Supporting Information

Gold-Catalyzed Assembly of Heterobicyclic Systems

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General. Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous dichloromethane (HPLC grade) was purified by distillation over calcium hydride. