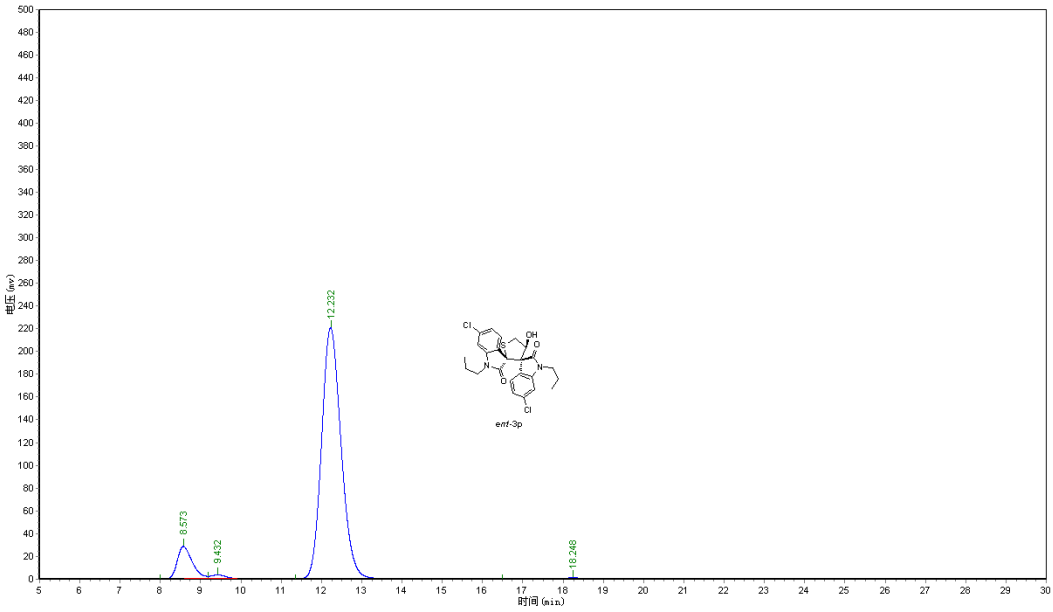
HPLC of 3p



Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	8.523	63202.742	1669647.500	31.0199
2	9.478	34300.695	1014424.438	18.8467
3	12.342	50984.449	1734510.500	32.2250
4	18.317	15201.221	963914.938	17.9083

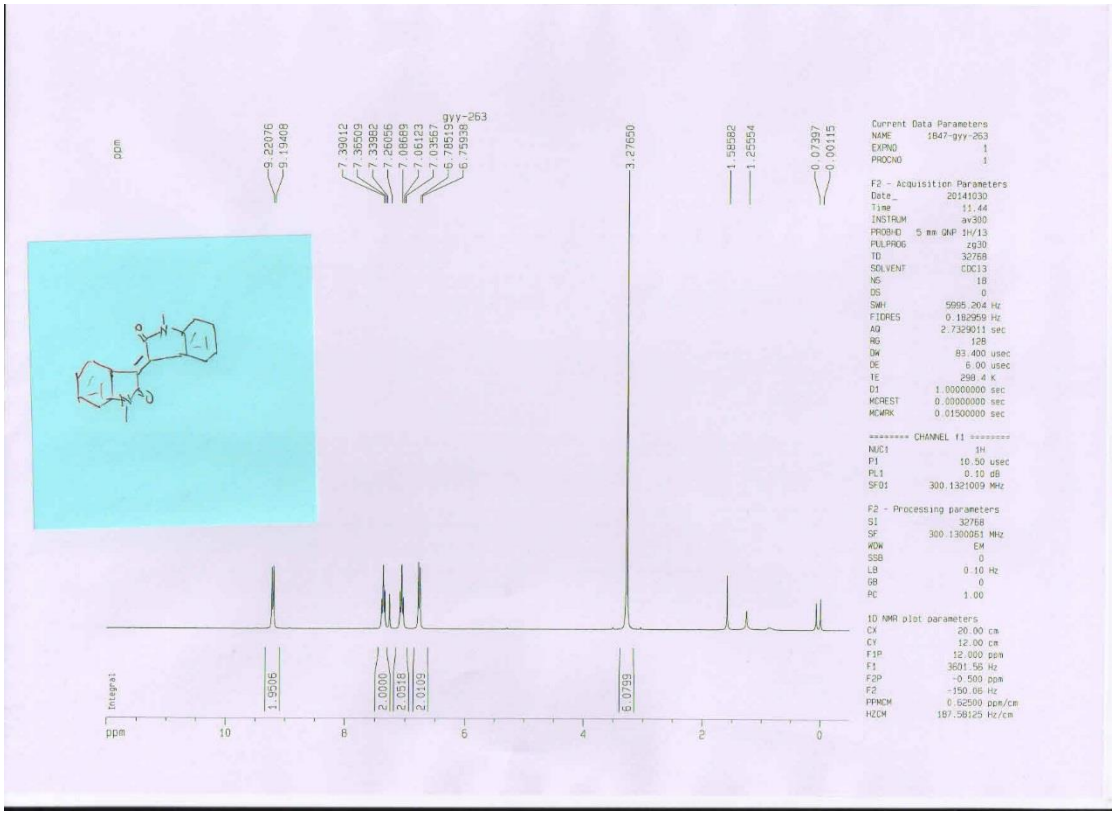


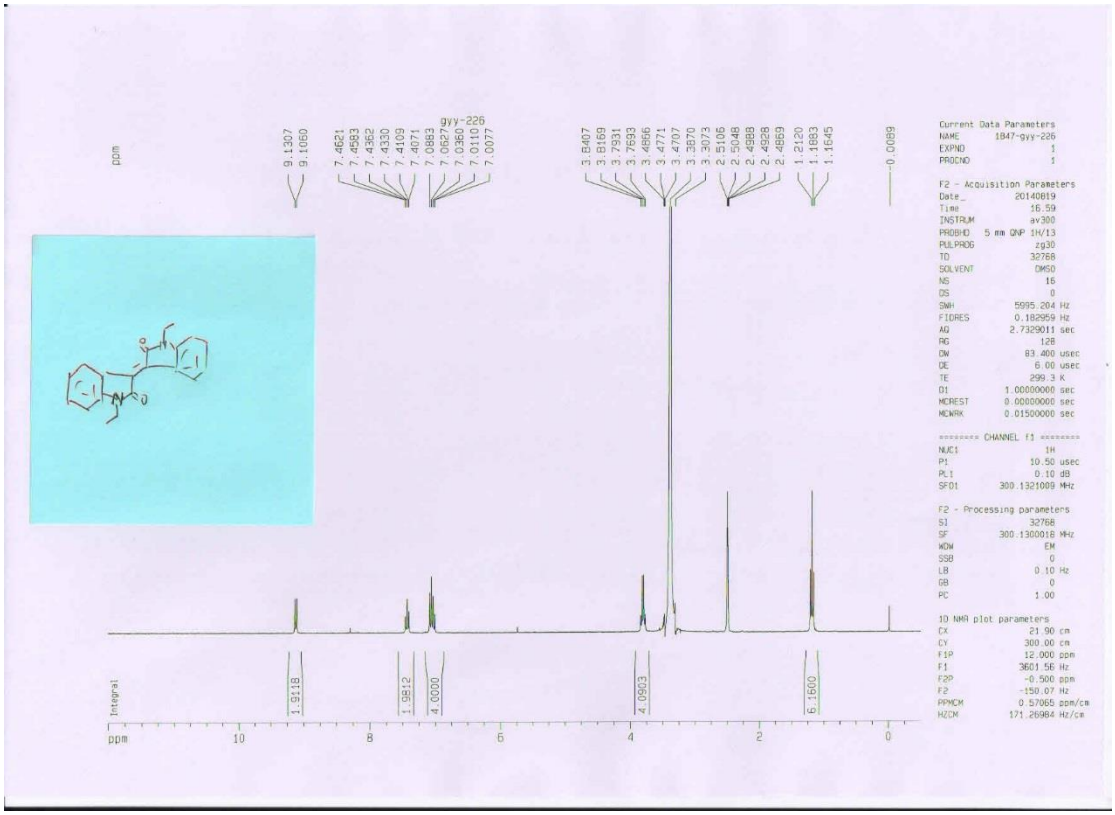
Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	8.457	91545.414	2464670.500	90.9878
2	12.323	7203.161	244122.703	9.0122

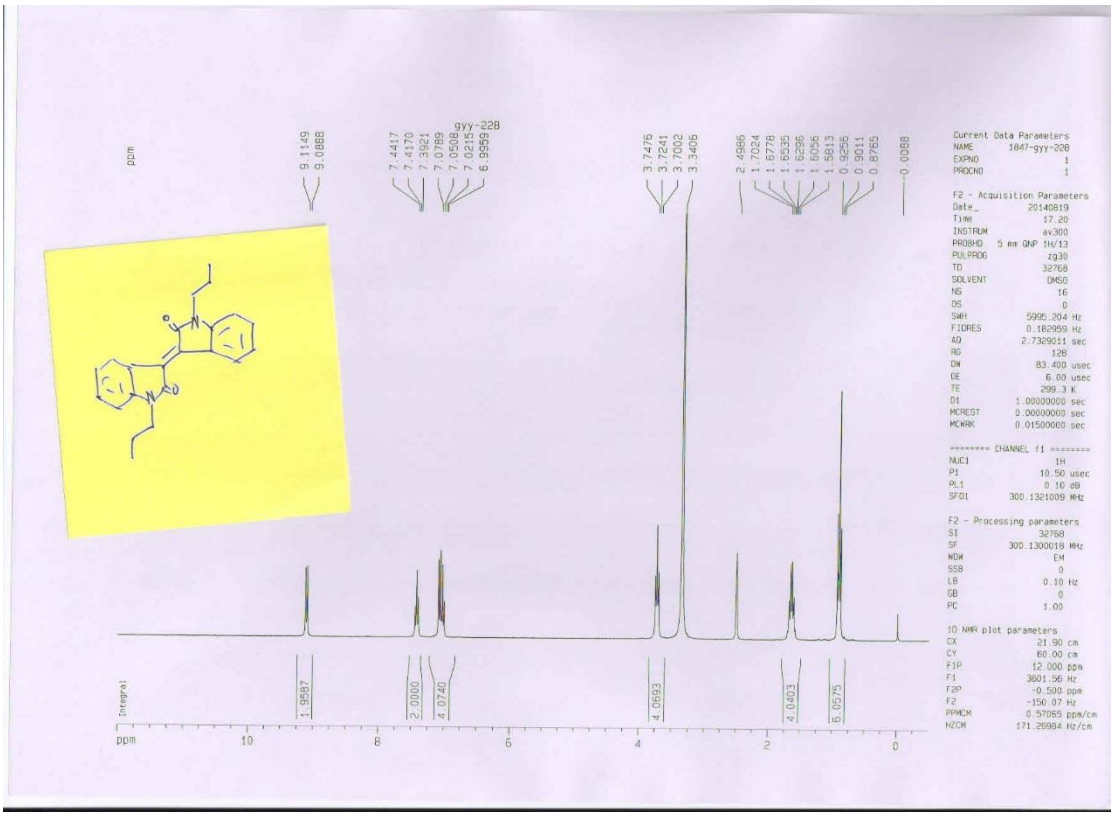


Peak	RT (min)	Height (mV*sec)	Area (mV)	Area (%)
1	8.573	28419.209	734969.750	8.8977
2	9.432	3097.795	78541.875	0.9508
3	12.232	220439.672	7395083.500	89.5263
4	18.248	880.094	51640.898	0.6252

6. Copies of NMR and MS Spectra



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7.4417
7.4170
7.3921
7.0789
7.0508
7.0215
6.9959
3.7476
3.7241
3.7002
3.3406
2.4986
1.7024
1.6778
1.6535
1.6286
1.6056
1.5813
0.9256
0.9011
0.8765
-0.0088
Integral
1.9587
2.0000
4.0740
4.0693
4.0403
6.0575
ppm
10
8
6
4
2
0
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NAME 1847-gyy-228
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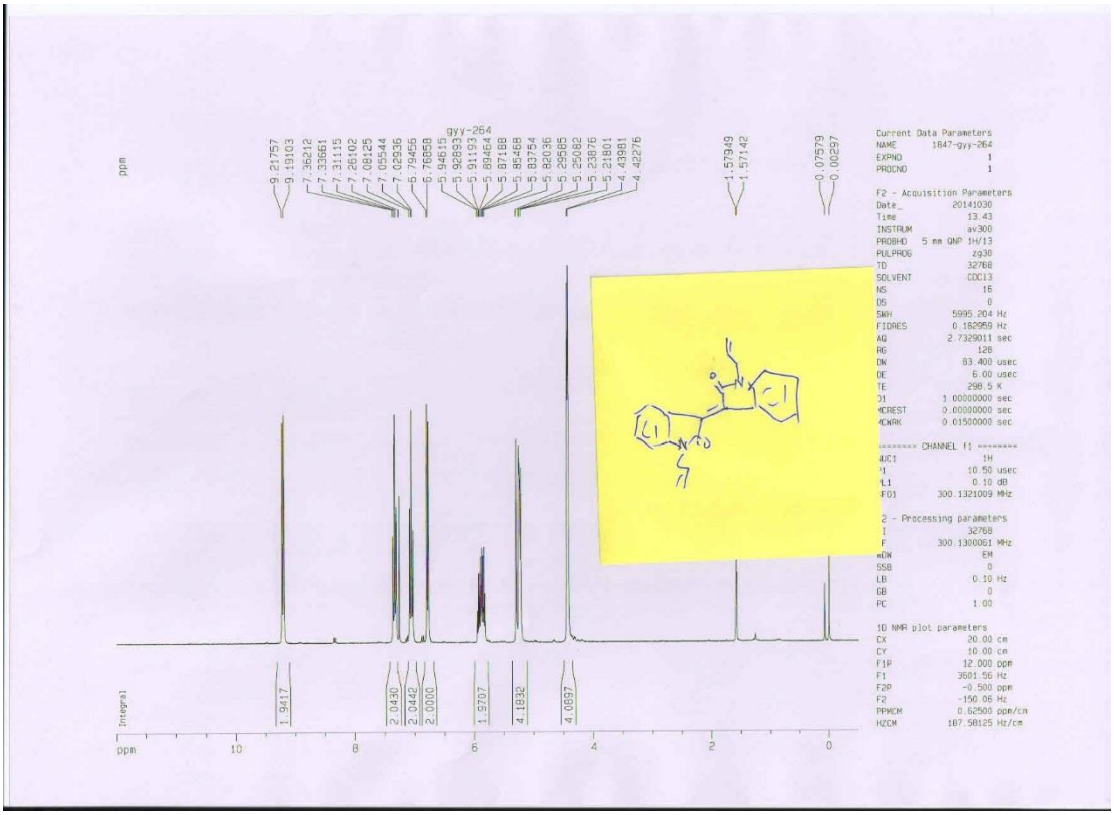
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140819
Time 17.20
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300018 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 60.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.57065 ppm/cm
HZCM 171.26984 Hz/cm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9.19103
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7.33661
7.31115
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7.08125
7.05544
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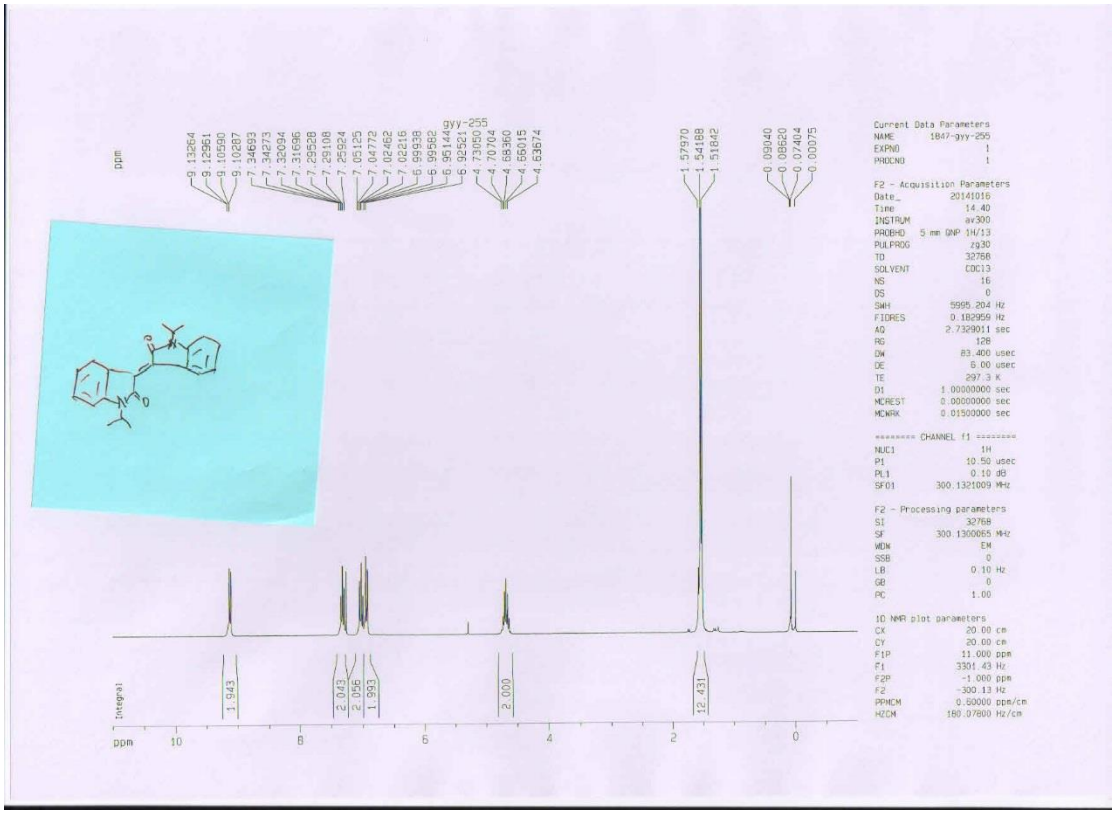
5.79456
5.76858
5.94615
5.92893
5.91193
5.89464
5.87188
5.85468
5.83754
5.82036
5.29565
5.25082
5.23876
5.21801
4.43981
4.42276
1.57949
1.57142
0.07579
0.00297
Integral
1.9417
2.0430
2.0442
2.0000
1.9707
4.1932
4.0897
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-264
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141030
Time 13.43
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.50125 Hz/cm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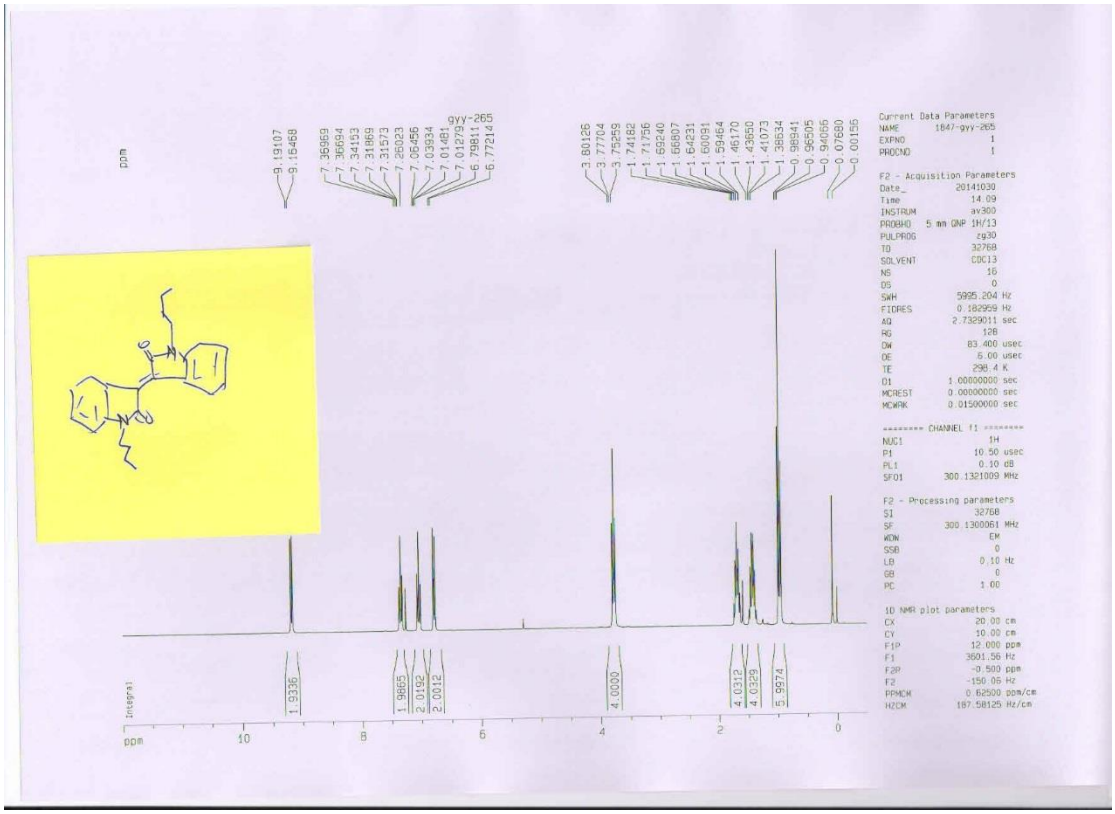
9.12961
9.10590
9.10287
7.34693
7.34273
7.32694
7.31586
7.29528
7.29108
7.25824
7.05125
7.04772
7.02462
7.02216
6.99938
6.99582
6.95144
6.92521
4.73050
4.70704
4.68360
4.66015
4.63674
1.57970
1.54188
1.51842
0.09040
0.08620
0.07404
0.00075
ppm
integral
1.943
2.043
2.056
1.993
2.000
12.431
Current Data Parameters
NAME 1847-gyy-255
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141016
Time 14.40
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.50000 ppm/cm
HZCM 150.07800 Hz/cm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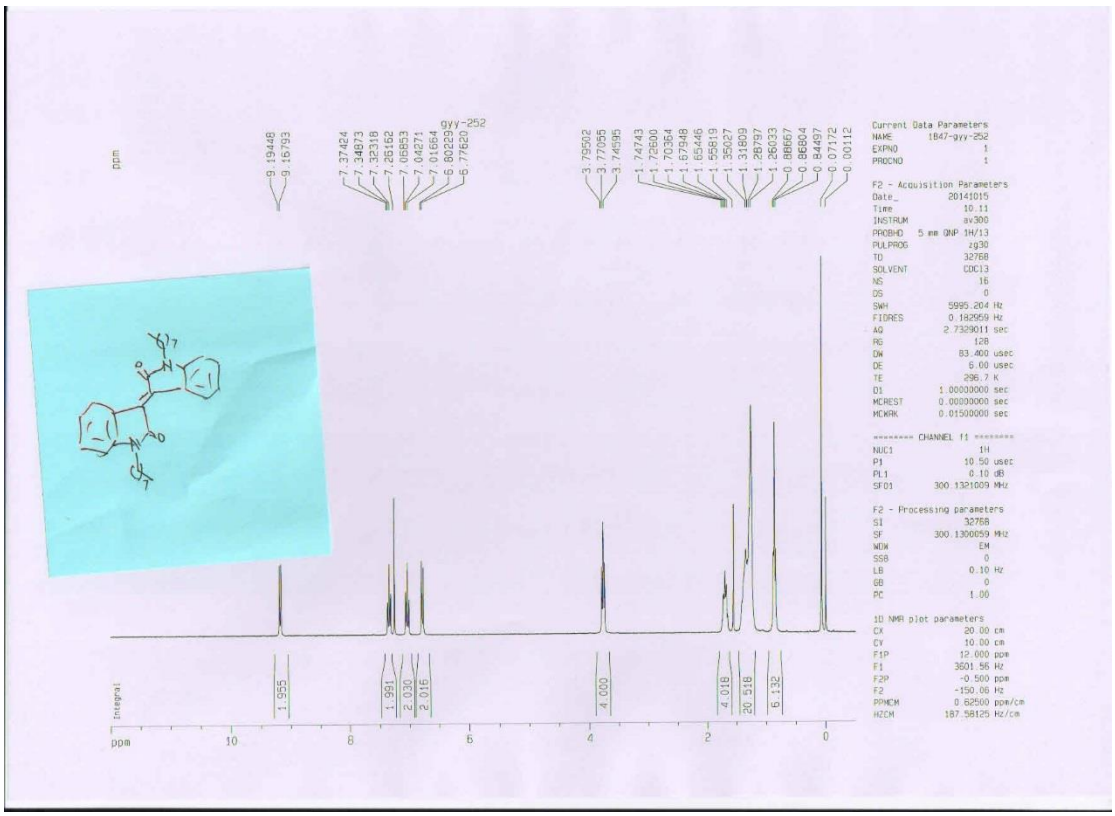
7.36694
7.34193
7.31869
7.31573
7.28023
7.06456
7.03934
7.01481
7.01279
6.79811
6.77214
3.80126
3.77704
3.75259
1.74182
1.71756
1.69340
1.66807
1.64231
1.60091
1.59464
1.46170
1.43650
1.41073
1.38634
0.98941
0.96505
0.94056
0.07680
0.00156
ppm
integral
1.9336
1.9865
2.0192
2.0012
4.0000
4.0312
4.0329
5.9974
Current Data Parameters
NAME 1847-gyy-265
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141030
Time 14.09
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.05 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm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7.06853
7.04271
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6.80229
6.77629
3.79502
3.77055
3.74595
1.74743
1.72600
1.70364
1.67948
1.65446
1.55819
1.35027
1.31809
1.28737
1.26033
0.88667
0.86804
0.84497
0.07172
0.00112
Integral
1.955
1.991
2.030
2.016
4.000
4.018
20.516
6.132
ppm
10
8
6
4
2
0
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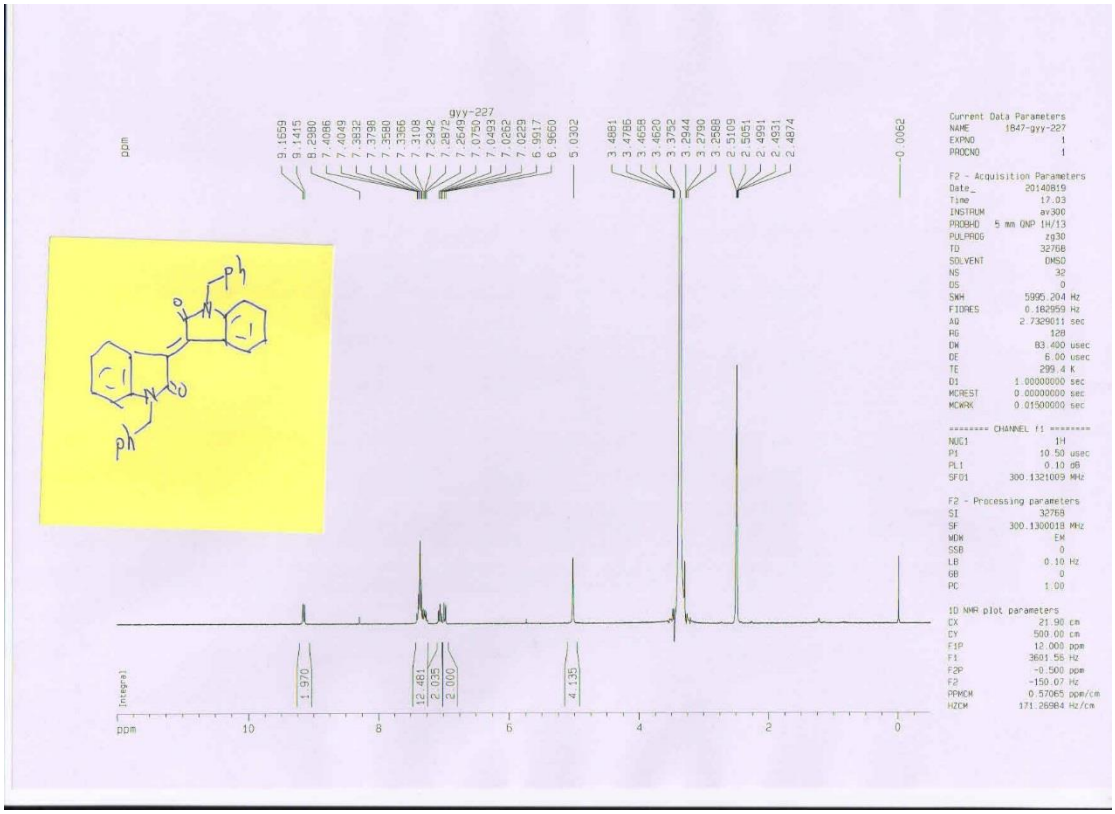
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 10.11
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm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7.2942
7.2872
7.2649
7.0750
7.0493
7.0282
7.0229
6.9917
6.9660
5.0302
3.4881
3.4785
3.4658
3.4620
3.3752
3.2944
3.2790
3.2588
2.5109
2.5051
2.4991
2.4931
2.4874
0.0062
Integral
1.970
12.481
2.035
2.000
4.135
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-227
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
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Time 17.03
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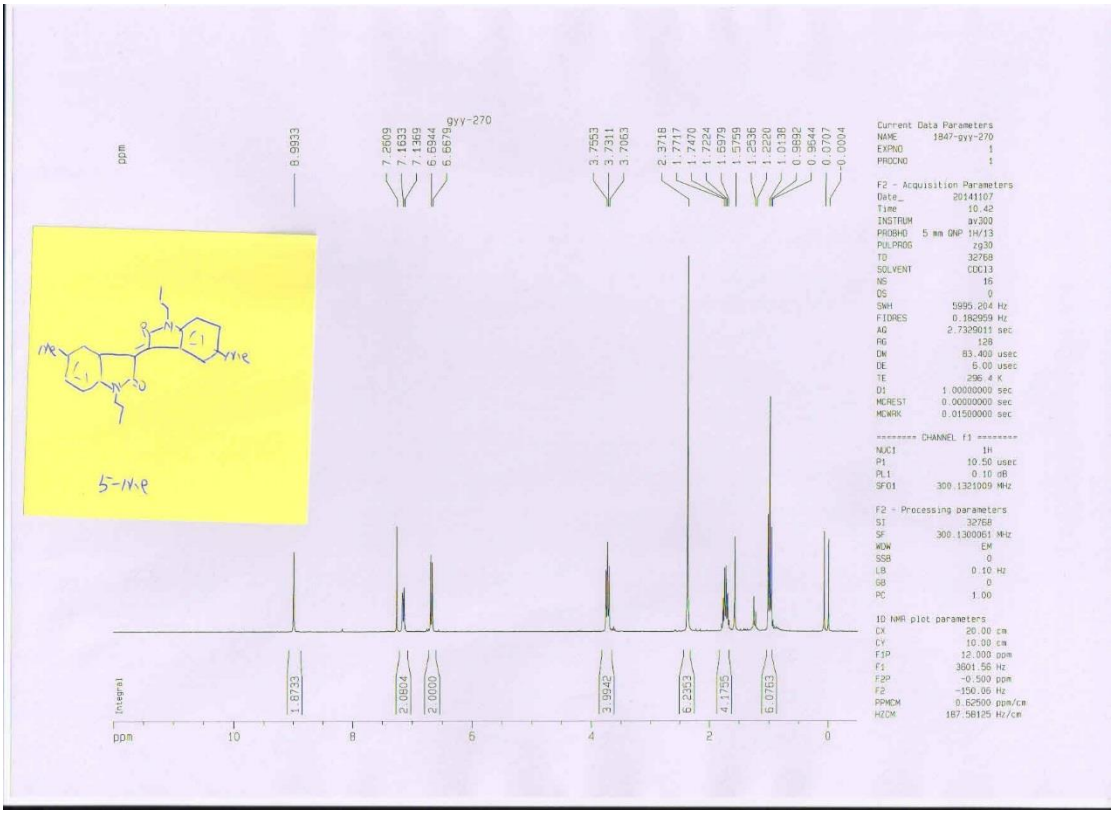
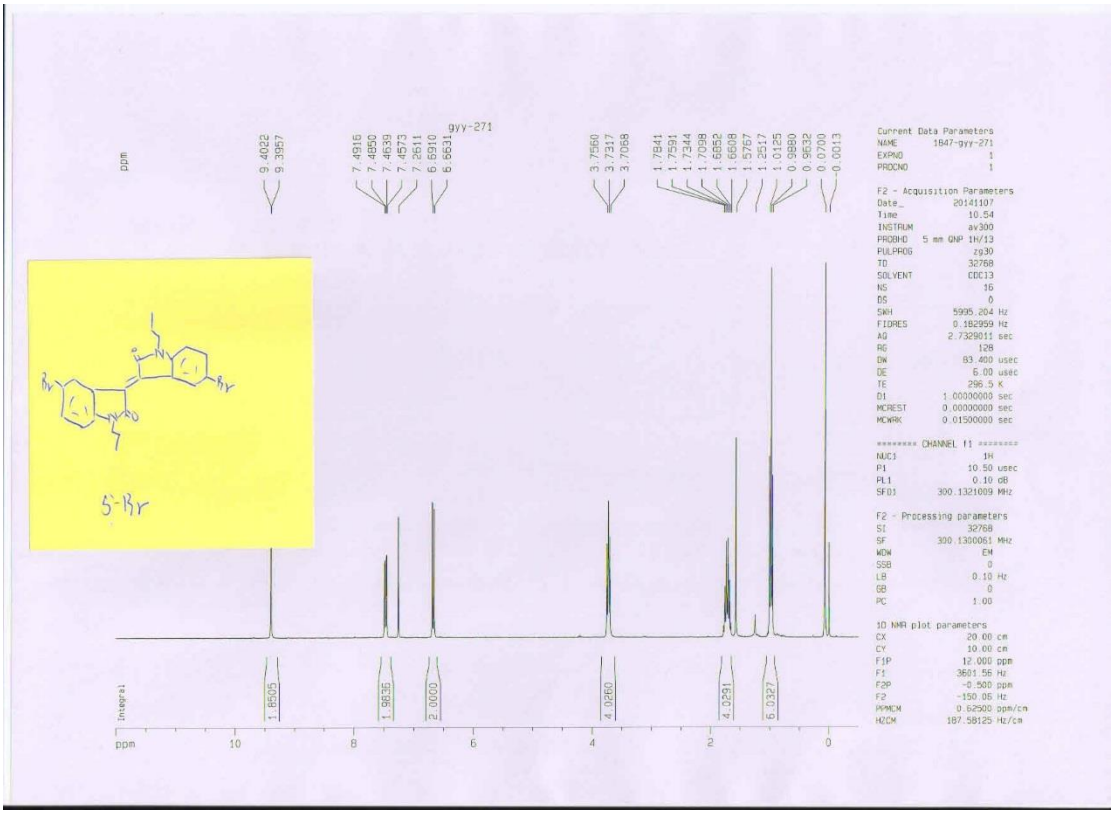
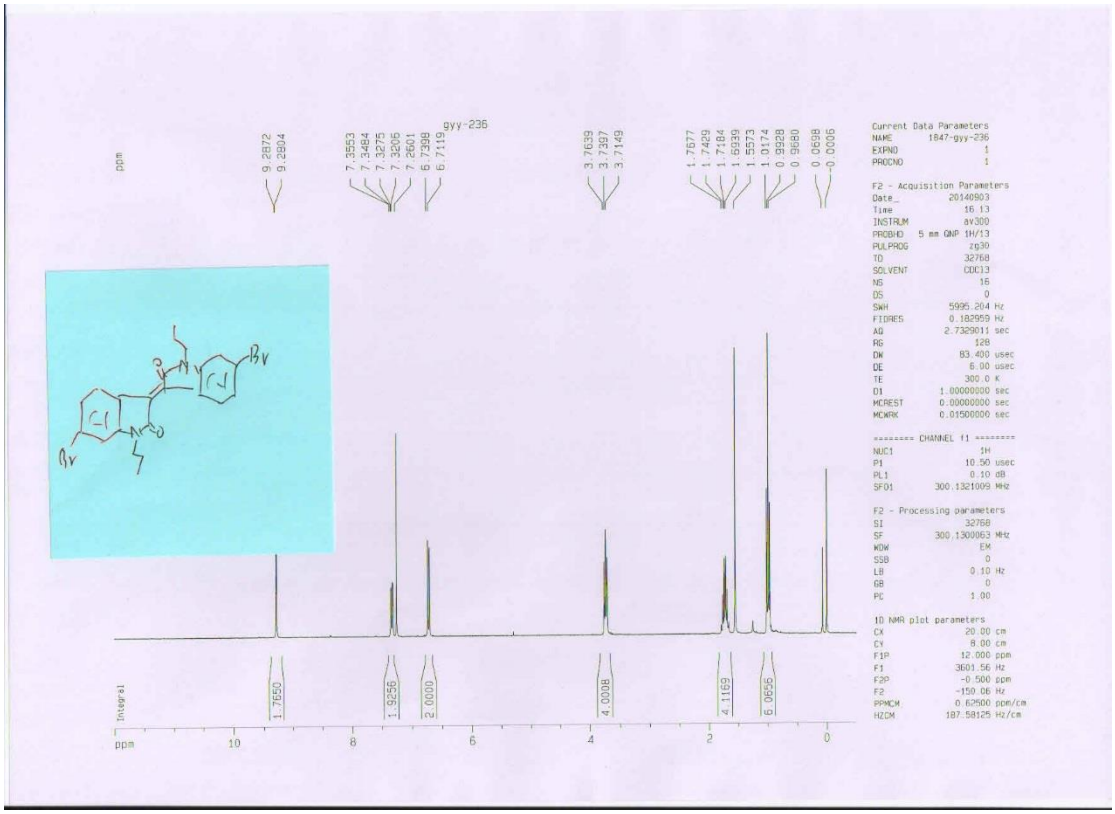
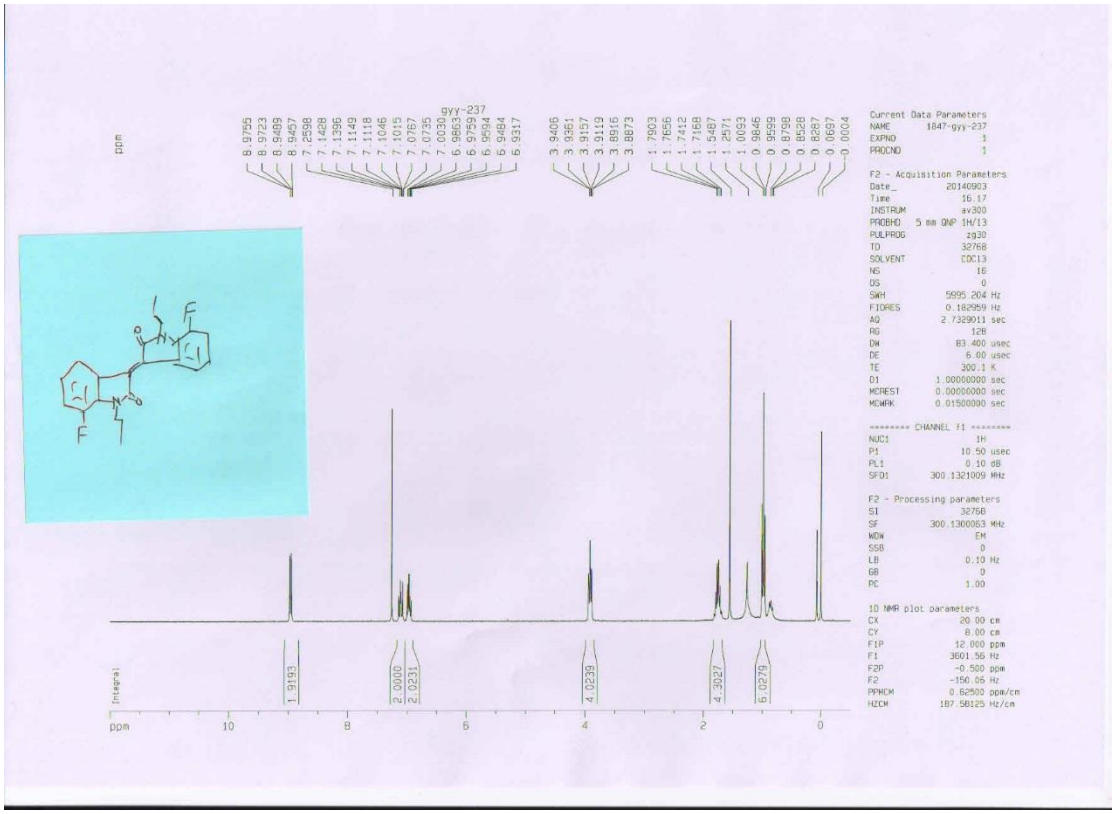
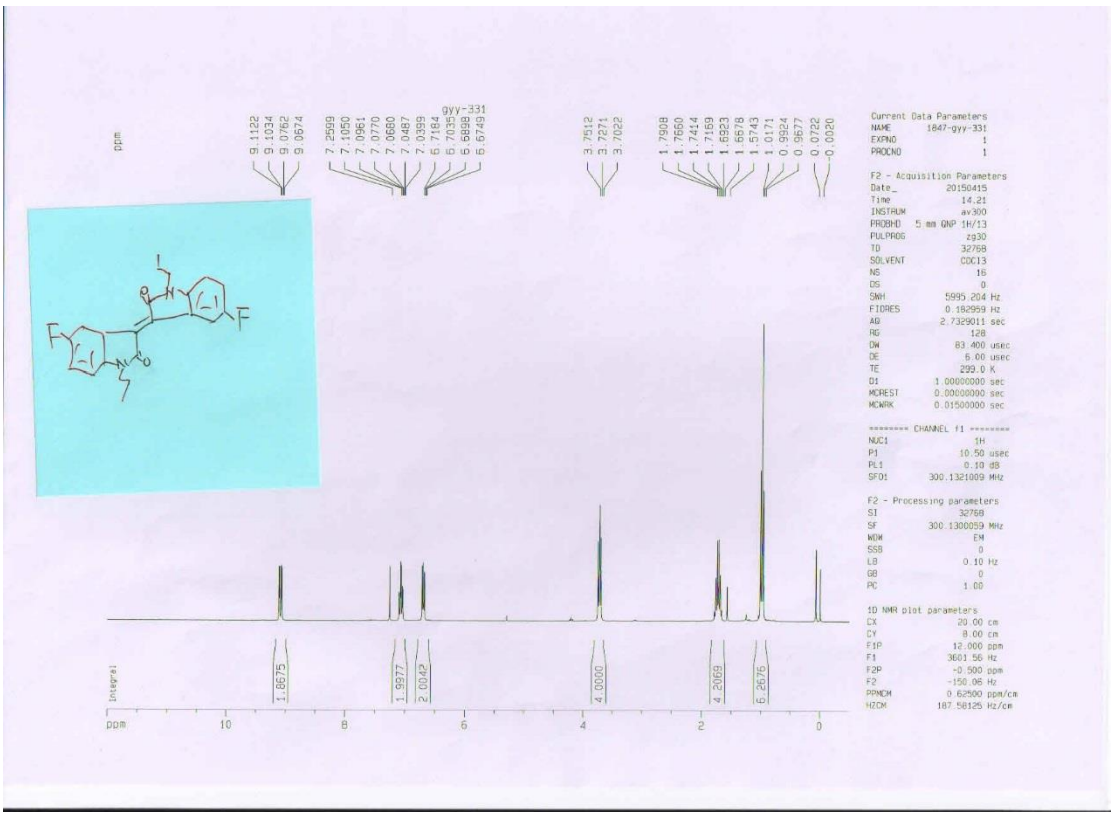
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300018 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 500.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.57065 ppm/cm
HZCM 171.26984 Hz/cm

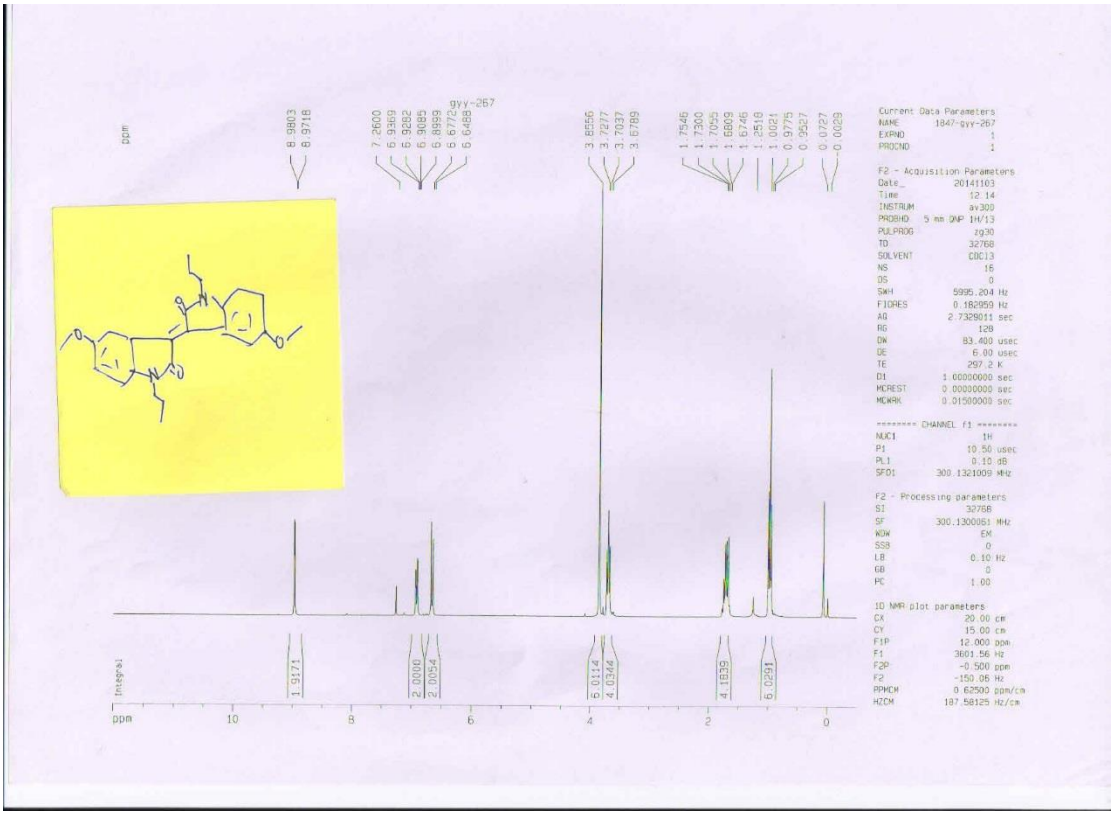

gyy-270
ppm
8.9933
7.2609
7.1633
7.1369
6.6944
6.6678
3.7553
3.7311
3.7063
2.3718
1.7717
1.7470
1.7224
1.6979
1.5759
1.2536
1.2220
1.0138
0.9892
0.9644
0.0707
-0.0004
Integral
1.8733
2.0804
2.0000
3.9942
6.2953
4.1795
6.0763
ppm
10
8
6
4
2
0
5-NHe
Current Data Parameters
NAME 1847-gyy-270
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141107
Time 10.42
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

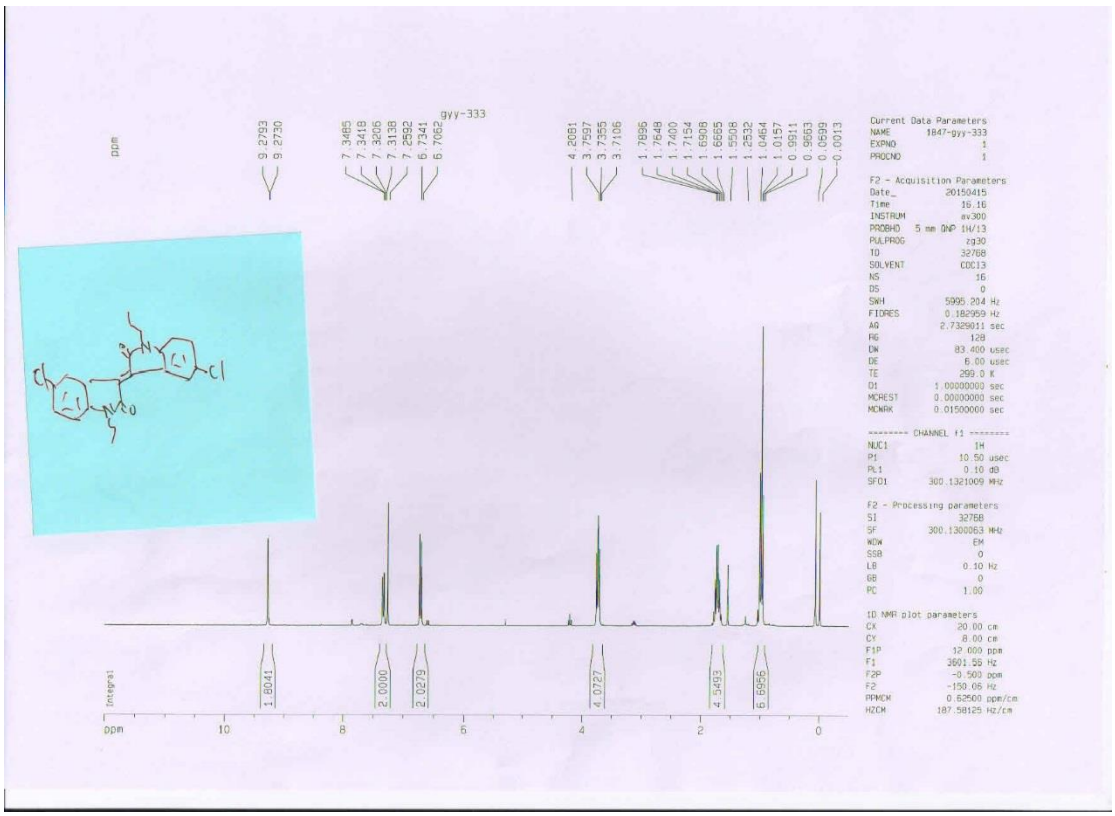

gyy-271
ppm
9.4022
9.3957
7.4916
7.4850
7.4639
7.4573
7.2611
6.6910
6.6631
3.7560
3.7317
3.7068
1.7841
1.7591
1.7344
1.7099
1.6852
1.6608
1.5767
1.2517
1.0125
0.9880
0.9632
0.0700
-0.0013
Integral
1.8505
1.9836
2.0000
4.0260
4.0291
6.0327
ppm
10
8
6
4
2
0
5-Br
Current Data Parameters
NAME 1847-gyy-271
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141107
Time 10.54
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

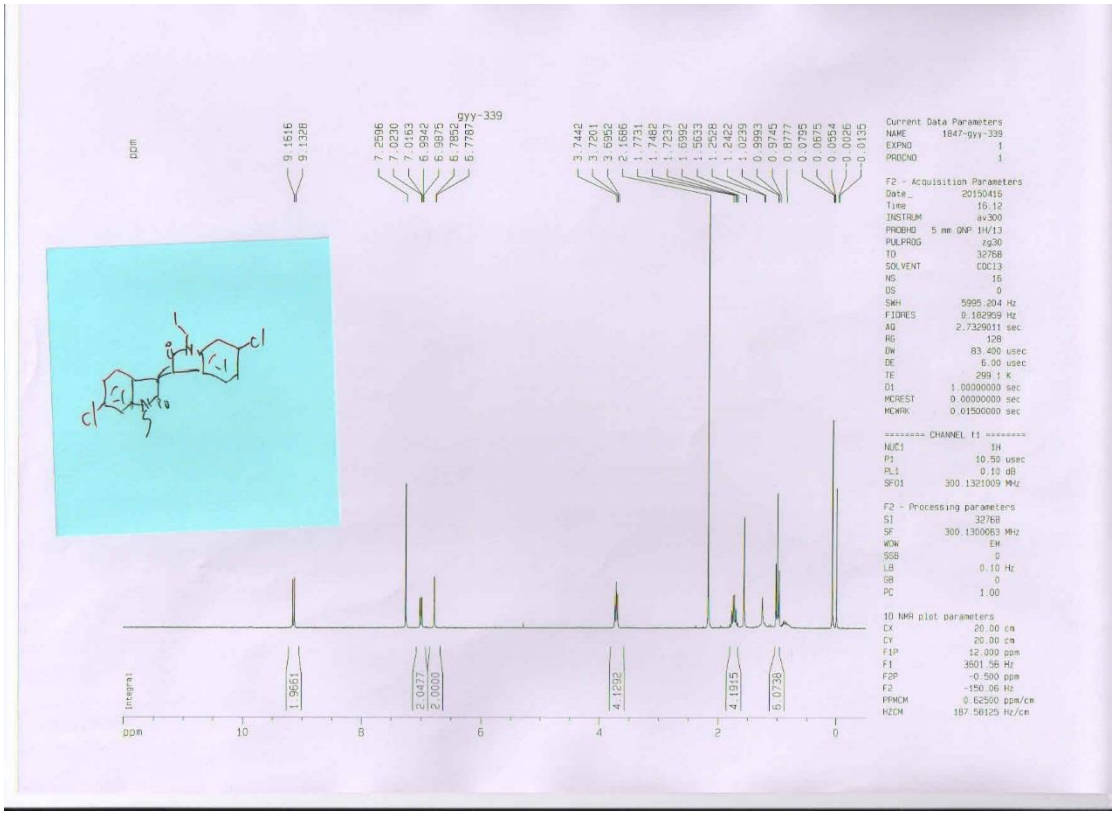

gyy-236
ppm
9.2872
9.2804
7.3563
7.3484
7.3275
7.3206
7.2601
6.7398
6.7119
3.7639
3.7397
3.7149
1.7677
1.7429
1.7184
1.6939
1.5573
1.0174
0.9928
0.9680
0.0698
-0.0006
Integral
1.7650
1.9256
2.0000
4.0008
4.1169
6.0656
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-236
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140903
Time 16.13
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm


gyy-237
ppm
8.9755
8.9723
8.9489
8.9457
7.2698
7.1428
7.1396
7.1149
7.1118
7.1046
7.1015
7.0767
7.0735
7.0039
6.9863
6.9759
6.9594
6.9484
6.9317
3.9406
3.9361
3.9157
3.9119
3.8916
3.8673
1.7903
1.7656
1.7412
1.7168
1.5487
1.2571
1.0093
0.9646
0.9598
0.8798
0.8528
0.8287
0.0697
-0.0004
Integral
1.9193
2.0000
2.0231
4.0239
4.3027
6.0279
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-237
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140903
Time 16.17
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 300.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

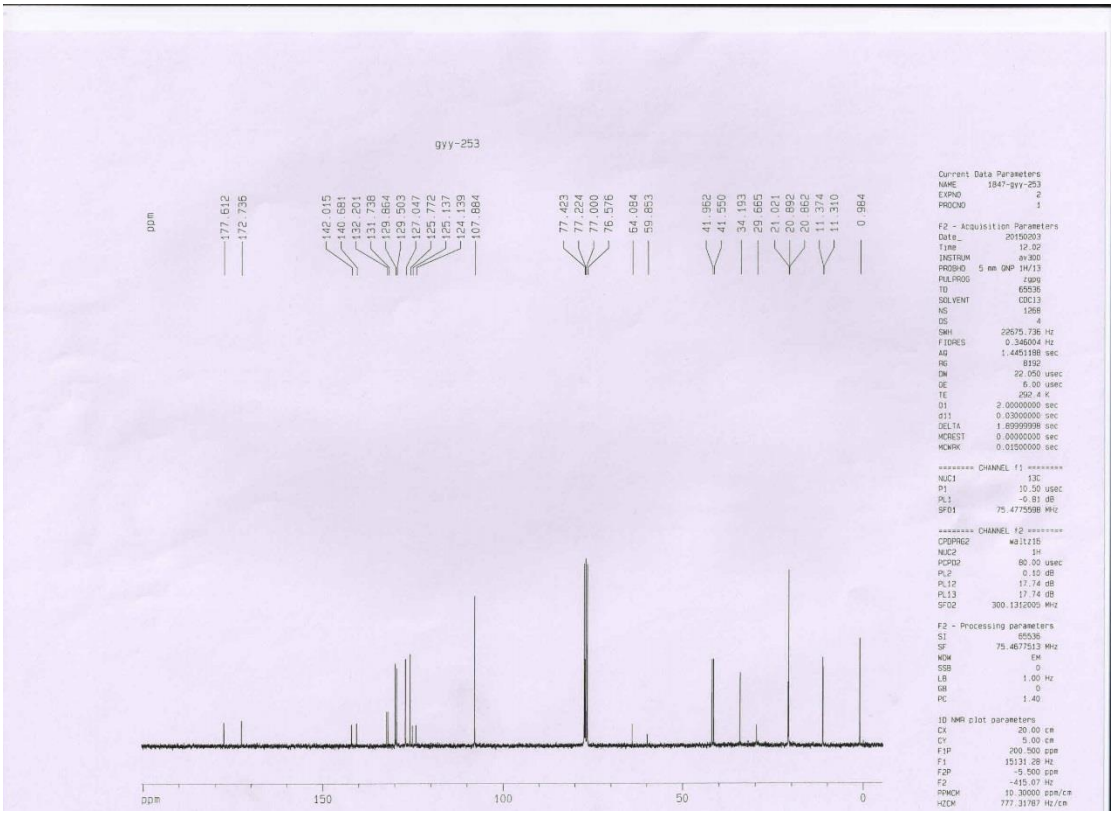

gyy-331
ppm
9.1122
9.1034
9.0762
9.0674
7.2599
7.1050
7.0961
7.0770
7.0680
7.0487
7.0399
6.7184
6.7035
6.6898
6.6749
3.7512
3.7271
3.7022
1.7908
1.7660
1.7414
1.7169
1.6923
1.6678
1.5743
1.0171
0.9924
0.9677
0.0722
-0.0020
Integral
1.8675
1.9977
2.0042
4.0000
4.2069
6.2676
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-331
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150415
Time 14.21
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

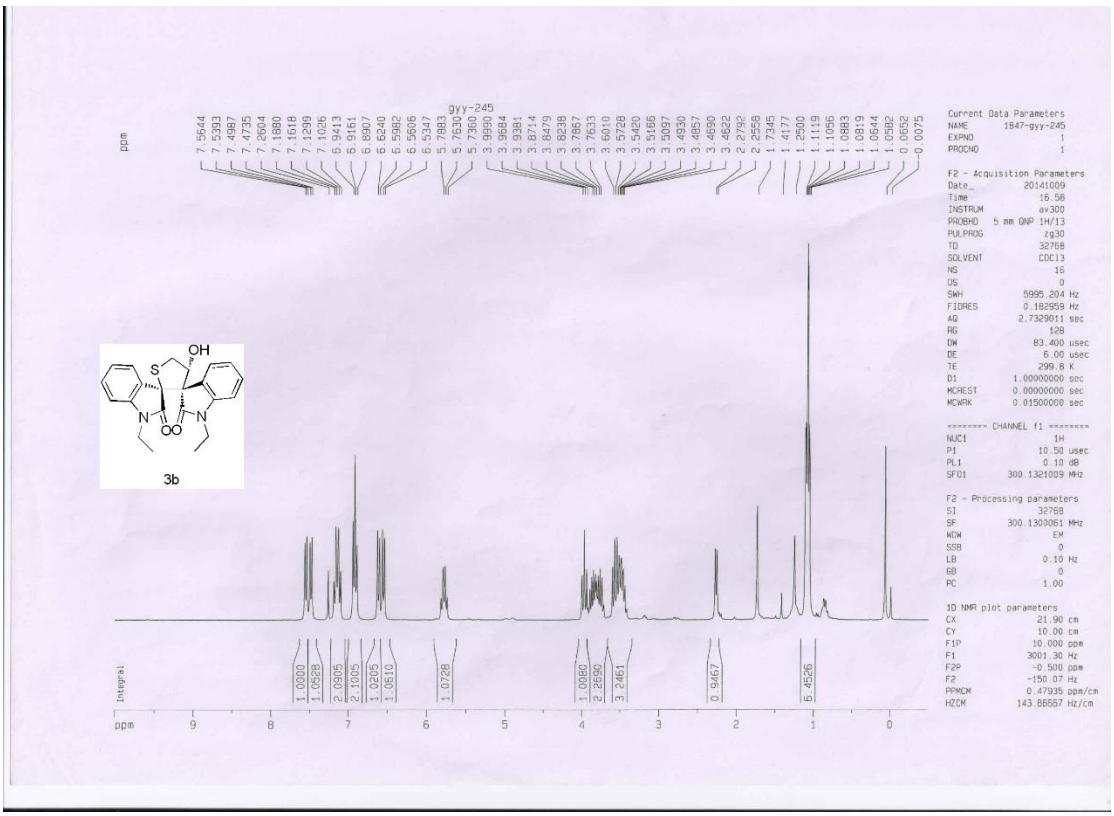

gyy-267
ppm
8.9803
8.9718
7.2600
6.9369
6.9282
6.9085
6.8999
6.6772
6.6488
3.8556
3.7277
3.7037
3.6789
1.7546
1.7300
1.7055
1.6809
1.6246
1.2518
1.0021
0.9775
0.9527
0.0727
-0.0029
Integral
1.9171
2.0006
2.0054
6.0114
4.0344
4.1839
6.0291
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-267
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141103
Time 12.14
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

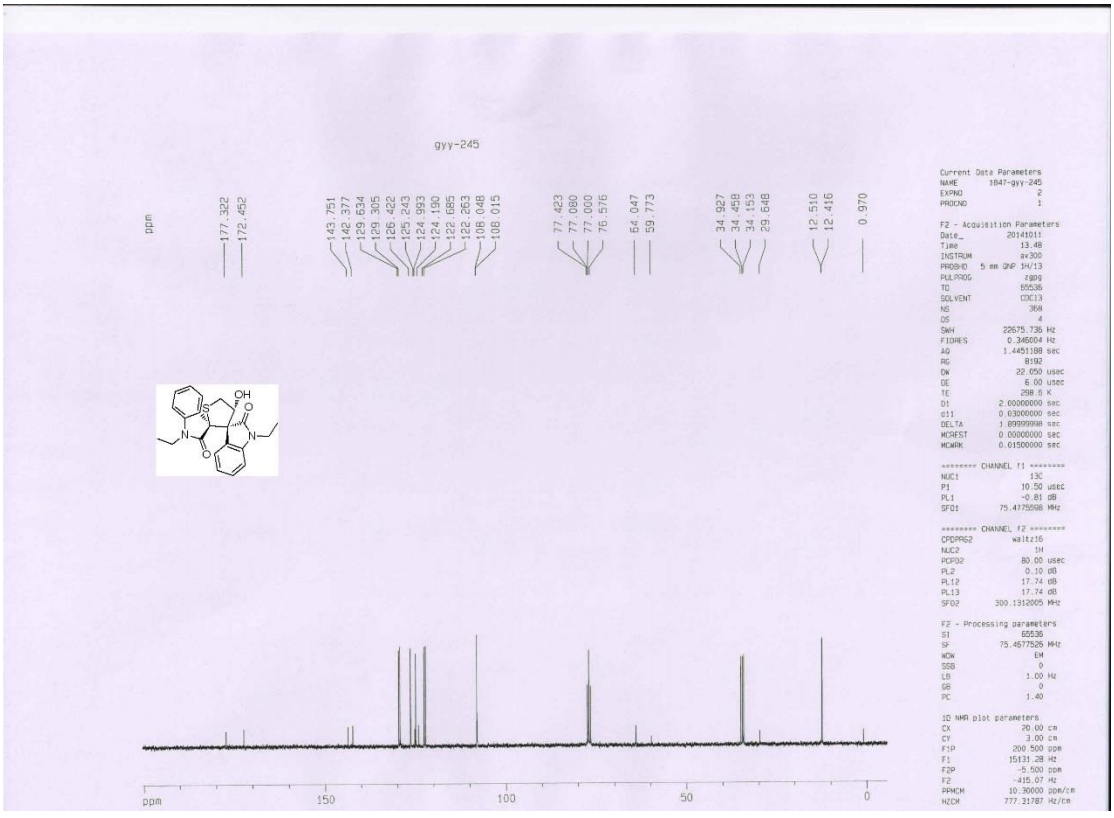

gyy-333
ppm
9.2793
9.2730
7.3485
7.3418
7.3206
7.3138
7.2592
6.7341
6.7062
4.2061
3.7597
3.7355
3.7106
1.7896
1.7648
1.7400
1.7164
1.6908
1.6685
1.5508
1.2532
1.0464
1.0157
0.9911
0.9663
0.0599
-0.0013
integral
1.8041
2.0000
2.0279
4.0727
4.5493
6.6956
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-333
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150415
Time 16.16
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 12.000 ppm
F1 3601.55 Hz
F2P -0.500 ppm
F2 -150.05 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

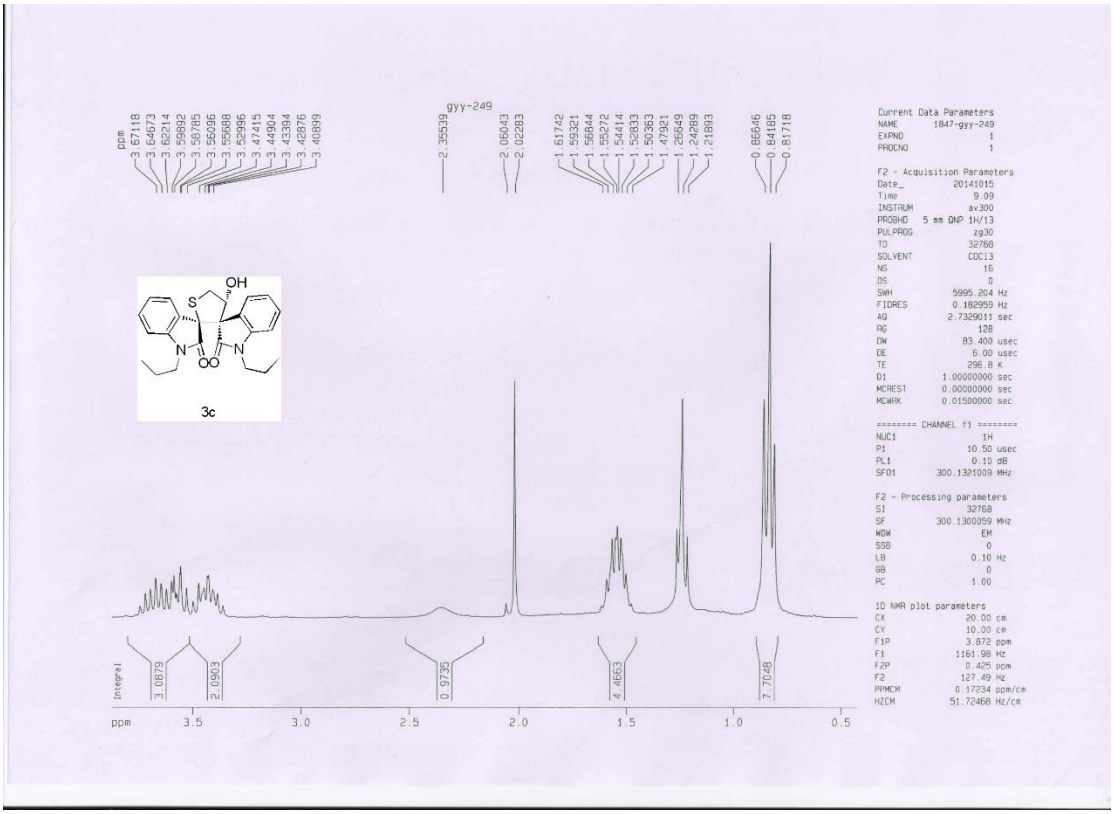

gyy-339
ppm
9.1616
9.1328
7.2596
7.0230
7.0163
6.9942
6.9875
6.7852
6.7787
3.7442
3.7201
3.6952
2.1686
1.7731
1.7482
1.7237
1.6992
1.5633
1.2528
1.2422
1.0239
0.9993
0.9745
0.8777
0.0795
0.0675
0.0554
-0.0026
-0.0135
integral
1.9661
2.0477
2.0000
4.1282
4.1915
6.0738
ppm
10
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-339
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 16.12
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

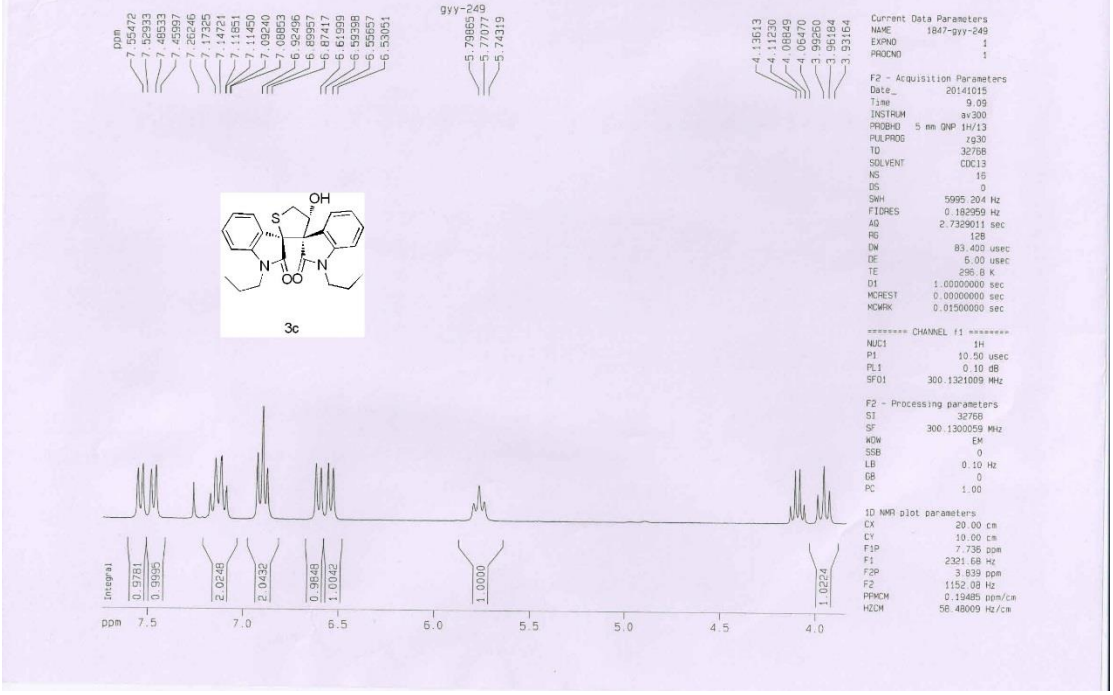

gyy-297
ppm
7.4997
7.4743
7.4503
7.4249
7.2611
7.2032
7.1771
7.1479
7.1201
6.9675
6.9422
6.9168
6.6099
6.5839
6.5466
6.5208
5.8362
5.8087
5.7836
5.7566
5.2957
4.0003
3.9694
3.9394
3.6384
3.6111
3.6075
3.5803
3.2925
3.0992
3.0610
3.0010
2.1457
2.1220
1.6577
1.4953
1.4190
1.2780
1.2476
0.8917
0.8751
0.8673
0.8452
0.0651
-0.0059
OH
S
N
O
O
N
3a
Integral
0.9607
1.0899
2.1028
2.0722
0.9834
1.0131
1.0000
1.0122
1.0067
2.9259
3.0223
0.9995
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-297
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150129
Time 10.22
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 291.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.58625 Hz/cm

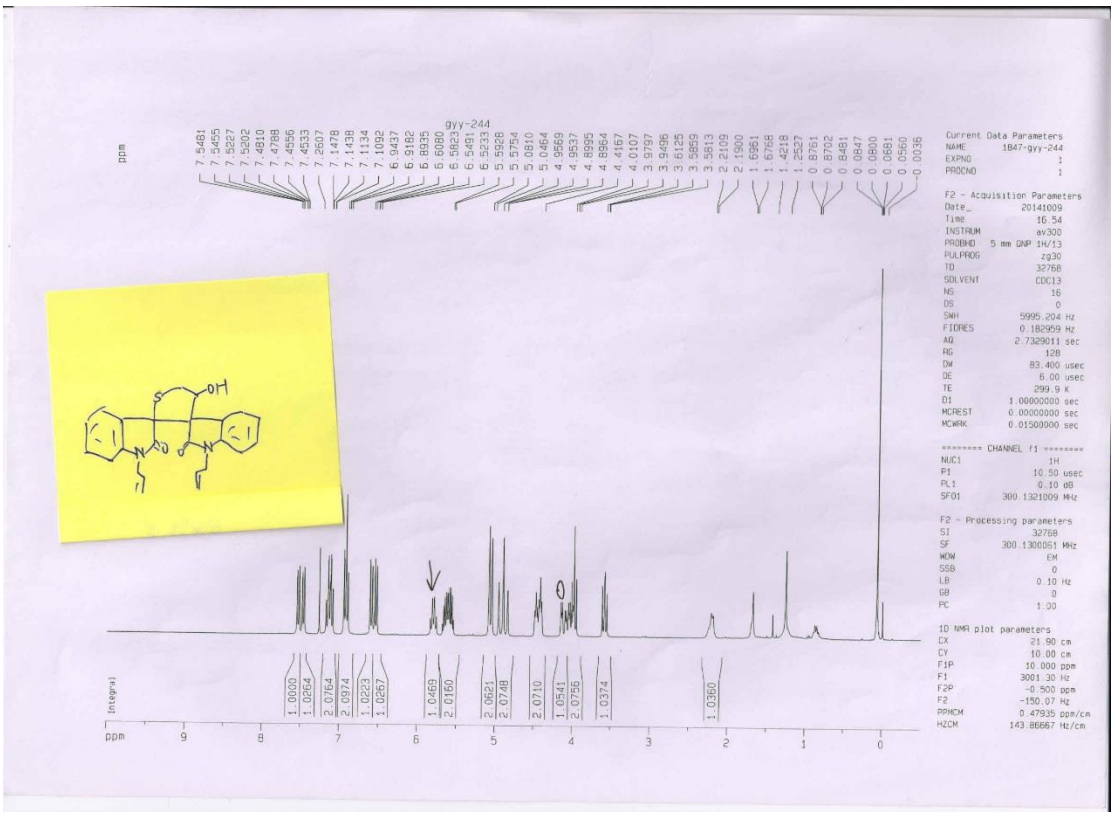

gyy-253
ppm
177.612
172.736
142.015
140.681
132.201
131.738
129.864
129.503
127.047
125.772
125.137
124.139
107.884
77.423
77.224
77.000
76.576
64.084
59.863
41.962
41.550
34.193
29.665
21.021
20.892
20.862
11.374
11.310
0.984
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-253
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150203
Time 12.02
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1268
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 292.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312009 MHz
F2 - Processing parameters
SI 65536
SF 75.4677513 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -9.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

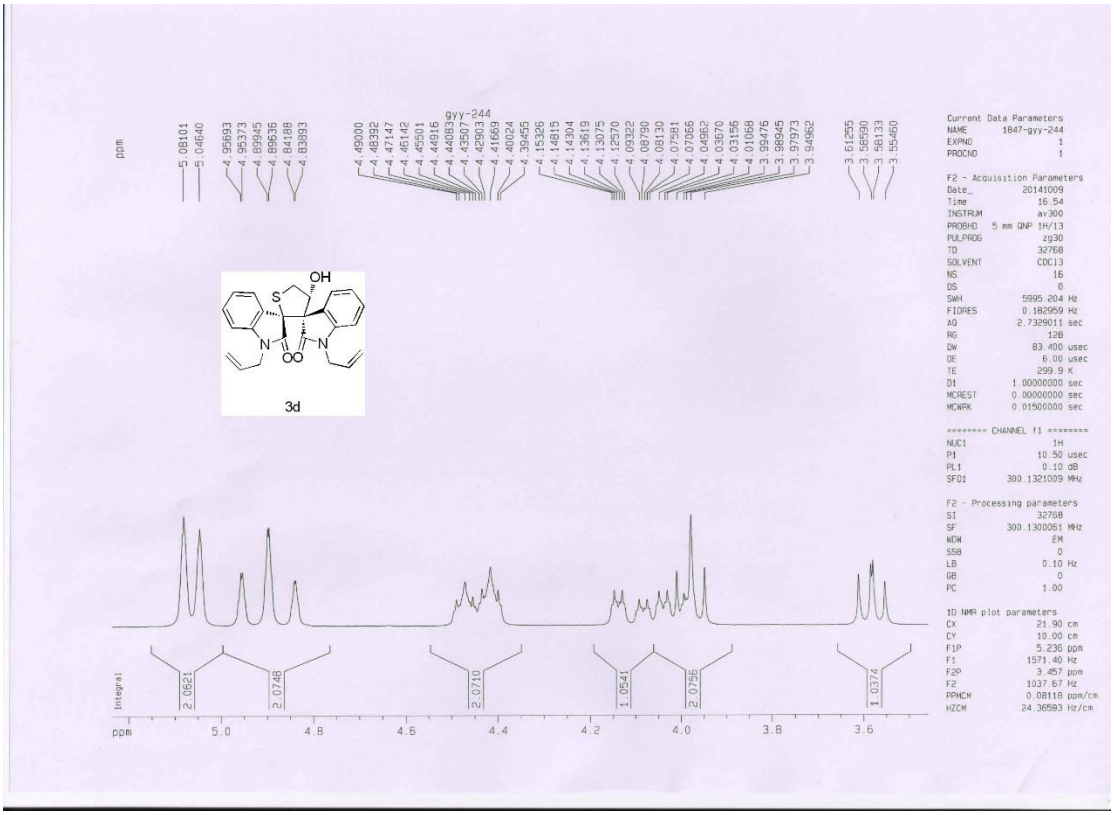

gyy-245
ppm
7.5644 7.5393 7.4987 7.4735 7.2604 7.1880 7.1618 7.1299 7.1026 6.9413 6.9161 6.8907 6.6240 6.5982 6.5606 6.5347 5.7883 5.7630 5.7360 3.9990 3.9684 3.9381 3.8714 3.8479 3.8238 3.7867 3.7633 3.6010 3.5728 3.5420 3.5166 3.5097 3.4930 3.4857 3.4690 3.4622 2.2792 2.2558 1.7245 1.4177 1.2500 1.1119 1.1056 1.0883 1.0819 1.0644 1.0582 0.0652 0.0075
Integral
1.0000 1.0528 2.0905 2.1005 1.0205 1.0610 1.0728 1.0086 2.2590 3.2461 0.9467 6.4526
ppm 9 8 7 6 5 4 3 2 1 0
OH
S
N
O
O
N
3b
Current Data Parameters
NAME 1847-gyy-245
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141009
Time 16.56
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.47935 ppm/cm
HZCM 143.86657 Hz/cm

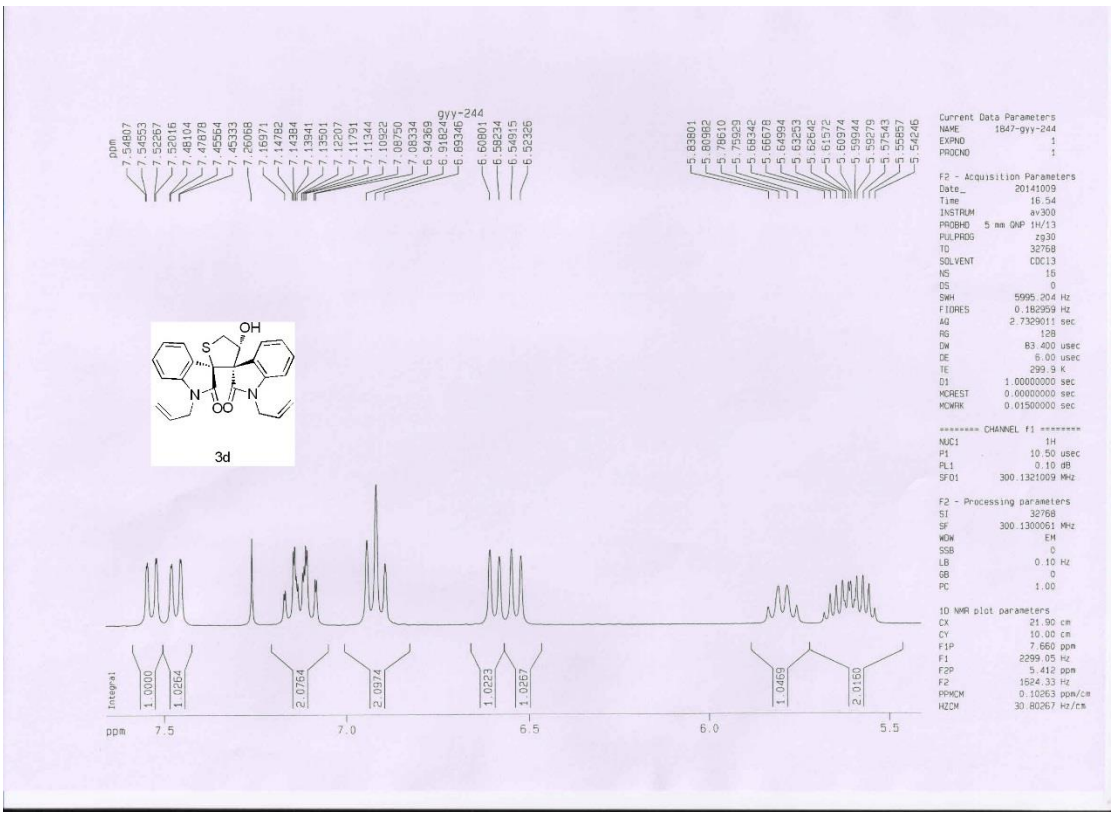

gyy-245
ppm
177.322 172.452
143.751 142.377 129.634 129.305 126.422 125.243 124.993 124.190 122.685 122.263 108.048 108.015
77.423 77.080 77.000 76.576
64.047 59.773
34.927 34.458 34.153 29.648
12.510 12.416
0.970
OH
S
O
N
O
N
ppm 150 100 50 0
Current Data Parameters
NAME 1847-gyy-245
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 13.48
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 368
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775998 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677526 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

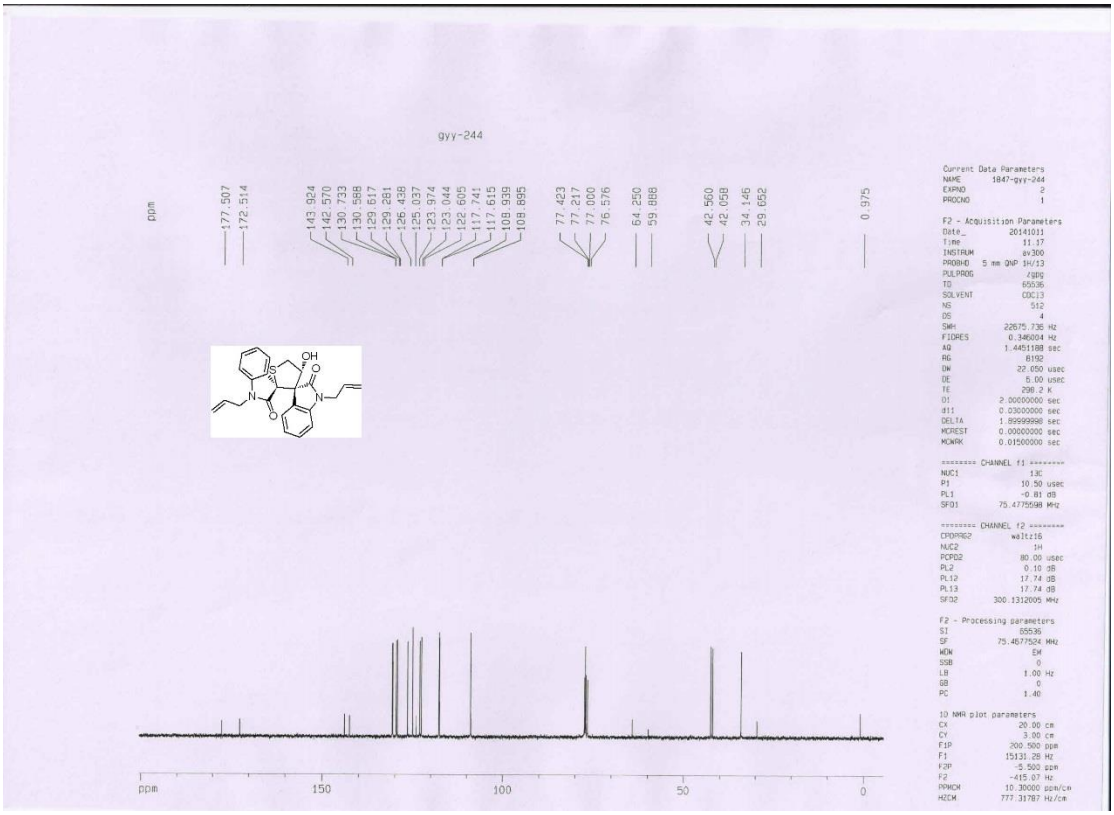

gyy-249
ppm
3.67118
3.64673
3.62214
3.59892
3.58785
3.56096
3.55608
3.52996
3.47415
3.44904
3.43394
3.42876
3.40899
2.35539
2.06043
2.02283
1.61742
1.59321
1.56844
1.55272
1.54414
1.52833
1.50363
1.47921
1.26649
1.24289
1.21893
0.86646
0.84185
0.81718
OH
S
N
O
O
N
3c
Integral
3.0879
2.0903
0.9735
4.4663
7.7048
ppm
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Current Data Parameters
NAME 1847-gyy-249
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 9.09
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 3.872 ppm
F1 1161.98 Hz
F2P 0.425 ppm
F2 127.49 Hz
PPMCM 0.17234 ppm/cm
HZCM 51.72468 Hz/cm

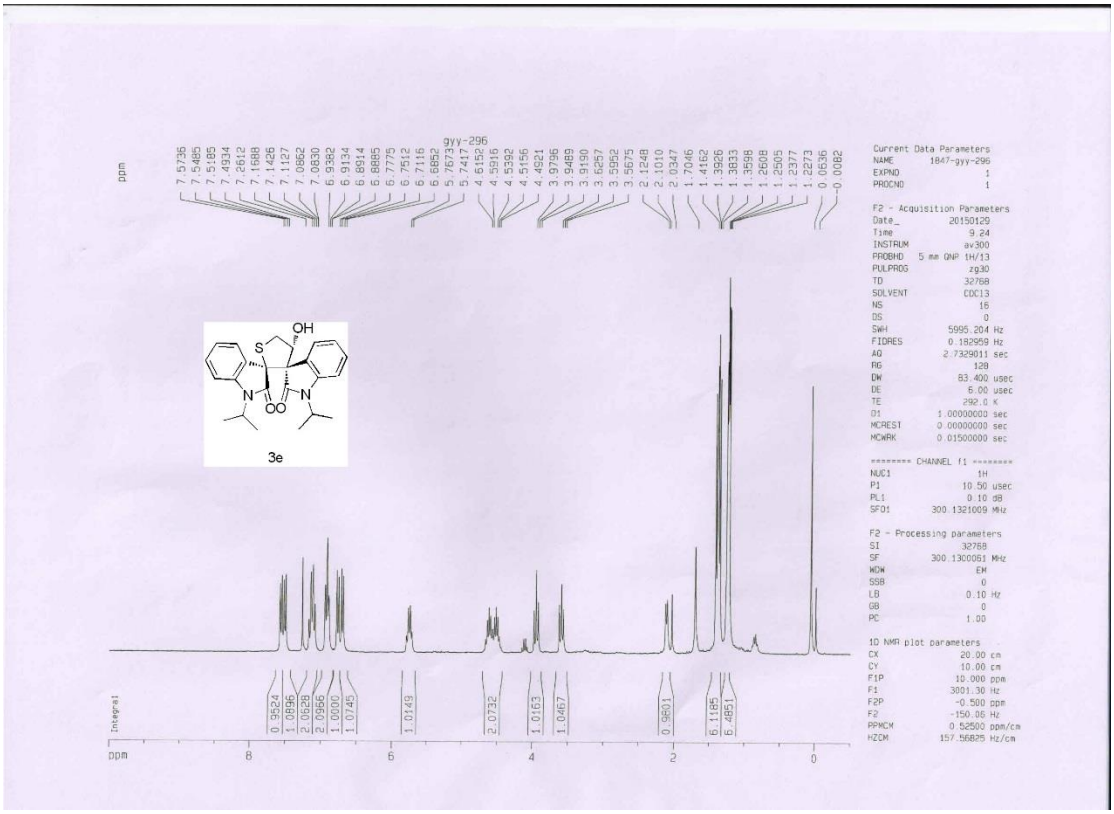

gyy-249
ppm
7.55472
7.52933
7.48533
7.45997
7.26246
7.17325
7.14721
7.11851
7.11450
7.09240
7.08853
6.92496
6.89957
6.87417
6.61999
6.59398
6.55657
6.53051
5.79865
5.77077
5.74319
4.13613
4.11230
4.08849
4.06470
3.99260
3.96184
3.93164
OH
S
N
O
O
N
3c
Integral
0.9781
0.9995
2.0248
2.0432
0.9848
1.0042
1.0000
1.0224
ppm
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
Current Data Parameters
NAME 1847-gyy-249
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 9.09
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 7.736 ppm
F1 2321.68 Hz
F2P 3.839 ppm
F2 1152.08 Hz
PPMCM 0.19485 ppm/cm
HZCM 58.48009 Hz/cm


gyy-244
ppm
7.5481 7.5455 7.5227 7.5202 7.4810 7.4788 7.4556 7.4533 7.2607 7.1478 7.1438 7.1134 7.1092 6.9437 6.9182 6.8935 6.6080 6.5823 6.5491 6.5233 5.5928 5.5754 5.0810 5.0464 4.9569 4.9537 4.8995 4.8964 4.4167 4.4107 3.9797 3.9496 3.6125 3.5859 3.5613 2.2109 2.1900 1.6961 1.6768 1.4219 1.2527 0.8761 0.8702 0.6481 0.0847 0.0800 0.0681 0.0560 0.0036
Integral
1.0000 1.0264 2.0764 2.0974 1.0223 1.0267 1.0469 2.0160 2.0621 2.0748 2.0710 1.0541 2.0756 1.0374 1.0360
ppm 9 8 7 6 5 4 3 2 1 0
Current Data Parameters
NAME 1847-gyy-244
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141009
Time 16.54
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.47935 ppm/cm
HZCM 143.86667 Hz/cm

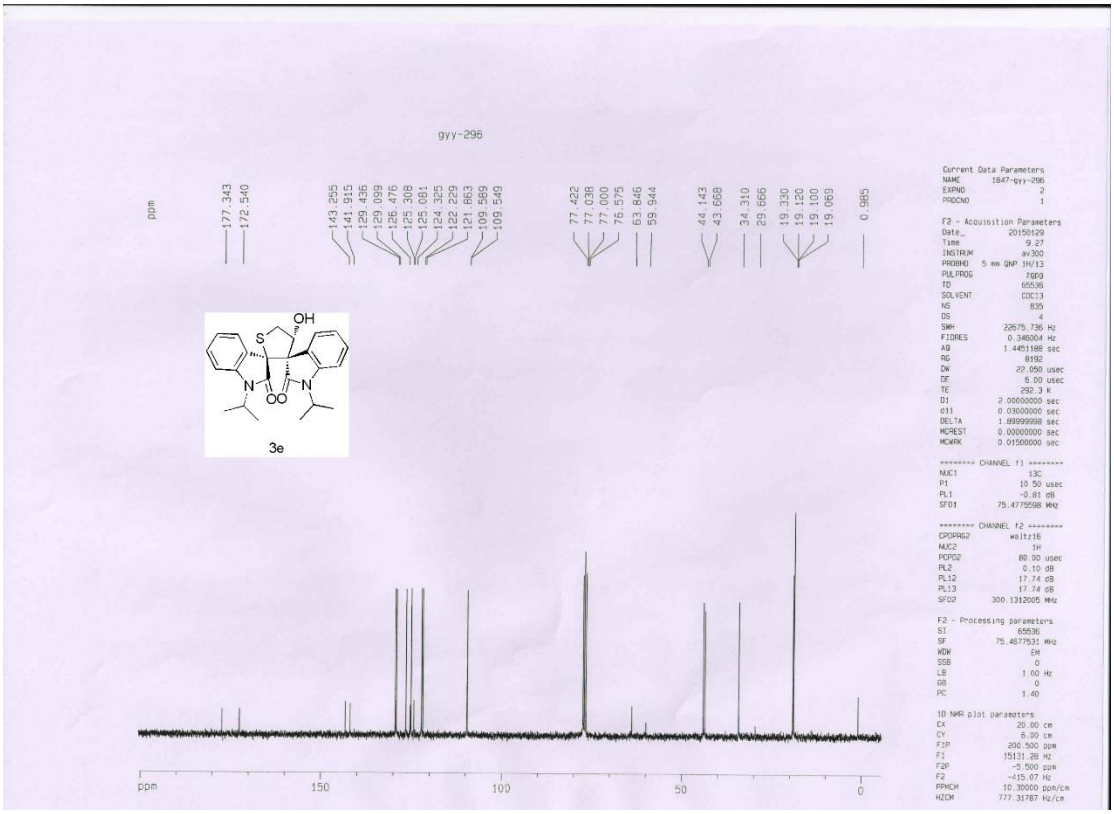

gyy-244
ppm
5.08101 5.04640 4.95693 4.95373 4.89945 4.89636 4.84188 4.83893 4.49000 4.48392 4.47147 4.46142 4.45501 4.44916 4.44083 4.43507 4.42903 4.41669 4.40024 4.39455 4.15326 4.14815 4.14304 4.13619 4.13075 4.12570 4.09322 4.08790 4.08130 4.07581 4.07066 4.04962 4.03670 4.03156 4.01068 3.99476 3.98945 3.97973 3.94962 3.61255 3.58590 3.58133 3.55460
OH
S
N
O
O
N
3d
Integral
2.0621 2.0748 2.0710 1.0541 2.0756 1.0374
ppm 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6
Current Data Parameters
NAME 1847-gyy-244
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141009
Time 16.54
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 10.00 cm
F1P 5.236 ppm
F1 1571.40 Hz
F2P 3.457 ppm
F2 1037.67 Hz
PPMCM 0.08118 ppm/cm
HZCM 24.36593 Hz/cm

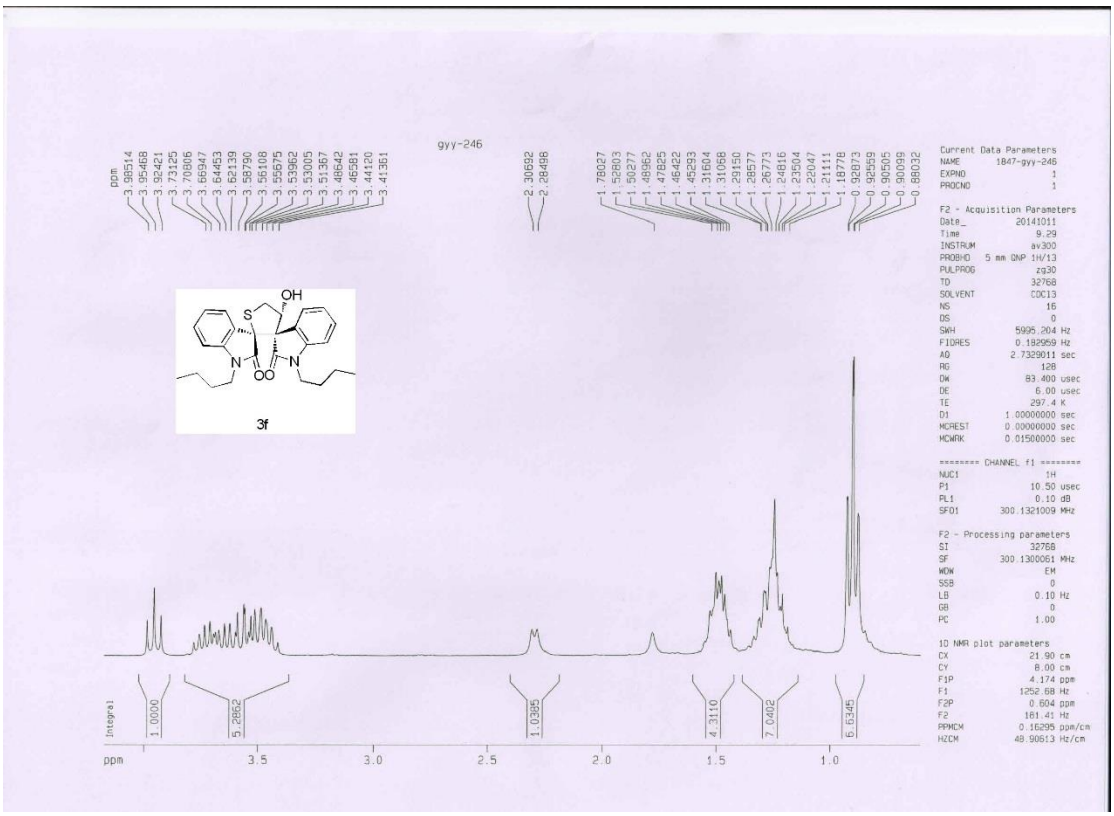

gyy-244
ppm
7.64807
7.54553
7.52267
7.52016
7.48104
7.47878
7.45564
7.45333
7.26068
7.16971
7.14782
7.14384
7.13941
7.13501
7.12207
7.11791
7.11344
7.10922
7.08750
7.08334
6.94369
6.91824
6.89346
6.60801
6.58234
6.54915
6.52326
5.83801
5.80982
5.78610
5.75929
5.68342
5.66678
5.64994
5.63253
5.62642
5.61572
5.60374
5.59944
5.59279
5.57543
5.55857
5.54246
OH
S
N
O
O
N
3d
Integral
1.0000
1.0264
2.0764
2.0974
1.0223
1.0267
1.0469
2.0160
ppm
7.5
7.0
6.5
6.0
5.5
Current Data Parameters
NAME 1847-gyy-244
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141009
Time 16.54
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 10.00 cm
F1P 7.660 ppm
F1 2299.05 Hz
F2P 5.412 ppm
F2 1624.33 Hz
PPMCM 0.10263 ppm/cm
HZCM 30.80267 Hz/cm

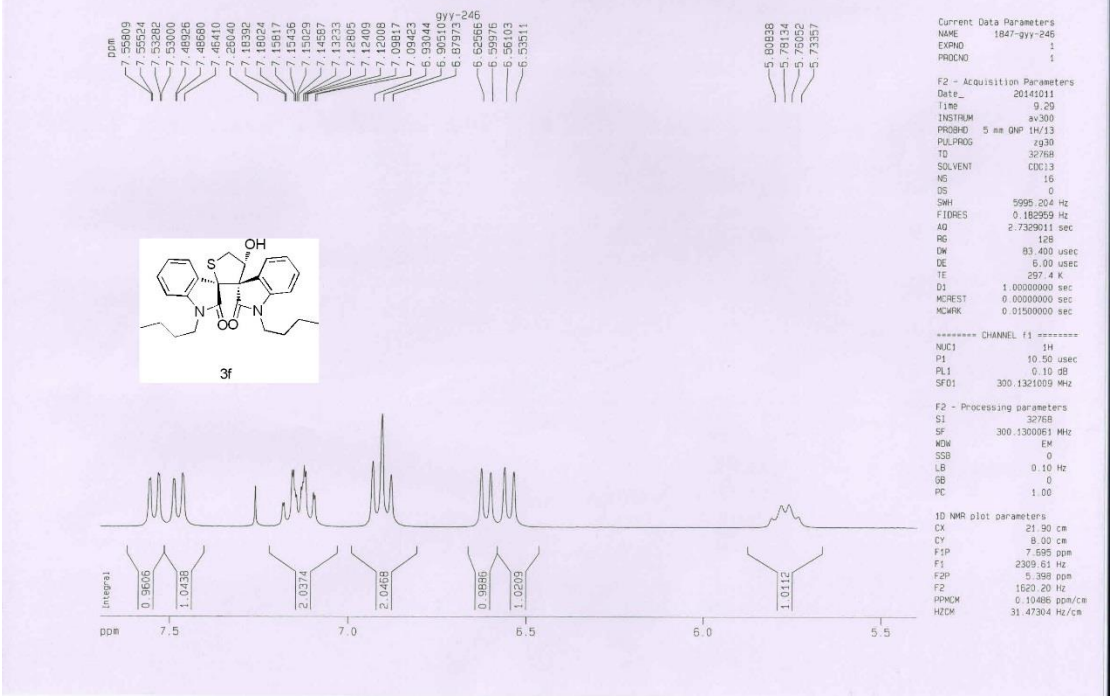

gyy-244
ppm
177.507
172.514
143.924
142.570
130.733
130.588
129.617
129.281
126.438
125.037
123.974
123.044
122.605
117.741
117.615
108.939
108.895
77.423
77.217
77.000
76.576
64.250
59.888
42.560
42.059
34.146
29.652
0.975
OH
S
N
O
O
N
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-244
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 11.17
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 22675.735 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

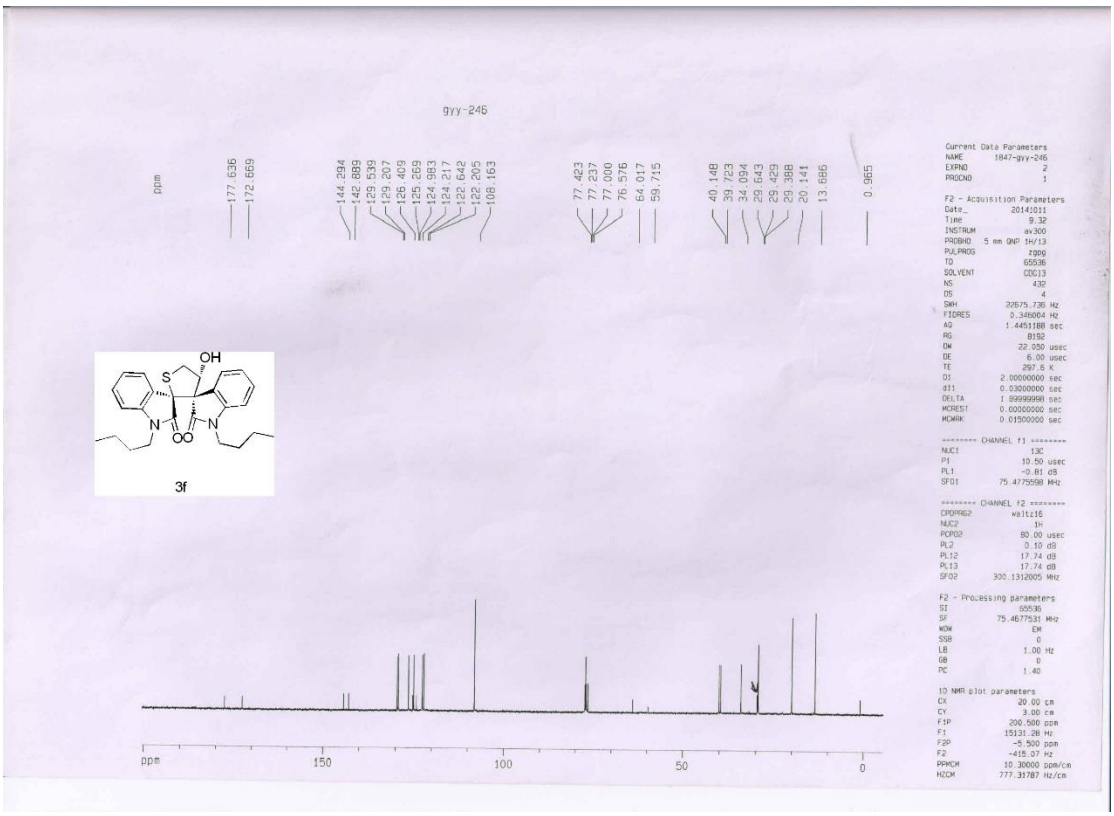

gyy-296
ppm
7.5735
7.5485
7.5185
7.4934
7.2612
7.1688
7.1426
7.1127
7.0862
7.0630
6.9382
6.9134
6.8914
6.8885
6.7775
6.7512
6.7116
6.6852
5.7613
5.7417
4.6156
4.5916
4.5392
4.5156
4.4921
3.9796
3.9489
3.9190
3.6257
3.5952
3.5675
2.1249
2.1010
2.0347
1.7046
1.4162
1.3926
1.3833
1.3598
1.2608
1.2505
1.2377
1.2273
0.0636
-0.0082
OH
S
N
O
O
N
3e
Current Data Parameters
NAME 1847-gyy-296
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150129
Time 9.24
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 292.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.05 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm
Integral
0.9524
1.0896
2.0628
2.0966
1.0000
1.0745
1.0149
2.0732
1.0163
1.0467
0.9801
6.1185
5.4851
ppm
8
6
4
2
0

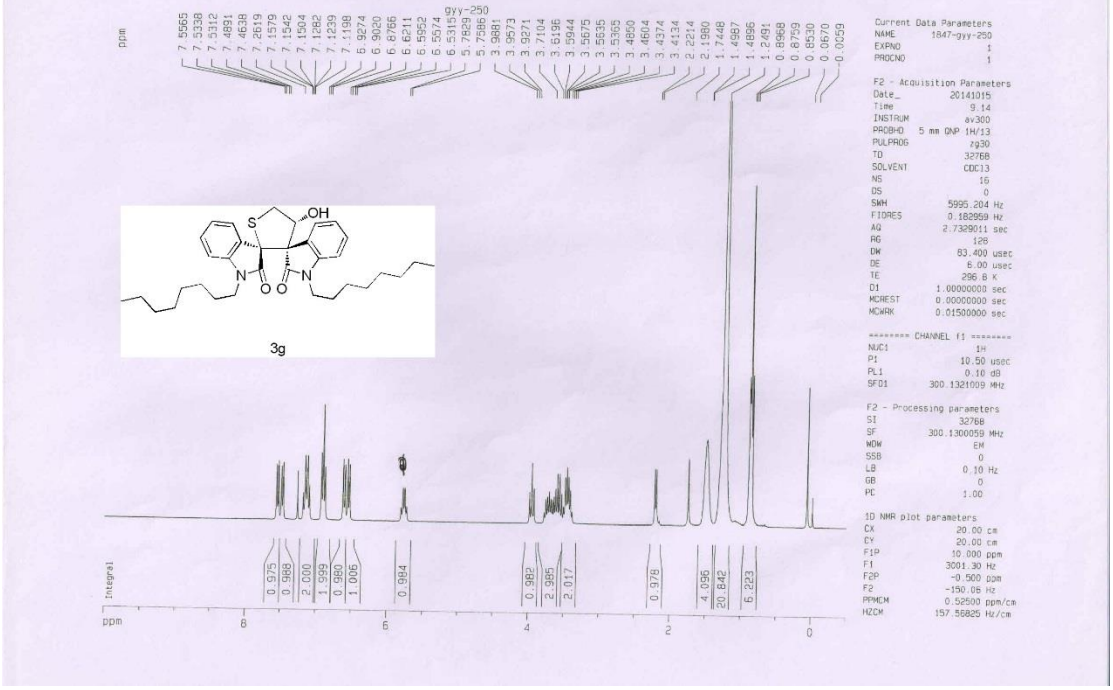
5

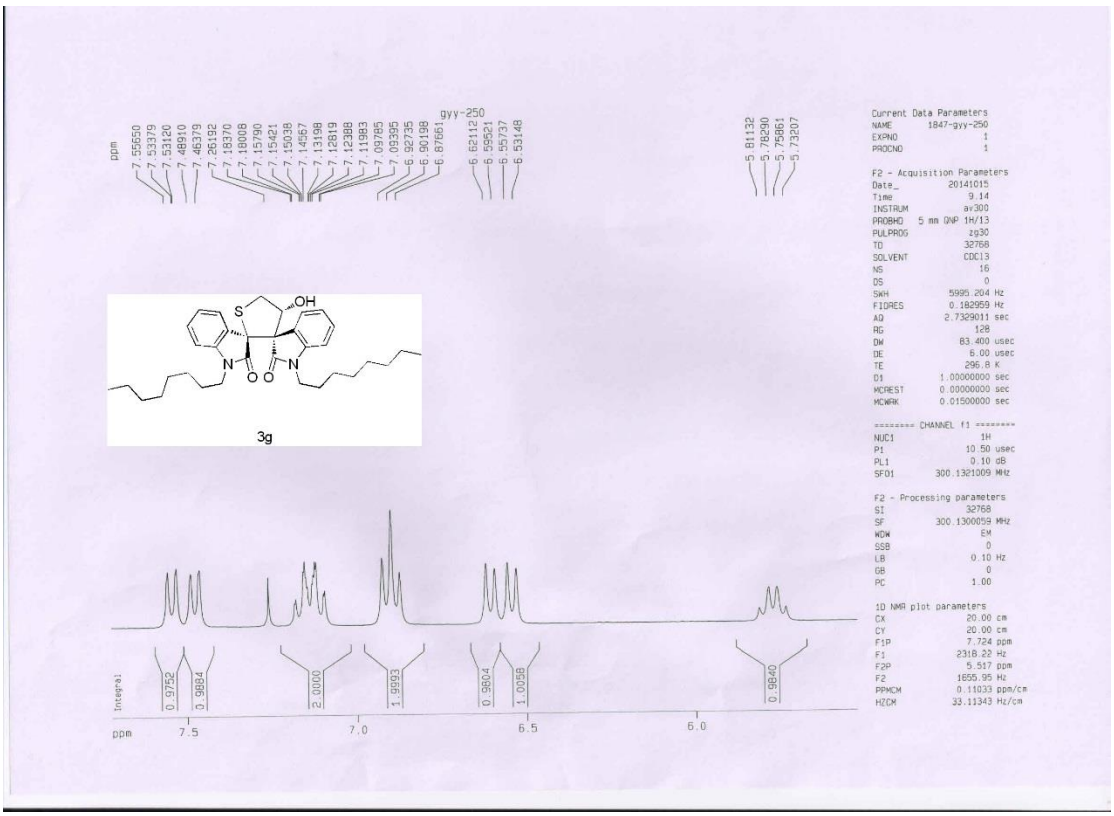

gyy-296
ppm
177.343
172.540
143.255
141.915
129.436
129.099
126.476
125.308
125.081
124.325
122.229
121.863
109.589
109.549
77.422
77.038
77.000
76.575
63.846
59.944
44.143
43.668
34.310
29.666
19.330
19.120
19.100
19.069
0.985
OH
S
N
O
O
N
3e
Current Data Parameters
NAME 1847-gyy-296
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150129
Time 9.27
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 835
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 292.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 206.500 ppm
F1 15131.28 Hz
F2P -0.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm
ppm
150
100
50
0

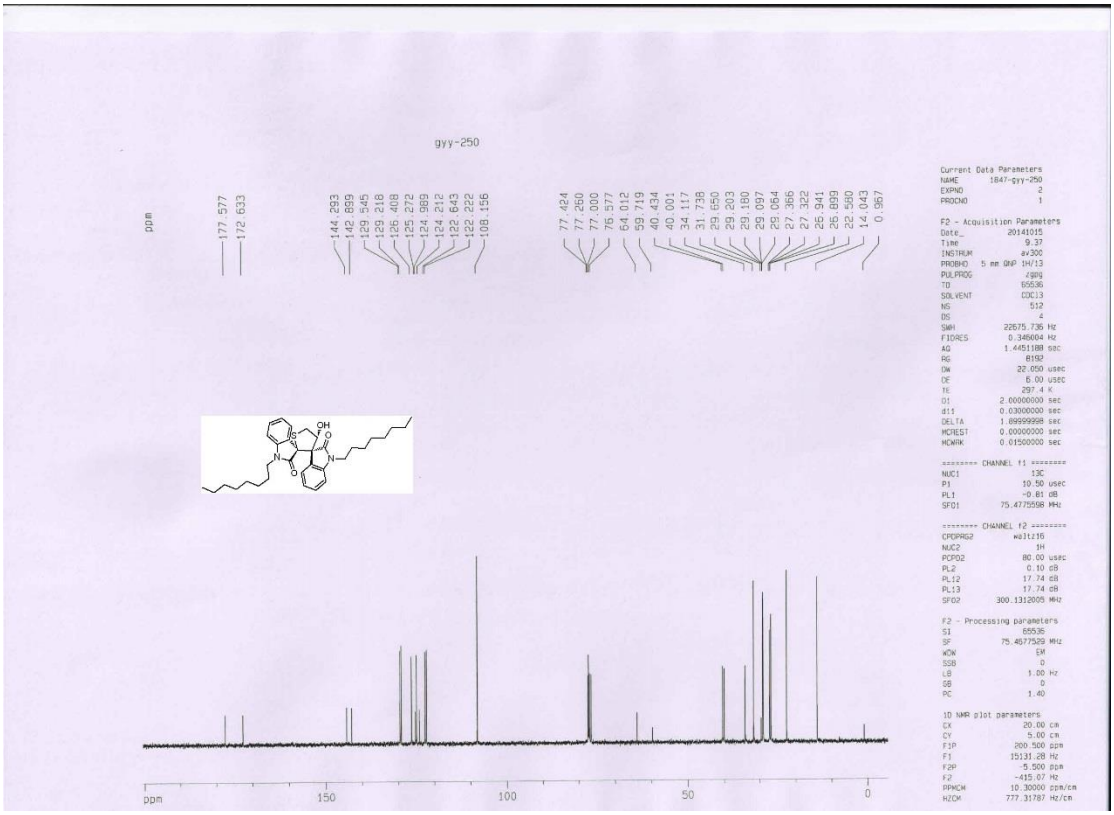

gyy-246
ppm
3.98514
3.95468
3.92421
3.73125
3.70806
3.66947
3.64453
3.62139
3.58790
3.56108
3.55675
3.53962
3.53005
3.51387
3.48542
3.46581
3.44120
3.41361
2.30692
2.28498
1.78027
1.52803
1.50277
1.49962
1.47825
1.46422
1.45293
1.31604
1.31068
1.29150
1.28577
1.26773
1.24816
1.23504
1.22047
1.21111
1.18778
0.92873
0.92559
0.90505
0.90099
0.88032
OH
S
N
O
O
N
3f
Integral
1.0000
5.2862
1.0385
4.3110
7.0402
6.6345
ppm
3.5
3.0
2.5
2.0
1.5
1.0
Current Data Parameters
NAME 1847-gyy-246
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 9.29
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 8.00 cm
F1P 4.174 ppm
F1 1252.68 Hz
F2P 0.604 ppm
F2 181.41 Hz
PPMCM 0.16295 ppm/cm
HZCM 48.90613 Hz/cm

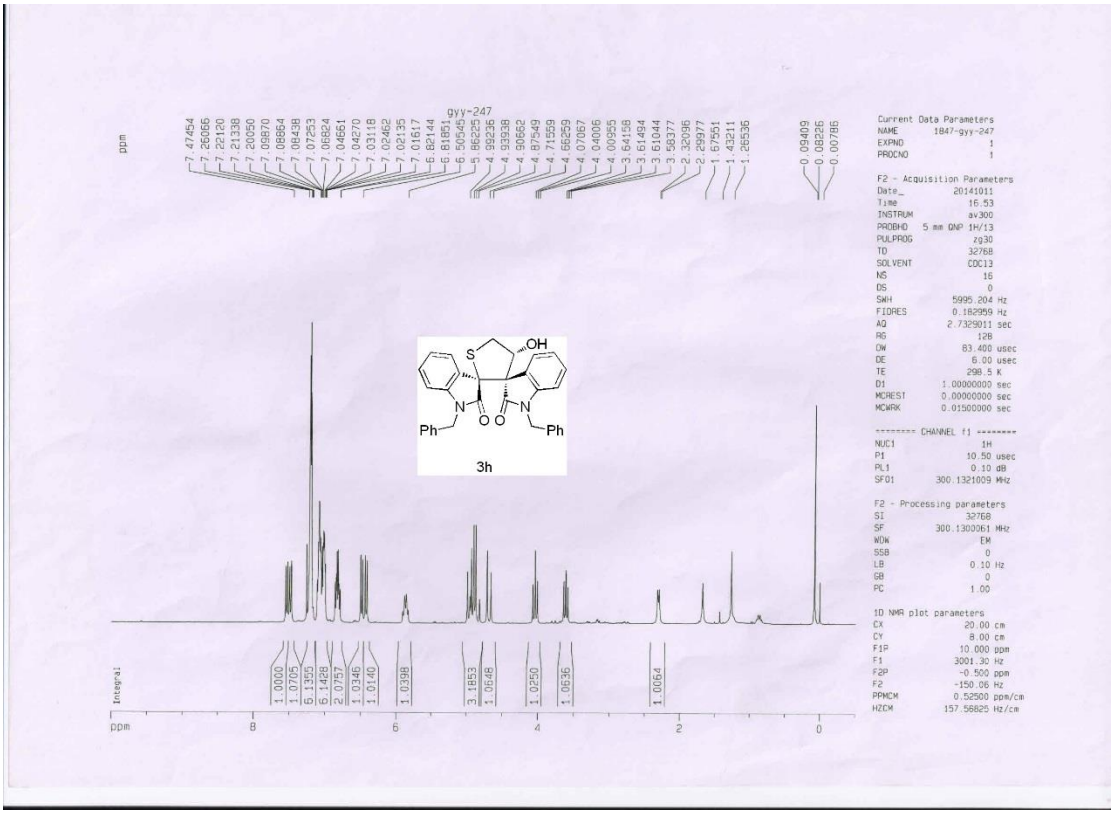

gyy-246
ppm
7.55809
7.55524
7.53282
7.53000
7.48926
7.48680
7.46410
7.26040
7.18392
7.18024
7.15817
7.15436
7.15029
7.14567
7.13233
7.12805
7.12409
7.12008
7.09817
7.09423
6.93044
6.90510
6.87973
6.62566
6.59976
6.56103
6.53511
5.80838
5.78134
5.76052
5.73357
OH
S
N
O
O
N
3f
Integral
0.9606
1.0438
2.0374
2.0468
0.9886
1.0209
1.0412
ppm
7.5
7.0
6.5
6.0
5.5
Current Data Parameters
NAME 1847-gyy-246
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 9.29
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.90 cm
CY 8.00 cm
F1P 7.595 ppm
F1 2309.61 Hz
F2P 5.398 ppm
F2 1620.20 Hz
PPMCM 0.10486 ppm/cm
HZCM 31.47304 Hz/cm

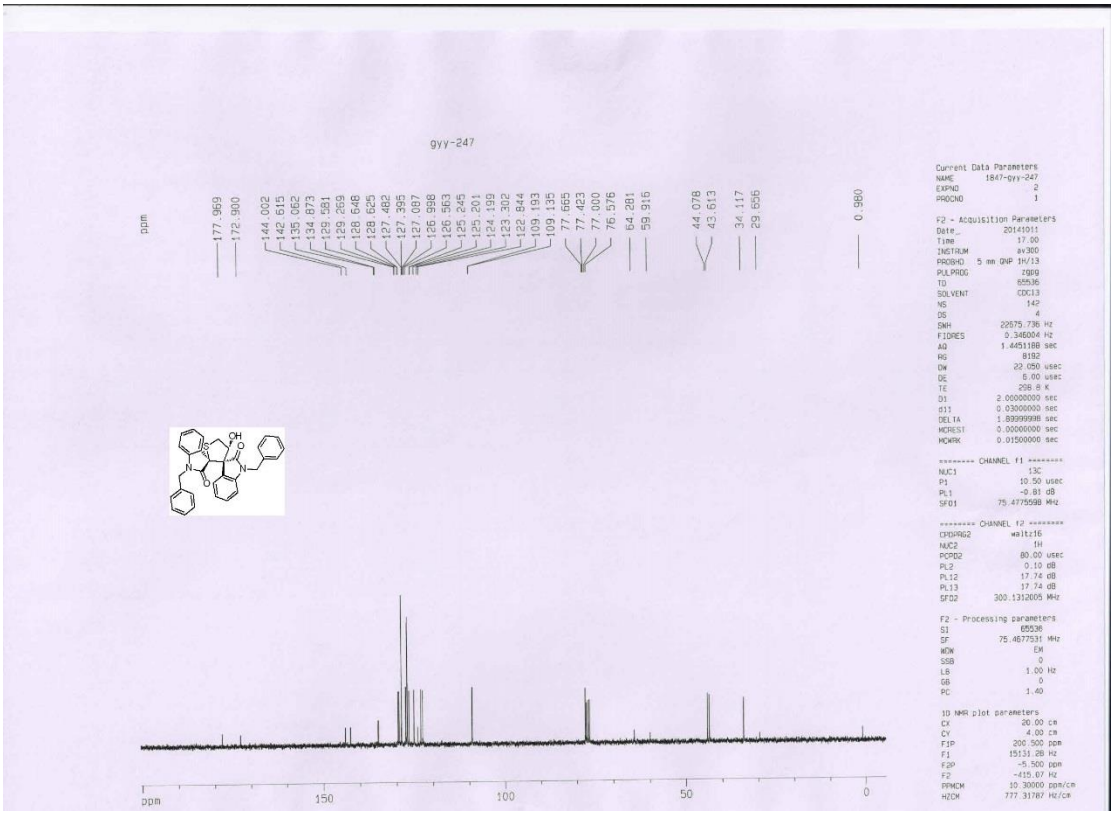

gyy-246
ppm
177.636
172.669
144.294
142.889
129.539
129.207
126.409
125.269
124.983
124.217
122.642
122.205
108.163
77.423
77.237
77.000
76.576
64.017
59.715
40.148
39.723
34.094
29.643
29.429
28.388
20.141
13.686
0.965
OH
S
N
O
O
N
3f
Current Data Parameters
NAME 1847-gyy-246
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 9.32
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 432
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -416.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm
ppm
150
100
50
0

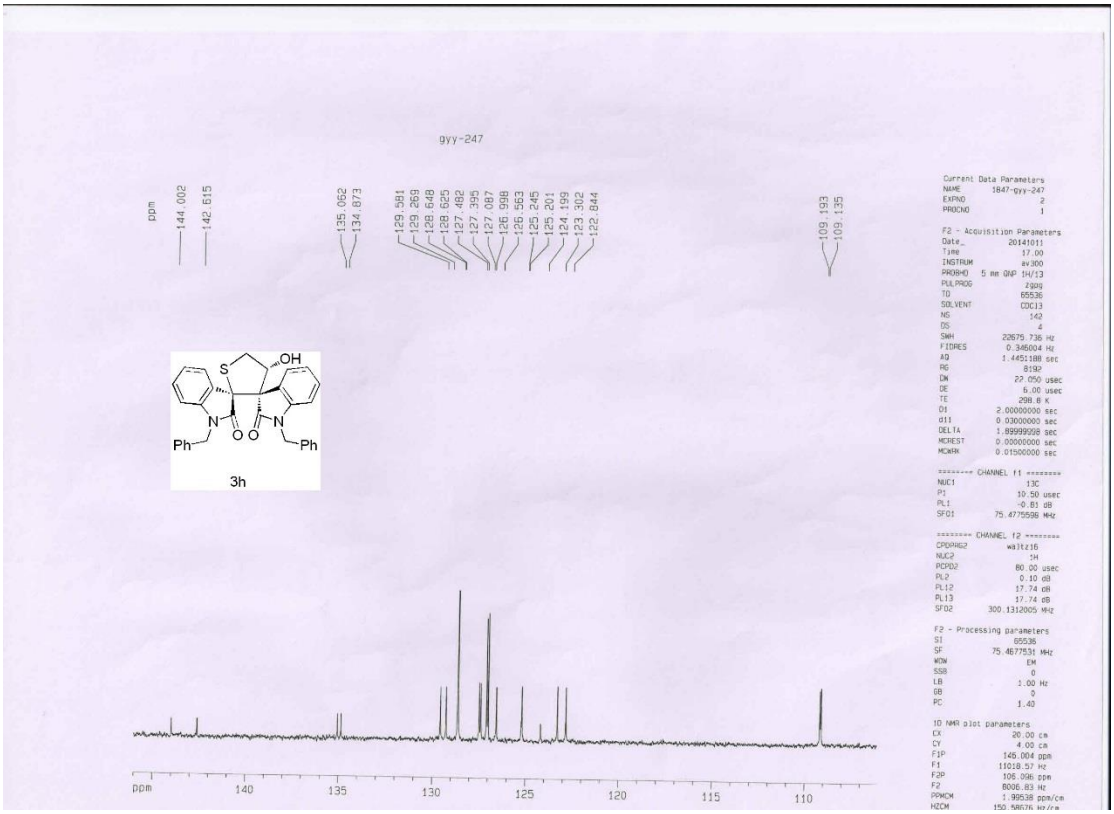

gyy-250
ppm
7.5665
7.5338
7.5312
7.4891
7.4638
7.2619
7.1579
7.1542
7.1504
7.1282
7.1239
7.1198
5.9274
5.9020
5.8766
5.6211
5.5952
5.5574
5.5315
5.7829
5.7586
3.9881
3.9573
3.9271
3.7104
3.6196
3.5944
3.5675
3.5635
3.5365
3.4850
3.4604
3.4374
3.4134
2.2214
2.1980
1.7448
1.4967
1.4896
1.2491
0.8968
0.8759
0.8530
0.0670
0.0259
OH
S
N
O
O
N
3g
Integral
0.975
0.988
2.000
1.999
0.980
1.006
0.984
0.982
2.985
2.017
0.978
4.096
20.842
6.223
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-250
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 9.14
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

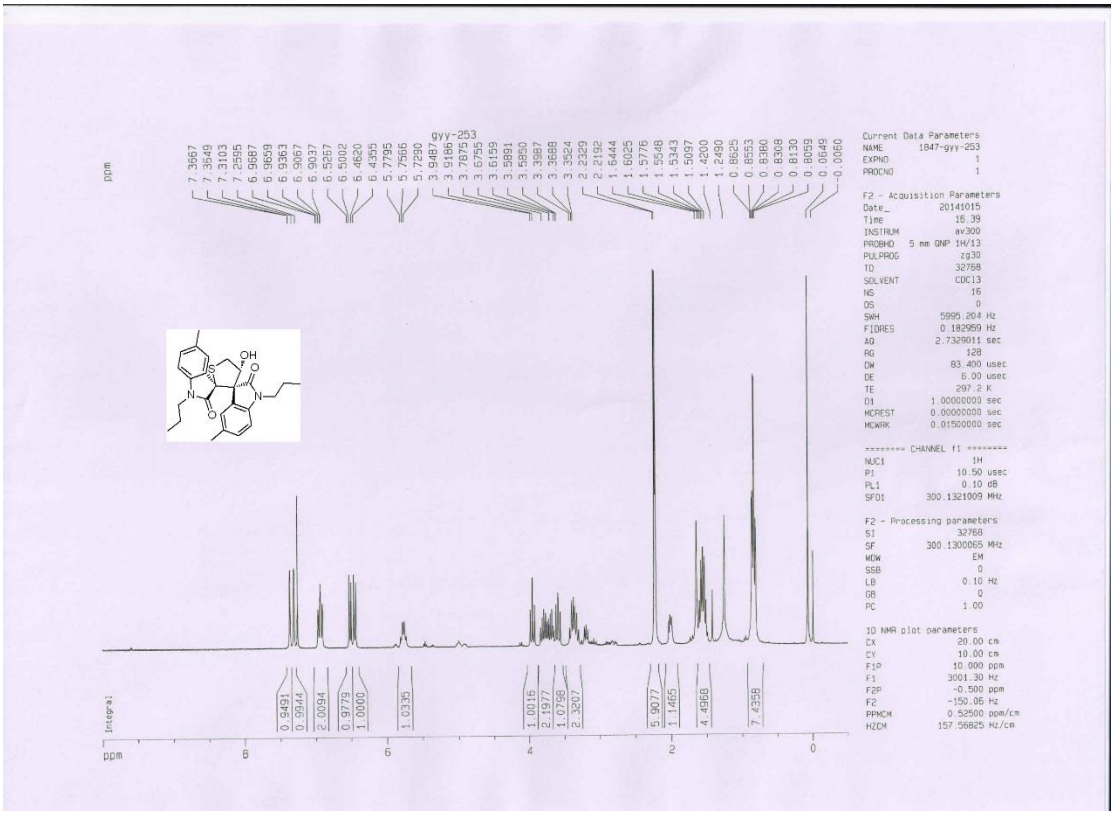

gyy-250
ppm
7.55650
7.53379
7.53120
7.48810
7.46379
7.26192
7.18370
7.18008
7.15790
7.15421
7.15038
7.14567
7.13198
7.12819
7.12388
7.11983
7.09785
7.09395
6.92735
6.90198
6.87661
6.62112
6.59521
6.55737
6.53148
5.81132
5.78290
5.75861
5.73207
OH
S
N
O
O
N
3g
Integral
0.9752
0.9884
2.0000
1.9993
0.9804
1.0058
0.9840
ppm
7.5
7.0
6.5
6.0
Current Data Parameters
NAME 1847-gyy-250
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 9.14
INSTRUM av300
PROBHD 5 mm DNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 7.724 ppm
F1 2318.22 Hz
F2P 5.517 ppm
F2 1655.95 Hz
PPMCM 0.11033 ppm/cm
HZCM 33.11343 Hz/cm

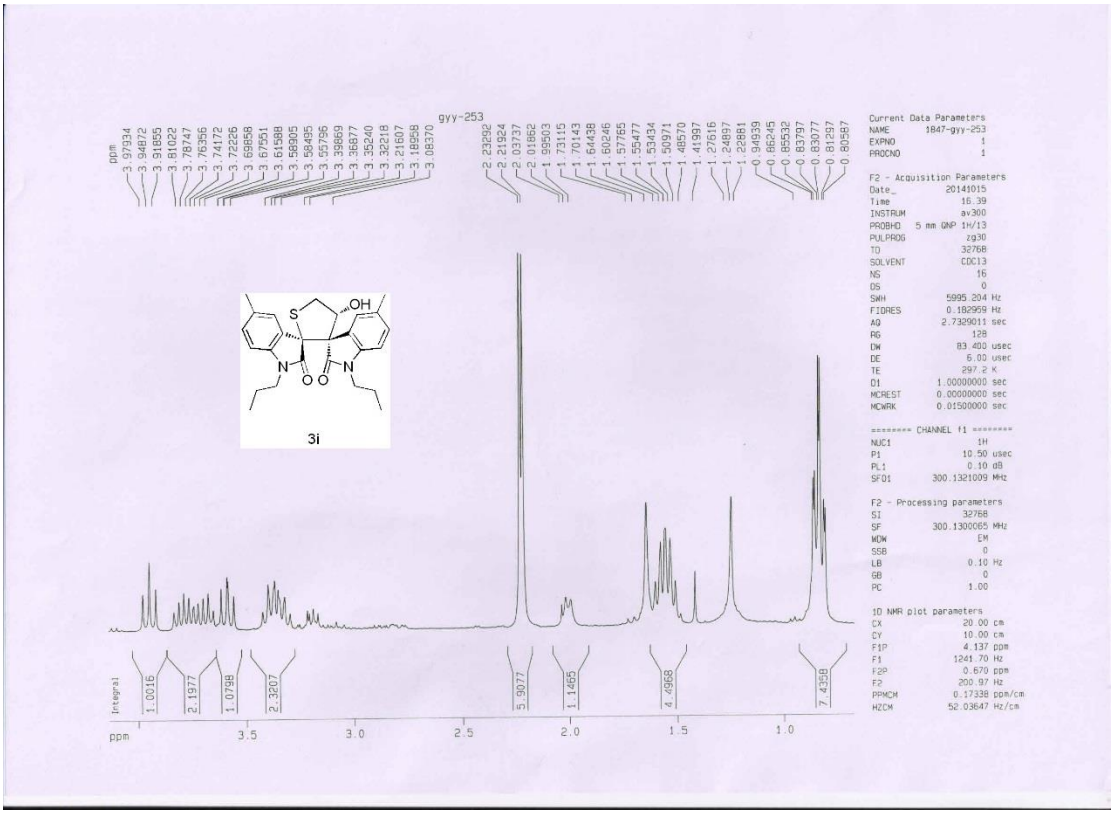

gyy-250
ppm
177.577
172.633
144.293
142.899
129.545
129.218
126.408
125.272
124.989
124.212
122.643
122.222
108.156
77.424
77.260
77.000
76.577
64.012
59.719
40.434
40.001
34.117
31.738
29.650
29.203
29.180
29.097
29.054
27.366
27.322
26.941
26.899
22.560
14.043
0.967
OH
O
S
N
O
N
O
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-250
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 9.37
INSTRUM av300
PROBHD 5 mm DNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775558 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677529 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

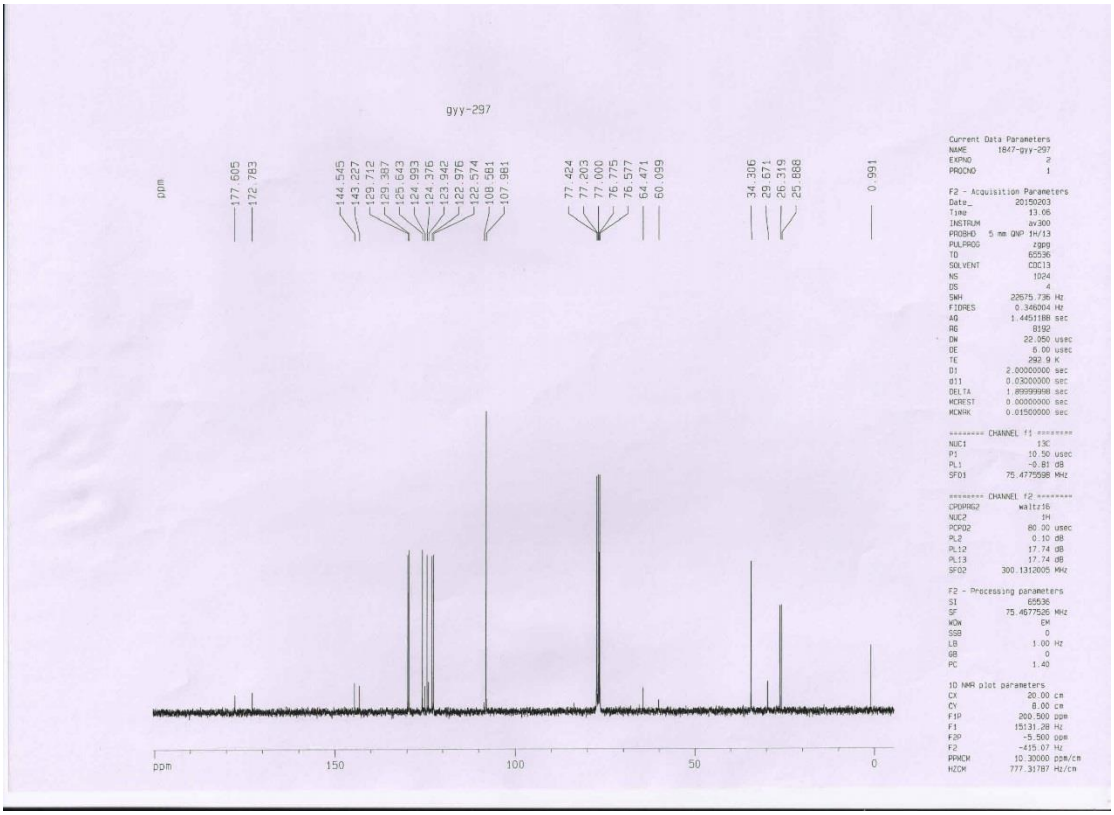

gyy-247
ppm
7.47454
7.26066
7.22120
7.21338
7.20050
7.09870
7.08864
7.08438
7.07253
7.06824
7.04661
7.04270
7.03118
7.02462
7.02135
7.01617
6.82144
6.81851
6.50945
5.86235
4.99236
4.99338
4.90662
4.87549
4.71559
4.66259
4.07067
4.04006
4.00955
3.64158
3.61494
3.61044
3.58377
2.32095
2.29977
1.67561
1.43211
1.26536
0.09409
0.08226
0.00786
OH
S
N
O
O
N
Ph
Ph
3h
Integral
1.0000
1.0705
5.1365
5.1489
2.0757
1.0346
1.0140
1.0398
3.1853
1.0648
1.0250
1.0636
1.0064
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-247
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 16.53
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

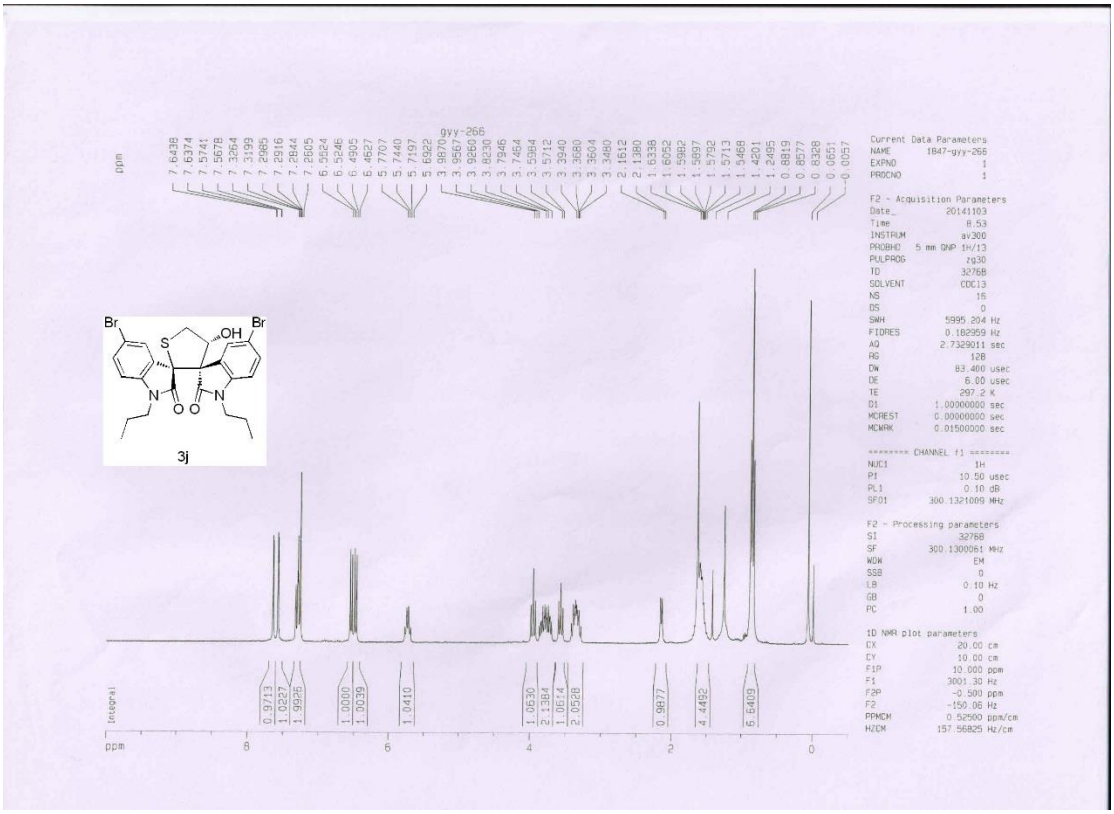

gyy-247
ppm
177.969
172.900
144.002
142.615
135.062
134.873
129.581
129.269
128.648
128.625
127.482
127.395
127.087
126.998
126.563
125.245
125.201
124.191
123.302
122.844
109.193
109.135
77.665
77.423
77.000
76.576
64.281
59.916
44.078
43.613
34.117
29.656
0.980
OH
S
N
O
O
N
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-247
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 17.00
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 142
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 10.50 usec
PL1 -0.83 dB
SFO1 75.4775598 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

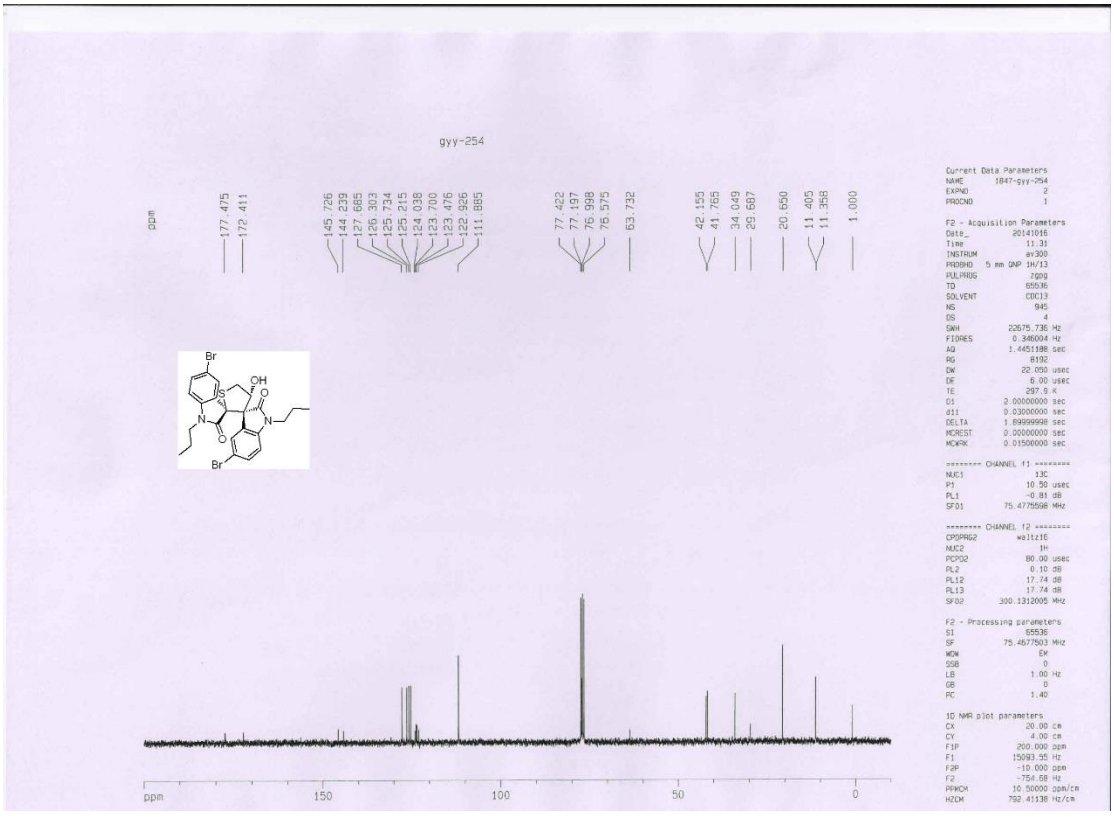

gyy-247
ppm
144.002
142.615
135.062
134.873
129.981
129.269
128.648
128.625
127.482
127.395
127.087
126.998
126.563
125.245
125.201
124.199
123.302
122.844
109.193
109.135
OH
S
N
O
O
N
Ph
Ph
3h
Current Data Parameters
NAME 1847-gyy-247
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141011
Time 17.00
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 142
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SF01 75.4775596 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 145.004 ppm
F1 11018.57 Hz
F2P 105.096 ppm
F2 8006.83 Hz
PPMCM 1.99538 ppm/cm
HZCM 150.58676 Hz/cm
ppm
140
135
130
125
120
115
110

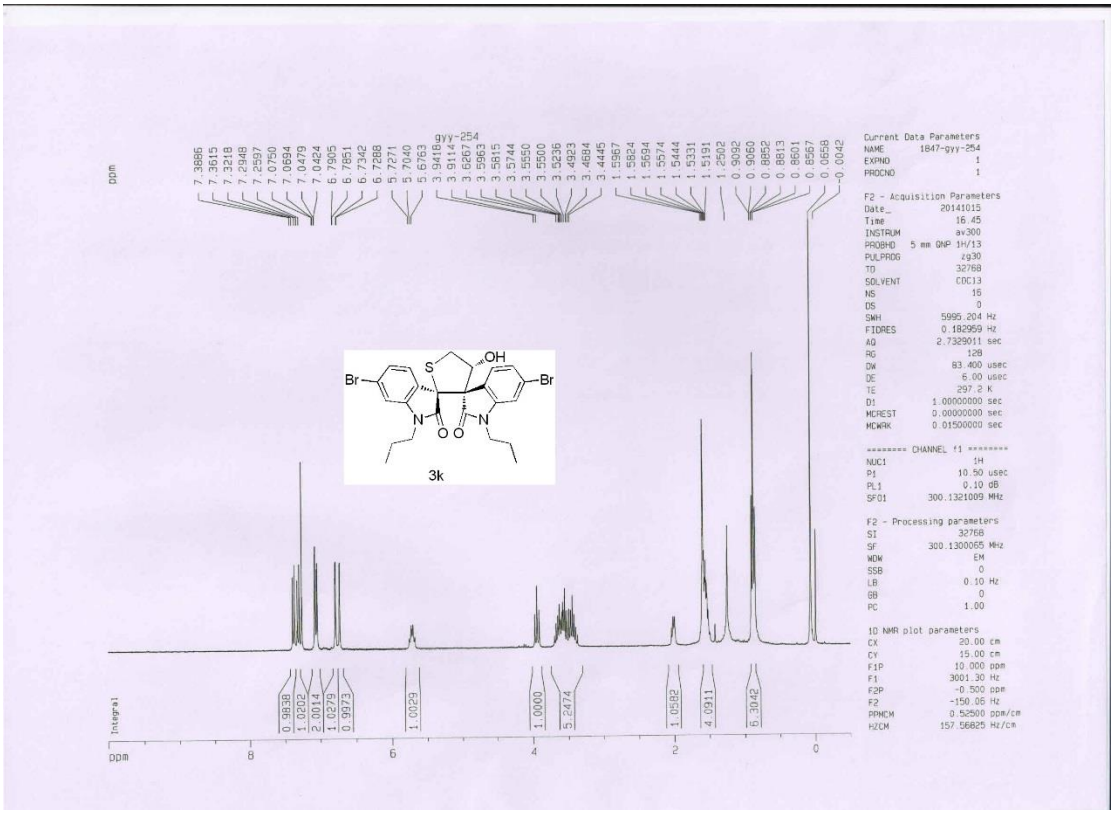

gyy-253
ppm
7.3667
7.3649
7.3103
7.2595
6.9687
6.9659
6.9363
6.9067
6.9037
6.5267
6.5002
6.4620
6.4355
5.7795
5.7566
5.7290
3.9487
3.9186
3.7675
3.6755
3.6159
3.5891
3.5850
3.3987
3.3688
3.3524
2.2329
2.2192
1.6444
1.6025
1.5776
1.5548
1.5343
1.5097
1.4200
1.2490
0.8625
0.8553
0.8380
0.8308
0.8130
0.8059
0.0649
-0.0060
OH
S
N
O
O
N
Integral
0.9491
0.9944
2.0094
0.9779
1.0000
1.0335
1.0016
2.1977
1.0798
2.3207
5.9077
1.1465
4.4968
7.4358
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-253
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 16.39
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

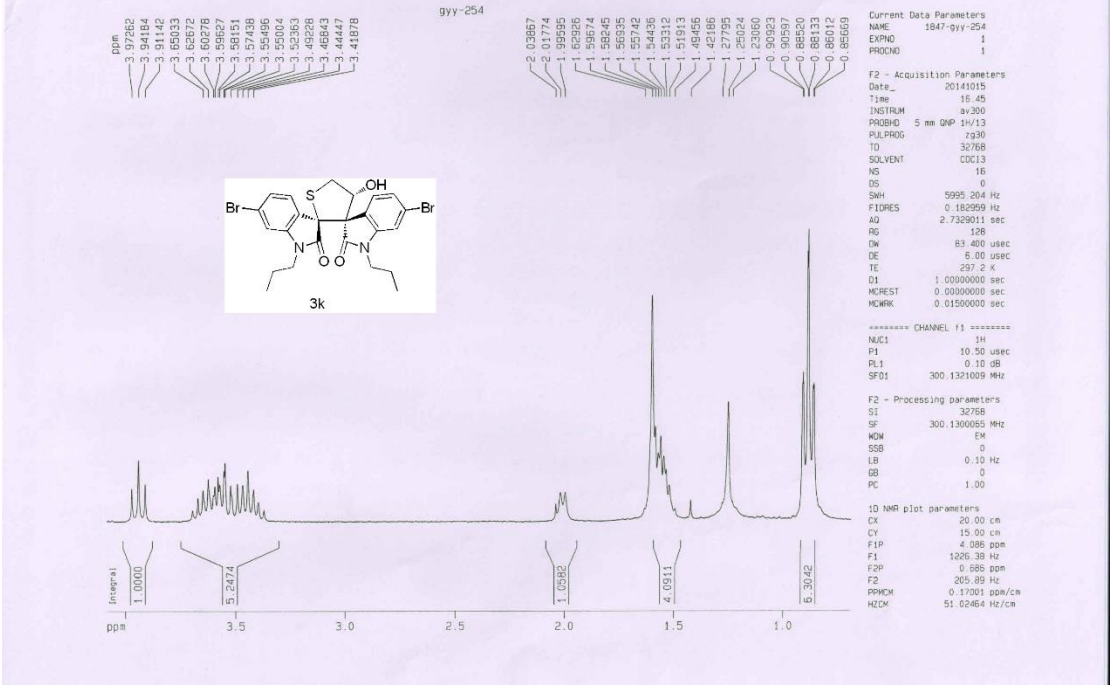

gyy-253
3i
Current Data Parameters
NAME 1847-gyy-253
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 16.39
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 4.137 ppm
F1 1241.70 Hz
F2P 0.670 ppm
F2 200.97 Hz
PPMCM 0.17338 ppm/cm
HZCM 52.03647 Hz/cm

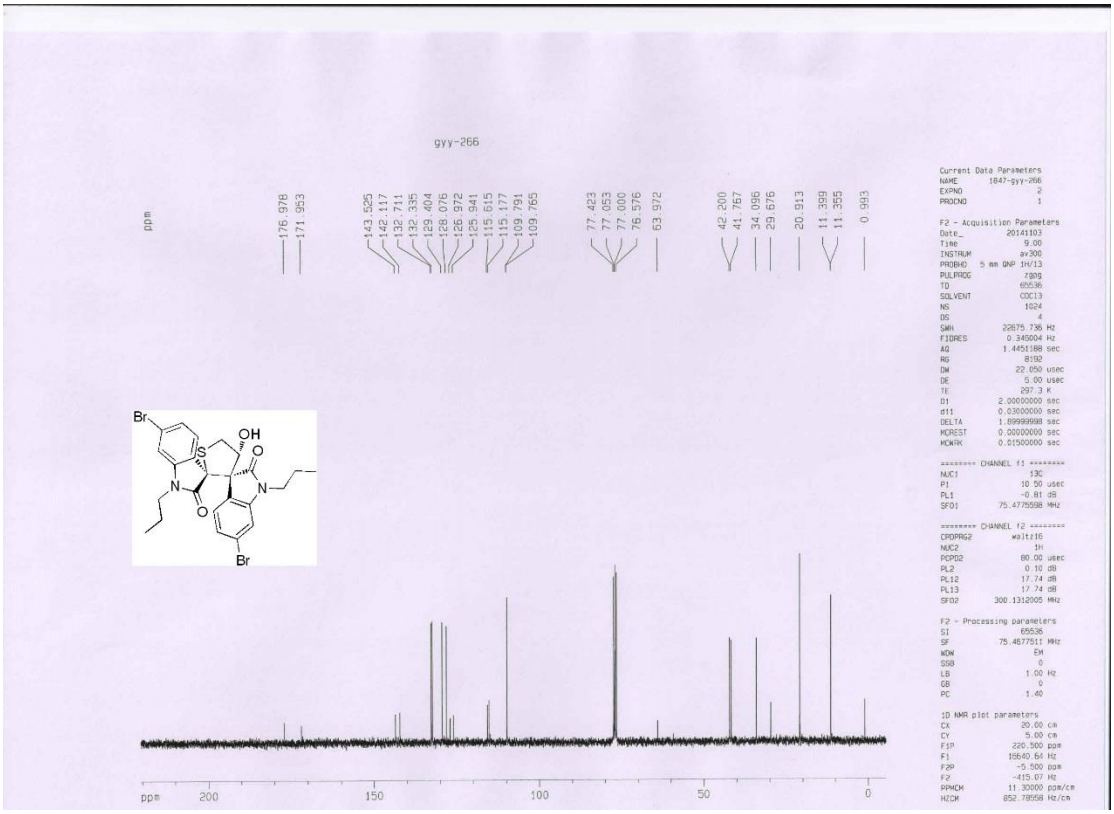

gyy-297
Current Data Parameters
NAME 1847-gyy-297
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150203
Time 13.08
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 292.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677526 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

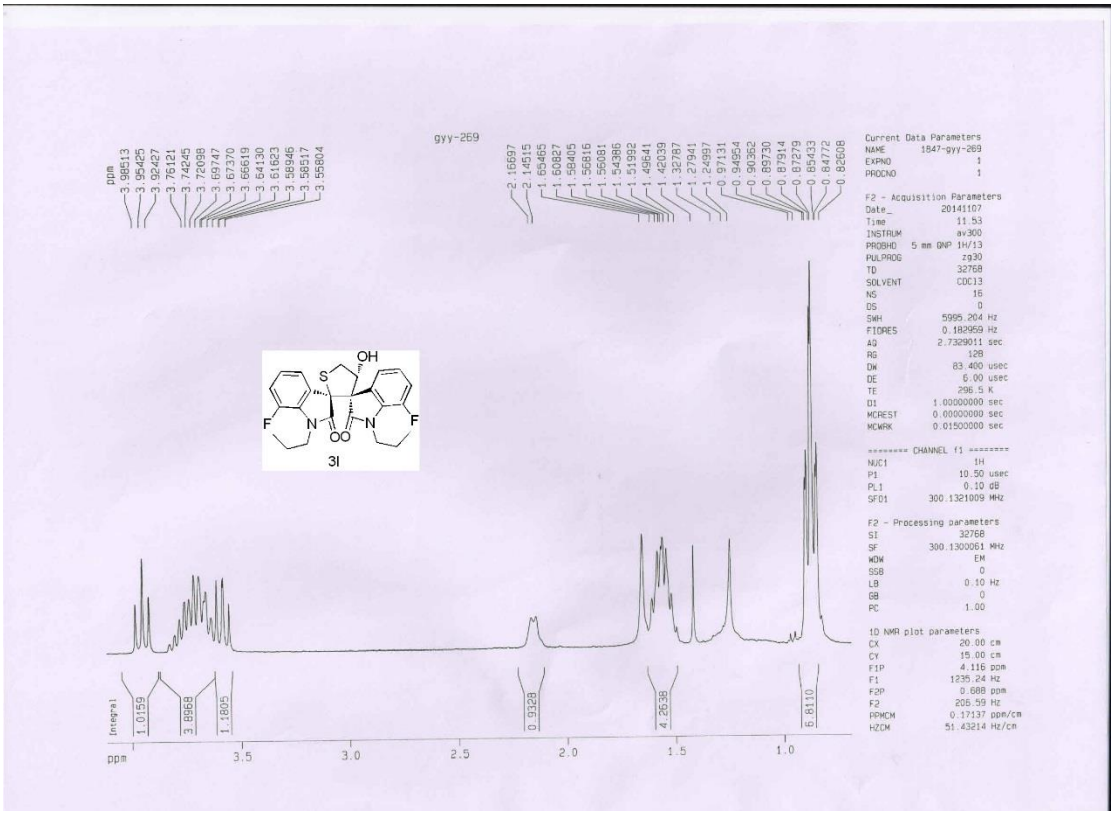

gyy-266
ppm
7.6438
7.6374
7.5741
7.5678
7.3264
7.3199
7.2985
7.2916
7.2844
7.2605
6.5524
6.5246
6.4905
6.4627
5.7707
5.7440
5.7197
5.6922
3.9870
3.9567
3.9260
3.8230
3.7946
3.7464
3.5984
3.5712
3.3940
3.3680
3.3604
3.3480
2.1612
2.1380
1.6338
1.6052
1.5982
1.5897
1.5732
1.5713
1.5468
1.4201
1.2495
0.9819
0.8577
0.8328
0.0651
0.0057
Br
OH
Br
S
N
O
O
N
3j
integral
0.9713
1.0227
1.9996
1.0000
1.0039
1.0410
1.0630
2.1384
1.0614
2.0528
0.9877
4.4492
5.6409
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-266
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141103
Time 8.53
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

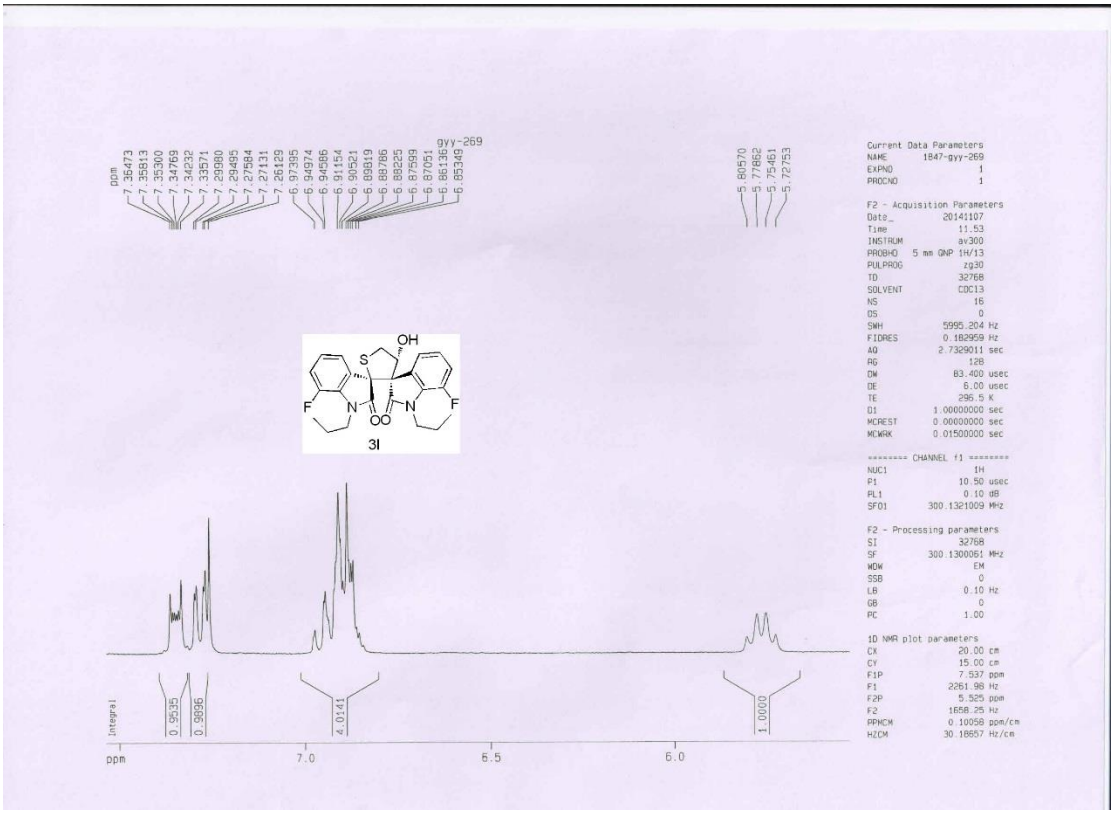

gyy-254
ppm
177.475
172.411
145.726
144.239
127.685
126.303
125.734
125.215
124.038
123.700
123.476
122.925
111.985
77.422
77.197
76.998
76.575
63.732
42.155
41.765
34.049
29.687
20.650
11.405
11.358
1.000
Br
OH
S
O
N
O
N
Br
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-254
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141016
Time 11.31
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 945
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451198 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SF01 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677503 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 15093.55 Hz
F2P -10.000 ppm
F2 -754.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 792.41138 Hz/cm

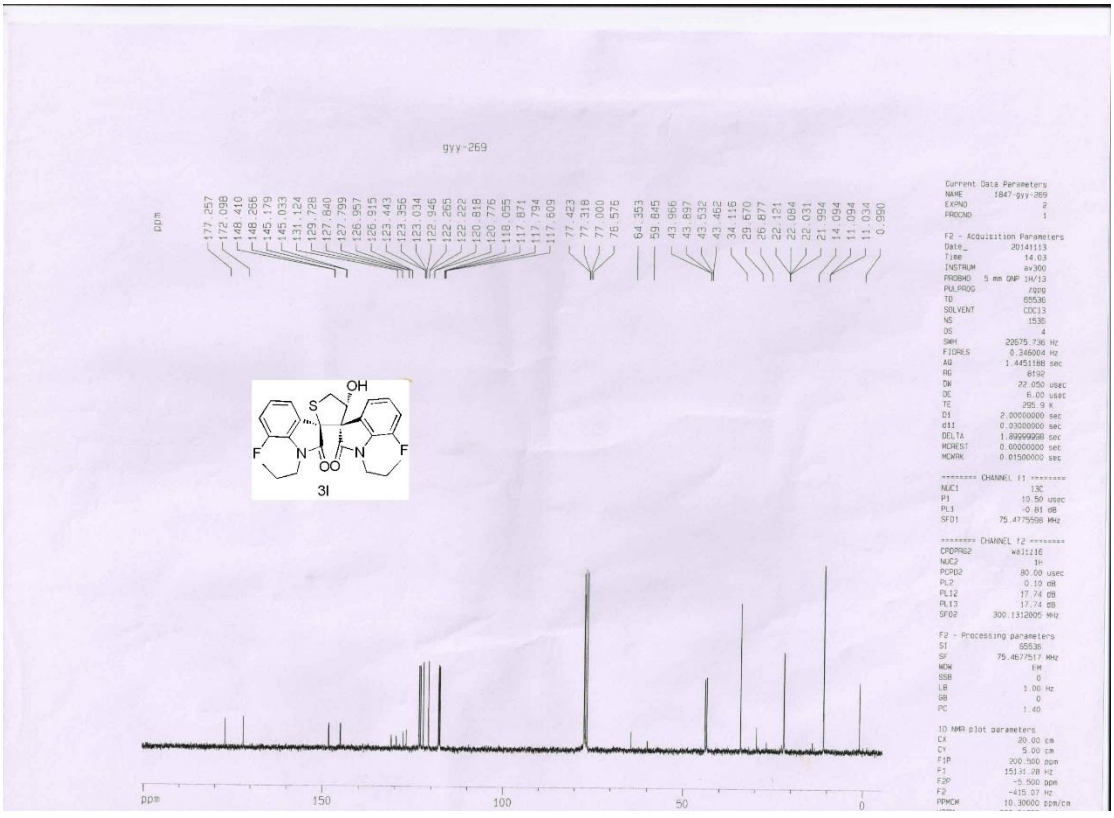

gyy-254
ppm
7.3866
7.3615
7.3218
7.2948
7.2597
7.0750
7.0694
7.0479
7.0424
6.7905
6.7851
6.7342
6.7288
5.7271
5.7040
5.6763
3.9410
3.9114
3.6267
3.5963
3.5815
3.5744
3.5550
3.5500
3.5236
3.4923
3.4684
3.4445
1.5967
1.5824
1.5694
1.5574
1.5444
1.5331
1.5191
1.2502
0.9092
0.9060
0.8852
0.8813
0.8601
0.8567
0.0558
-0.0042
Br
S
OH
N
O
O
N
Br
3k
Integral
0.9838
1.0202
2.0014
1.0279
0.9973
1.0029
1.0000
5.2474
1.0582
4.0911
6.3042
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-254
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 16.45
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.05 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

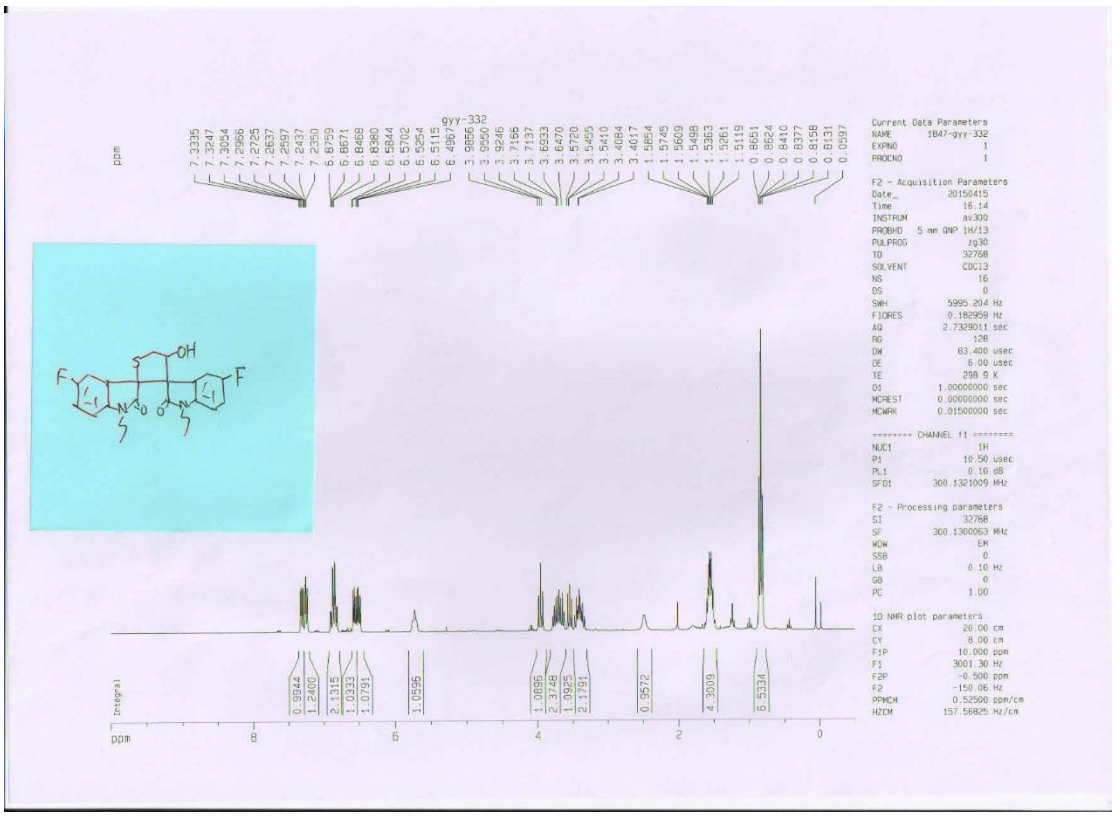

gyy-254
ppm
3.97262
3.94184
3.91142
3.65033
3.62672
3.60278
3.59627
3.58151
3.57438
3.55496
3.55004
3.53263
3.49228
3.46843
3.44447
3.41878
2.03867
2.01774
1.99995
1.62926
1.59674
1.58245
1.56935
1.55742
1.54436
1.53312
1.51913
1.49456
1.42186
1.27795
1.25024
1.23060
0.90923
0.90597
0.88520
0.88133
0.86012
0.85669
Br
S
OH
N
O
O
N
Br
3k
Integral
1.0000
5.2474
1.0582
4.0911
6.3042
ppm
3.5
3.0
2.5
2.0
1.5
1.0
Current Data Parameters
NAME 1847-gyy-254
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141015
Time 16.45
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 4.086 ppm
F1 1226.38 Hz
F2P 0.686 ppm
F2 205.89 Hz
PPMCM 0.17001 ppm/cm
HZCM 51.02464 Hz/cm

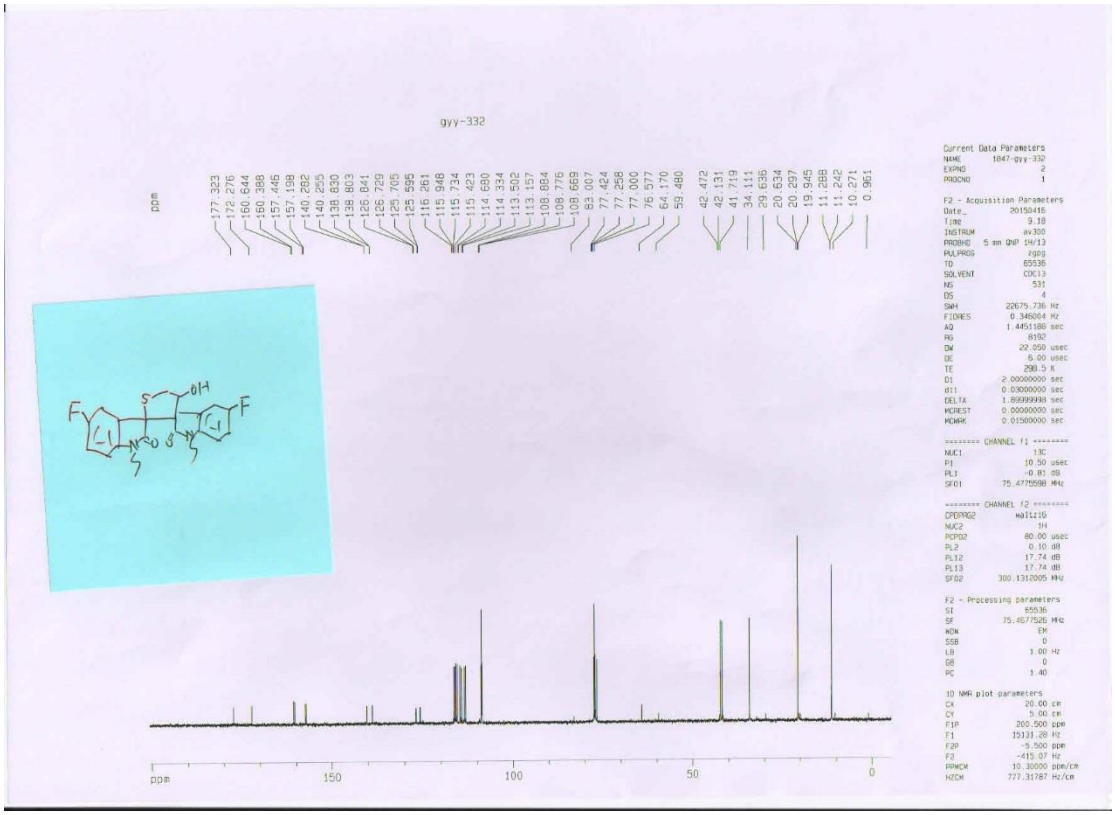

gyy-266
ppm
176.978
171.953
143.525
142.117
132.711
132.335
129.404
128.076
126.972
125.941
115.615
115.177
109.791
109.765
77.423
77.053
77.000
76.576
63.972
42.200
41.767
34.096
29.676
20.913
11.399
11.355
0.993
Br
OH
S
O
N
O
N
Br
ppm
200
150
100
50
0
Current Data Parameters
NAME 1847-gyy-266
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141103
Time 9.00
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 22675.736 Hz
FIDRES 0.345004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 5.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677511 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 220.500 ppm
F1 16640.64 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 11.30000 ppm/cm
HZCM 852.78558 Hz/cm

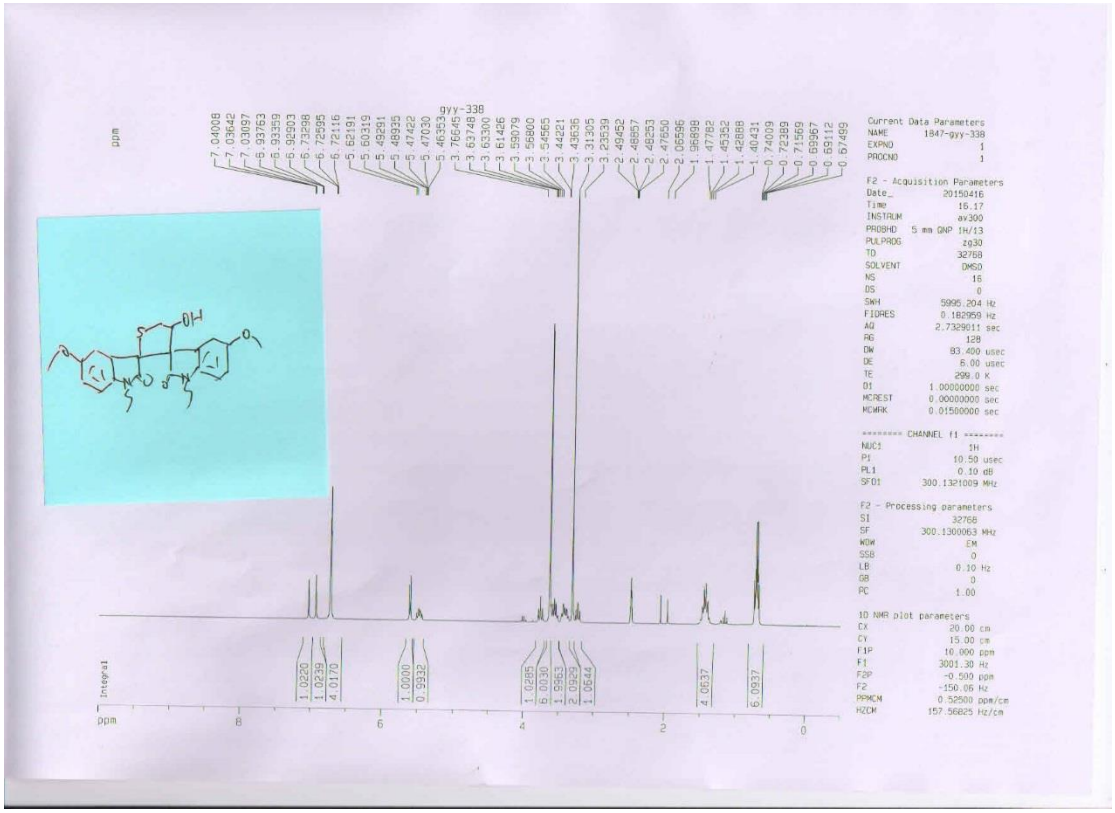

gyy-269
ppm
3.98513
3.95425
3.92427
3.76121
3.74245
3.72098
3.69747
3.67370
3.66619
3.64130
3.61623
3.58946
3.58517
3.55804
2.16697
2.14515
1.69465
1.60827
1.58405
1.56816
1.56081
1.54386
1.51932
1.49641
1.42039
1.32787
1.27941
1.24997
0.97131
0.94954
0.90362
0.89730
0.87914
0.87279
0.85433
0.84772
0.82608
OH
S
F
N
O
O
N
F
3l
Integral
1.0159
3.8968
1.1805
0.9328
4.2638
6.8110
ppm
3.5
3.0
2.5
2.0
1.5
1.0
Current Data Parameters
NAME 1847-gyy-269
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141107
Time 11.53
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 4.116 ppm
F1 1235.24 Hz
F2P 0.688 ppm
F2 206.59 Hz
PPMCM 0.17137 ppm/cm
HZCM 51.43214 Hz/cm

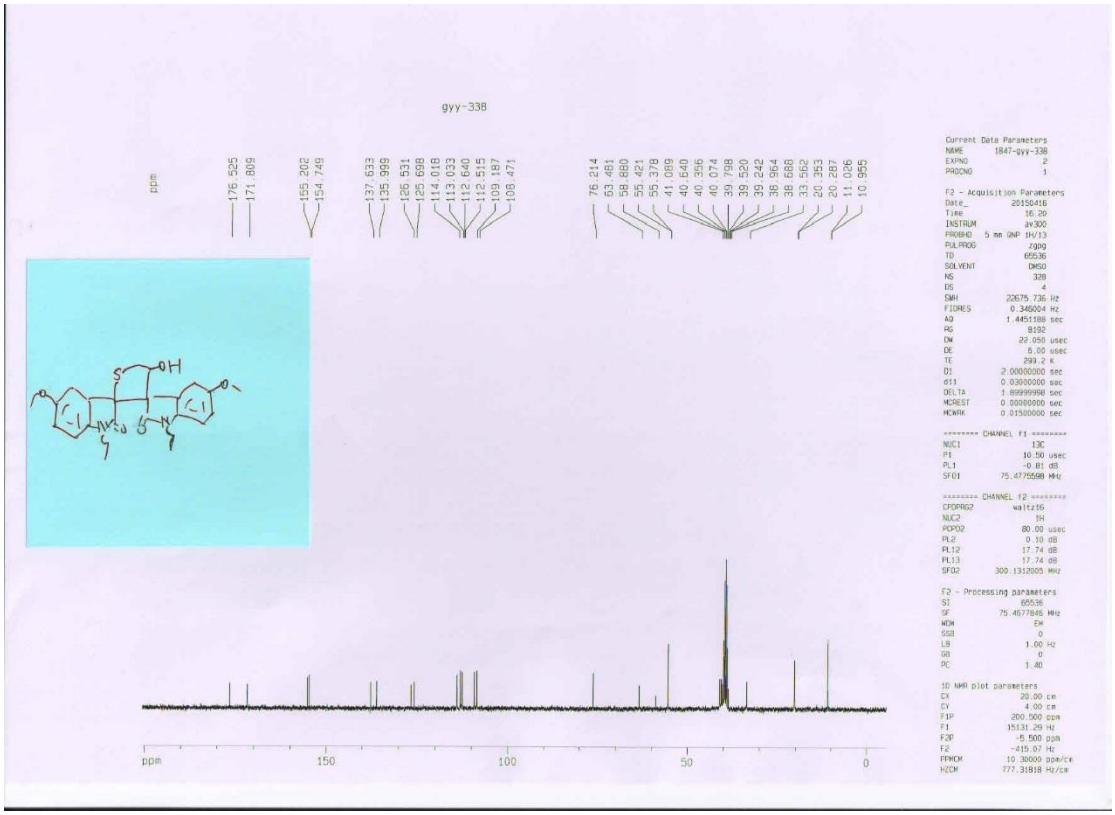

gyy-269
ppm
7.36473
7.35813
7.35300
7.34769
7.34232
7.33571
7.29980
7.29495
7.27584
7.27131
7.26129
6.97395
6.94974
6.94566
6.91154
6.90521
6.89819
6.88786
6.88225
6.87599
6.87051
6.86136
6.85349
5.80570
5.77862
5.75461
5.72753
OH
S
F
N
O
O
N
F
3l
Integral
0.9535
0.9696
4.0141
1.0000
ppm
7.0
6.5
6.0
Current Data Parameters
NAME 1847-gyy-269
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141107
Time 11.53
INSTRUM av300
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 7.537 ppm
F1 2261.98 Hz
F2P 5.525 ppm
F2 1658.25 Hz
PPMCM 0.10058 ppm/cm
HZCM 30.18657 Hz/cm

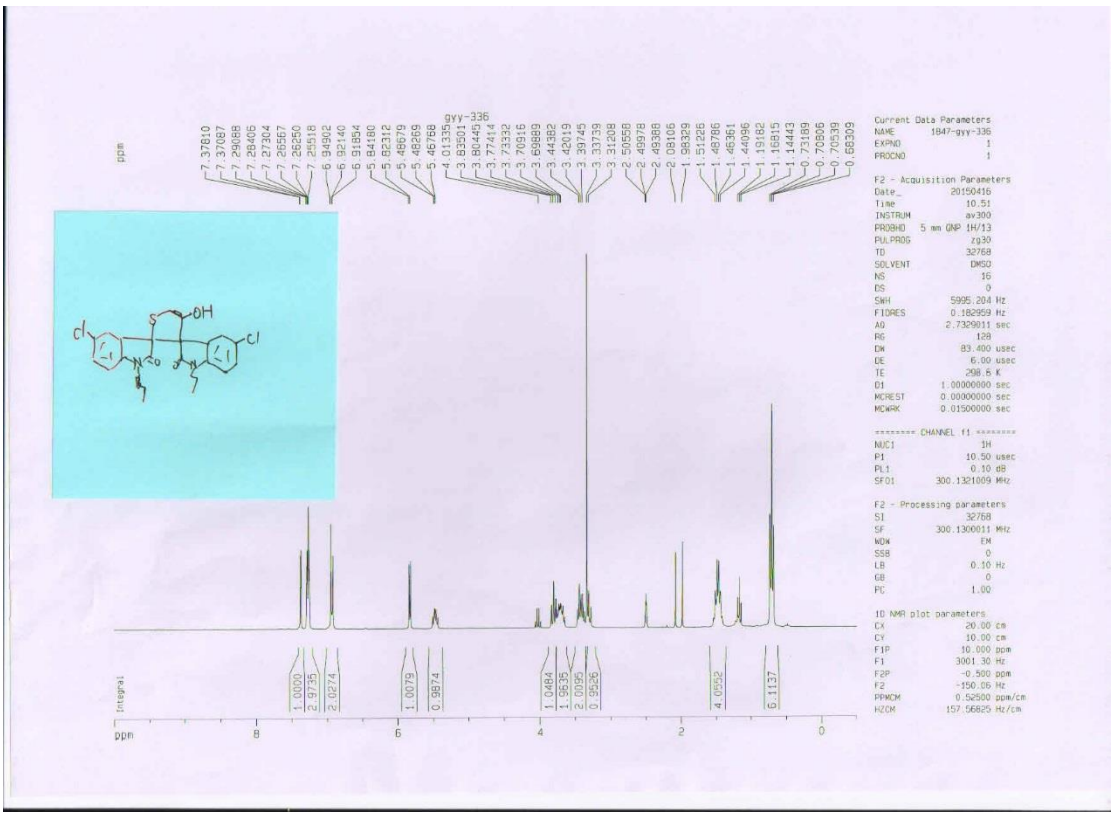

gyy-269
ppm
177.257
172.098
148.410
148.266
145.779
145.033
131.124
129.728
127.840
127.799
126.957
126.915
123.443
123.356
123.034
122.946
122.265
122.222
120.818
120.776
118.055
117.871
117.794
117.609
77.423
77.318
77.000
76.576
64.353
59.845
43.966
43.837
43.532
43.462
34.116
29.670
26.877
22.121
22.084
22.031
21.994
14.094
11.094
11.034
0.990
OH
S
F
N
O
O
N
F
3l
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-269
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141113
Time 14.03
INSTRUM av300
PROBHD 5 mm GNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1536
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451186 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677517 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.500 ppm
F1 15131.98 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm

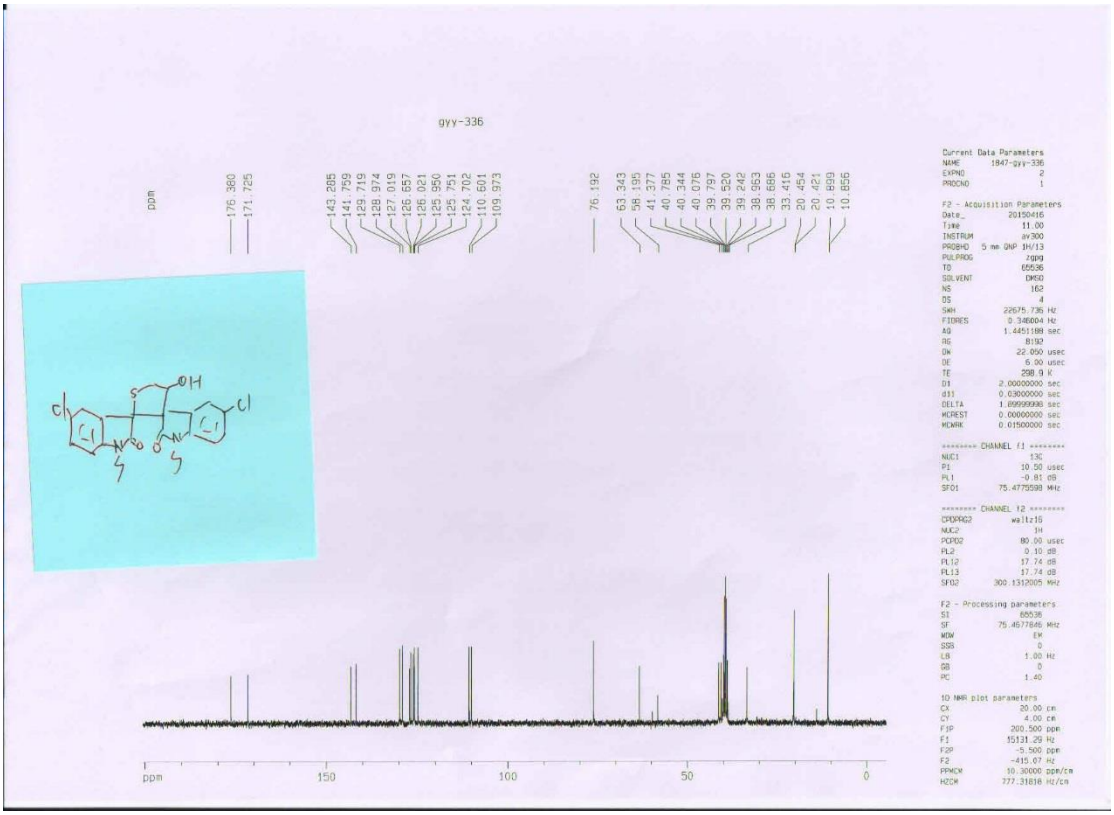

gyy-332
ppm
7.3335 7.3247 7.3054 7.2966 7.2725 7.2637 7.2597 7.2437 7.2350 6.8759 6.8671 6.8468 6.8380 6.5844 6.5702 6.5254 6.5115 6.4967 3.9856 3.9550 3.9246 3.7166 3.7137 3.6933 3.6470 3.5720 3.5465 3.5410 3.4064 3.4017 1.5854 1.5745 1.5609 1.5498 1.5363 1.5261 1.5119 0.8651 0.8624 0.8410 0.8377 0.8158 0.8131 0.0597
Integral
0.9844 1.2400 2.1315 1.0333 1.0791 1.0596 1.0696 2.3748 1.0925 2.1791 0.9572 4.3009 6.5334
ppm
8 6 4 2 0
Current Data Parameters
NAME 1847-gyy-332
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150415
Time 16.14
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

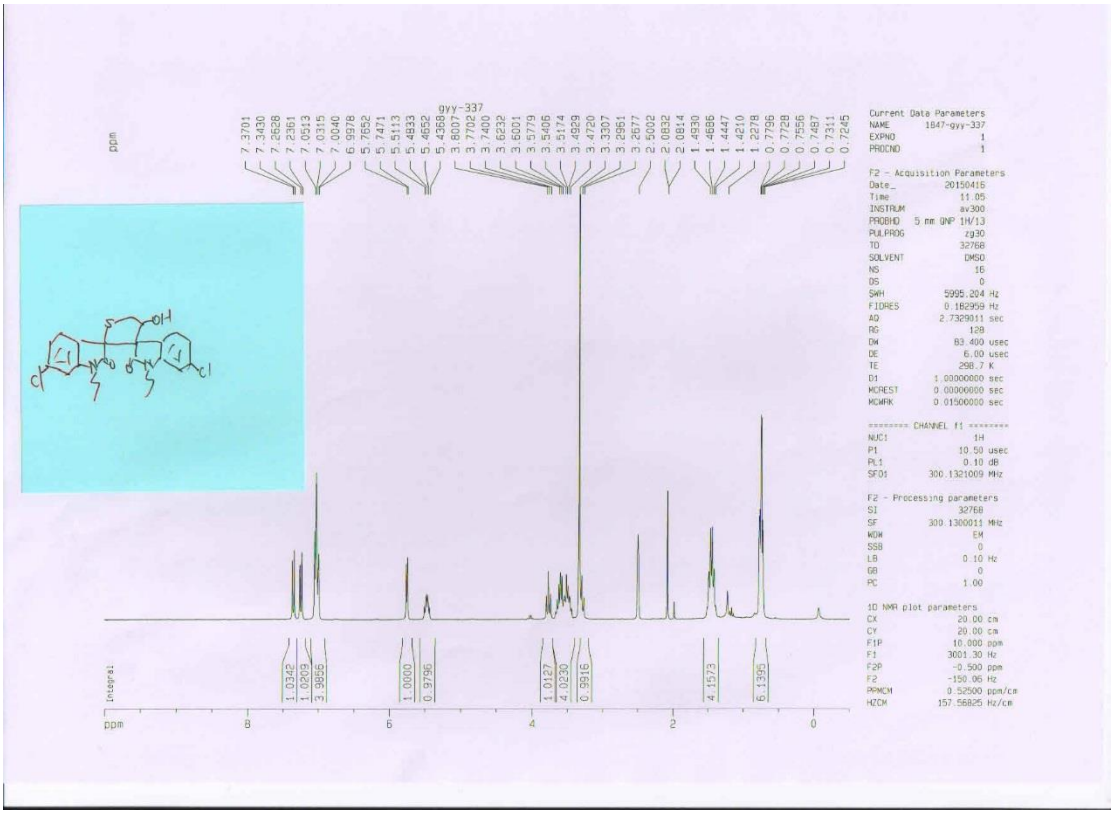

gyy-332
ppm
177.323 172.276 160.644 160.388 157.446 157.198 140.282 140.255 138.830 138.803 126.841 126.729 125.765 125.595 116.261 115.948 115.734 115.423 114.680 114.334 113.502 113.157 108.884 108.776 108.669 83.007 77.424 77.258 77.000 76.577 64.170 59.480 42.472 42.131 41.719 34.111 29.636 20.634 20.297 19.945 11.288 11.242 10.271 0.961
ppm
150 100 50 0
Current Data Parameters
NAME 1847-gyy-332
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 9.18
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 531
DS 4
SWH 22675.736 Hz
FIDRES 0.346084 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677526 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm

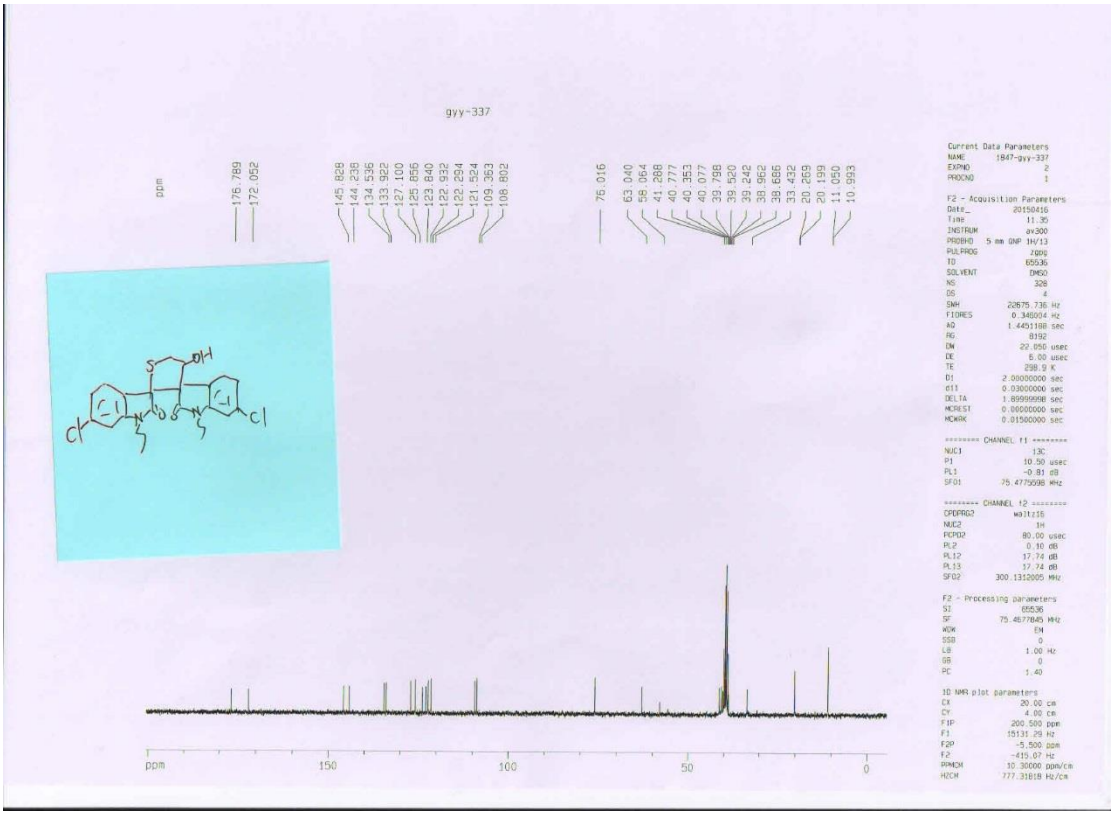

gyy-338
ppm
7.04008
7.03642
7.03097
6.93763
6.93359
6.92903
6.73298
6.72695
6.72116
5.62191
5.60319
5.49291
5.48935
5.47422
5.47030
5.46353
3.76645
3.63748
3.63300
3.61426
3.59079
3.56800
3.54565
3.44221
3.43636
3.31395
3.28339
2.49452
2.48857
2.48353
2.47850
2.06596
1.96898
1.47782
1.45352
1.42888
1.40431
0.74009
0.72389
0.71569
0.69967
0.69312
0.67499
Integral
1.0220
1.0239
4.0170
1.0000
0.9938
1.0285
6.0030
1.9963
2.0929
1.0644
4.0637
6.0937
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-338
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 16.17
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329611 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 299.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

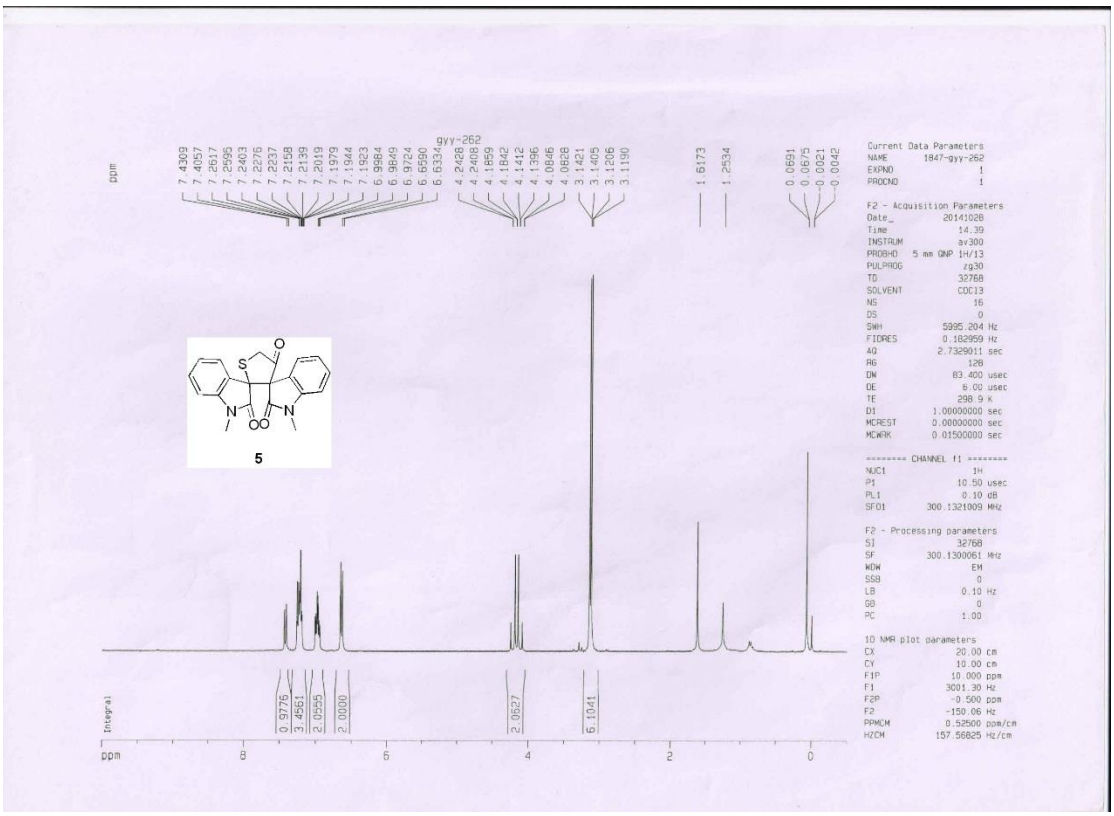

gyy-338
ppm
176.525
171.809
155.202
154.749
137.633
135.999
126.531
125.698
114.018
113.033
112.640
112.515
109.187
105.471
76.214
63.461
58.880
55.421
55.378
41.089
40.640
40.356
40.074
39.798
39.520
39.242
38.964
38.686
33.562
20.353
20.287
11.026
10.955
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-338
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 16.20
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 328
DS 4
SWH 22675.736 Hz
FIDRES 0.346064 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4770588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677845 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.500 ppm
F1 15131.29 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31818 Hz/cm

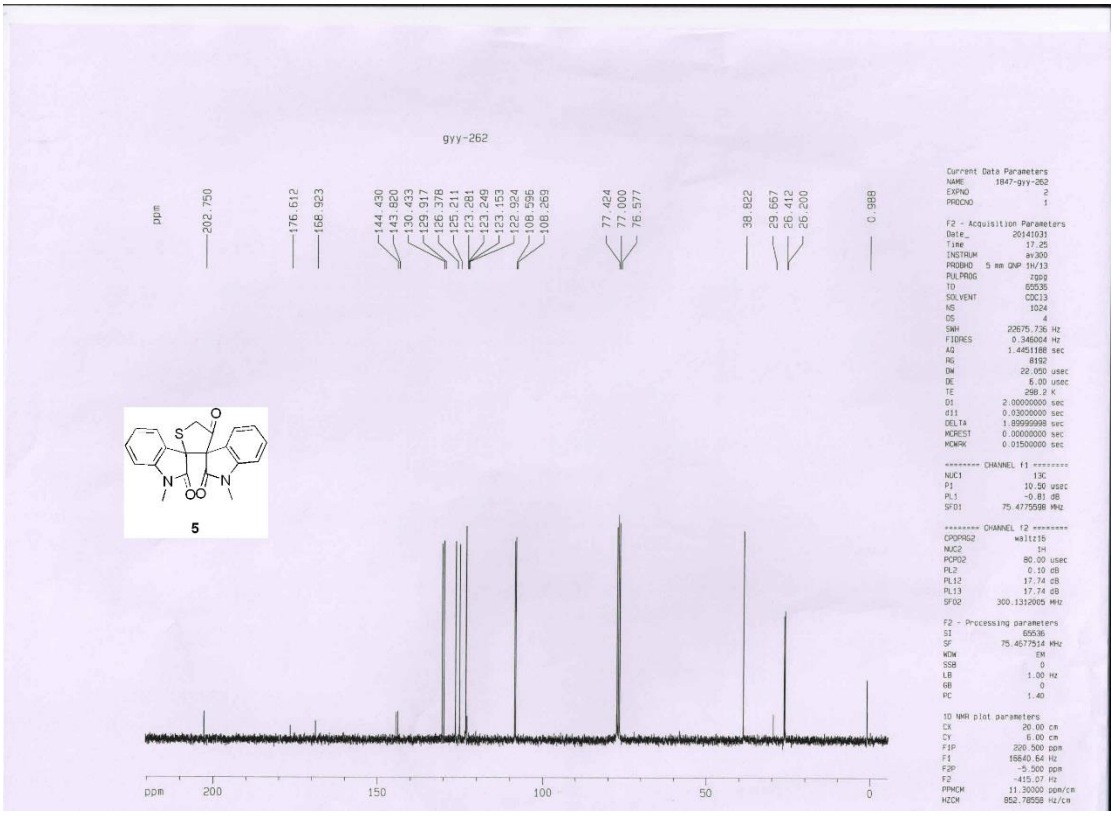

gyy-336
ppm
7.37610
7.37087
7.29068
7.28405
7.27304
7.26567
7.26250
7.25518
6.94902
6.92140
6.91854
5.84180
5.82312
5.48679
5.48269
5.46768
4.01335
3.83501
3.80445
3.77414
3.73332
3.70916
3.69889
3.44382
3.42019
3.39745
3.33739
3.31208
2.50558
2.49978
2.49388
2.08106
1.98329
1.51126
1.48786
1.46361
1.44096
1.19182
1.16815
1.14443
0.73189
0.70806
0.70539
0.68309
Integral
1.0000
2.9735
2.0274
1.0079
0.9874
1.0484
1.9635
2.0095
0.9526
4.0952
6.1137
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-336
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 10.51
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

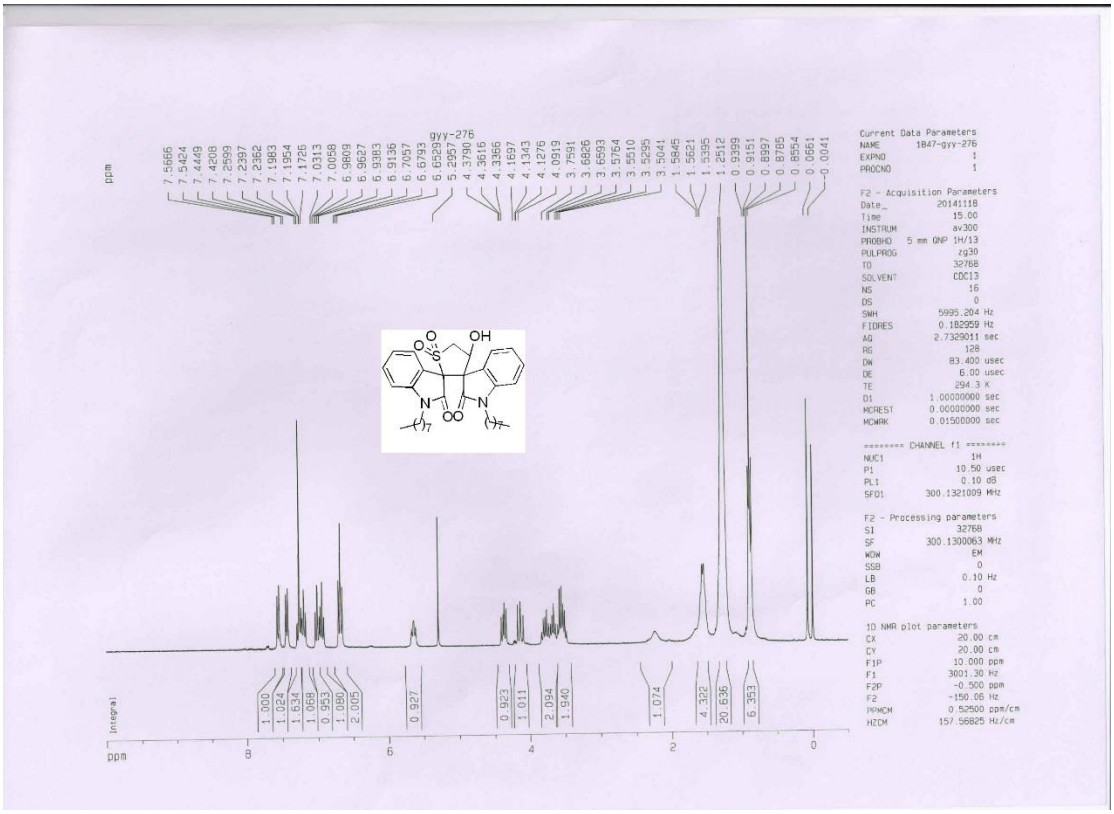

gyy-336
ppm
176.360
171.725
143.285
141.759
129.719
128.974
127.019
126.657
126.021
125.950
125.751
124.702
110.601
109.973
76.192
63.343
58.195
41.377
40.785
40.344
40.076
39.797
39.520
39.242
38.963
38.686
33.416
20.454
20.421
10.899
10.856
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-336
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 11.00
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 162
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.91 dB
SF01 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677846 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.500 ppm
F1 15131.29 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31818 Hz/cm

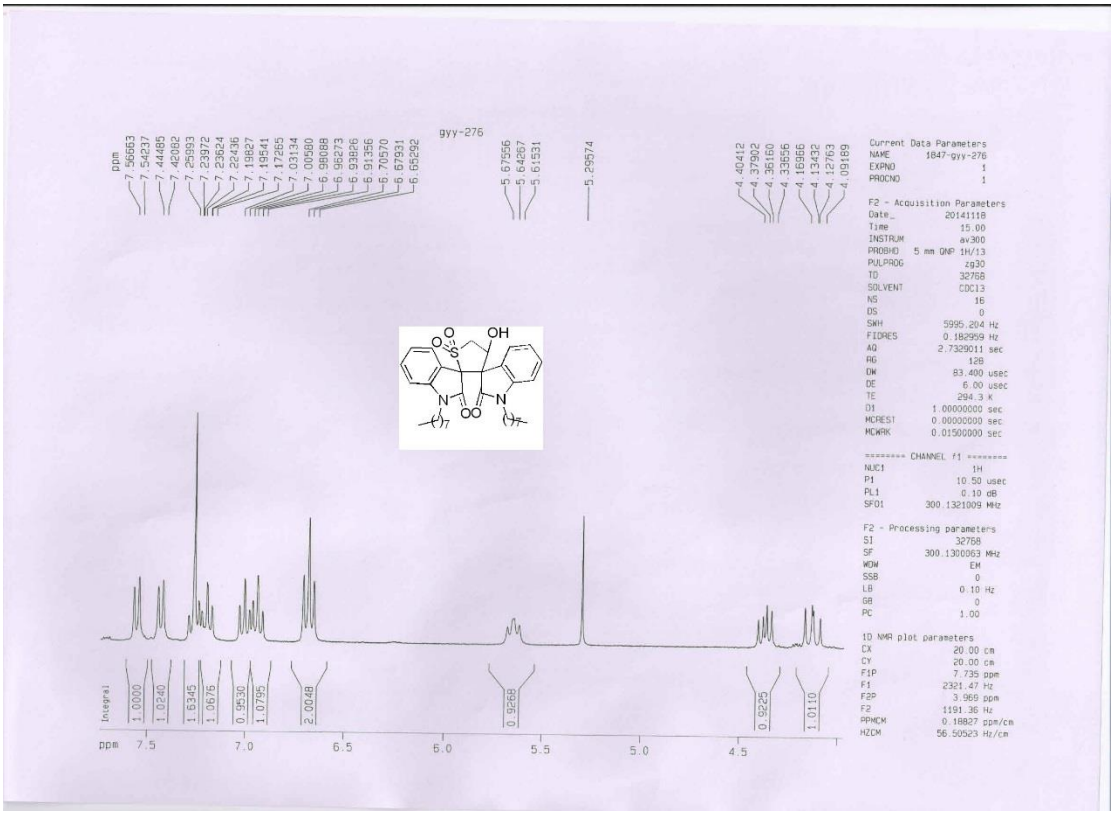

gyy-337
ppm
7.3701
7.3430
7.2628
7.2361
7.0513
7.0315
7.0040
6.9978
5.7652
5.7471
5.5113
5.4893
5.4652
5.4368
3.8007
3.7702
3.7400
3.6232
3.6001
3.5779
3.5406
3.5174
3.4929
3.4720
3.3307
3.2961
3.2677
2.5002
2.0832
2.0814
1.4930
1.4686
1.4447
1.4210
1.2278
0.7796
0.7728
0.7556
0.7487
0.7311
0.7245
Integral
1.0342
1.0209
3.9855
1.0000
0.9796
1.0127
4.0230
0.9816
4.1573
6.1395
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-337
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 11.05
INSTRUM av300
PROBHD 5 mm BNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

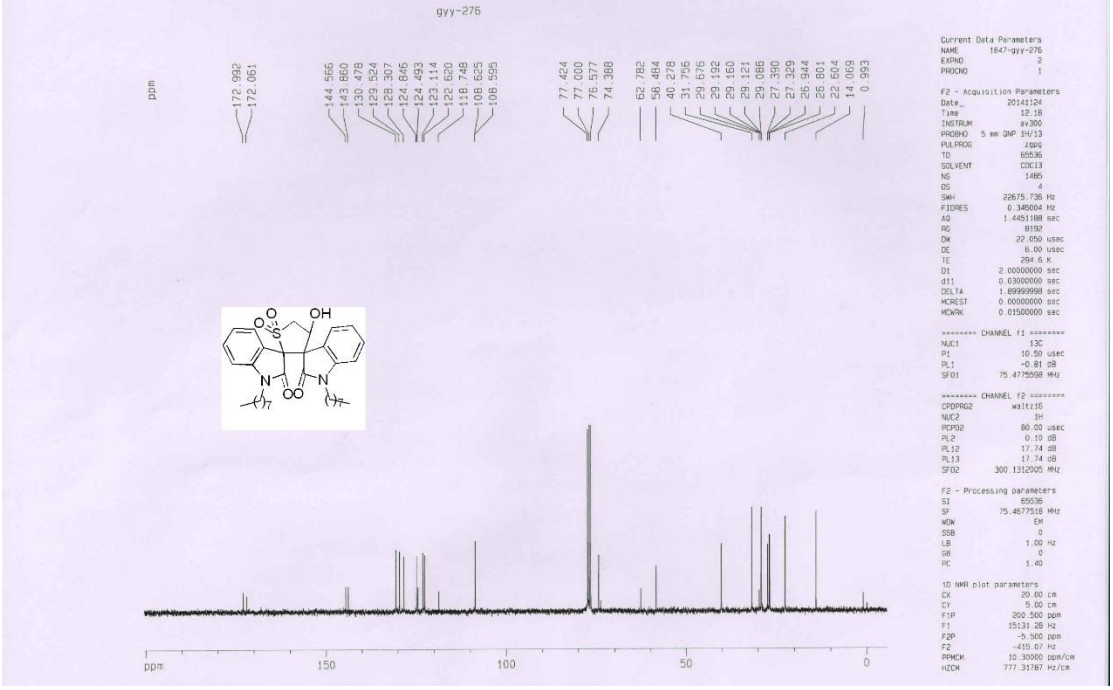

gyy-337
ppm
176.789
172.052
145.828
144.238
134.536
133.922
127.100
125.856
123.840
122.932
122.254
121.524
109.363
108.802
76.016
63.040
58.064
41.288
40.777
40.353
40.077
39.798
39.520
39.242
38.962
38.686
33.432
20.269
20.199
11.050
10.993
ppm
150
100
50
0
Current Data Parameters
NAME 1847-gyy-337
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 11.35
INSTRUM av300
PROBHD 5 mm BNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 328
DS 4
SWH 20575.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SF01 75.4775098 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677845 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.500 ppm
F1 15131.29 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31818 Hz/cm


gyy-262
ppm
7.4309
7.4057
7.2617
7.2595
7.2403
7.2276
7.2237
7.2158
7.2139
7.2019
7.1979
7.1944
7.1823
6.9984
6.9849
6.9724
6.6590
6.6334
4.2428
4.2408
4.1859
4.1842
4.1412
4.1396
4.0846
4.0828
3.1421
3.1405
3.1206
3.1190
1.6173
1.2534
0.0691
0.0675
-0.0021
-0.0042
5
Integral
0.9775
3.4561
2.0555
2.0000
2.0627
6.1041
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-262
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141028
Time 14.39
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SF01 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm


gyy-262
ppm
202.750
176.612
168.923
144.430
143.820
130.433
129.917
126.378
125.211
123.281
123.249
123.153
122.924
108.596
108.269
77.424
77.000
76.577
38.822
29.667
26.412
26.200
0.988
5
ppm
200
150
100
50
0
Current Data Parameters
NAME 1847-gyy-262
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141031
Time 17.25
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SF01 75.4775598 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 220.500 ppm
F1 16640.64 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 11.30000 ppm/cm
HZCM 852.78558 Hz/cm


gyy-276
ppm
7.5666
7.5424
7.4449
7.4208
7.2599
7.2397
7.2362
7.1983
7.1954
7.1726
7.0313
7.0058
6.9809
6.9627
6.9383
6.9136
6.7057
6.6793
6.6529
5.2957
4.3790
4.3616
4.3366
4.1697
4.1343
4.1276
4.0919
3.7591
3.6826
3.6593
3.5764
3.5510
3.5295
3.5041
1.5845
1.5621
1.5395
1.2512
0.9399
0.9151
0.8997
0.8785
0.8554
0.0661
-0.0041
Integral
1.000
1.024
1.634
1.008
0.953
1.090
2.005
0.927
0.923
1.011
2.094
1.940
1.074
4.322
20.636
6.353
ppm
8
6
4
2
0
Current Data Parameters
NAME 1847-gyy-276
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141118
Time 15.00
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm


gyy-276
ppm
7.56663
7.54237
7.44485
7.42082
7.25993
7.23972
7.23624
7.22436
7.19827
7.19541
7.17265
7.03134
7.00580
6.99088
6.96273
6.93826
6.91356
6.70570
6.67931
6.65292
5.67566
5.64267
5.61531
5.29574
4.40412
4.37902
4.36160
4.33556
4.16966
4.13432
4.12763
4.09189
Integral
1.0000
1.0240
1.6345
1.0676
0.9530
1.0795
2.0048
0.9268
0.9225
1.0110
ppm
7.5
7.0
6.5
6.0
5.5
5.0
4.5
Current Data Parameters
NAME 1847-gyy-276
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141118
Time 15.00
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 7.735 ppm
F1 2321.47 Hz
F2P 3.969 ppm
F2 1191.36 Hz
PPMCM 0.18827 ppm/cm
HZCM 56.50523 Hz/cm



Current Data Parameters
NAME 1847-gyy-276
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141124
Time 12.18
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1486
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 294.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -0.81 dB
SFO1 75.4775598 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.10 dB
PL12 17.74 dB
PL13 17.74 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677518 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.500 ppm
F1 15131.28 Hz
F2P -5.500 ppm
F2 -415.07 Hz
PPMCM 10.30000 ppm/cm
HZCM 777.31787 Hz/cm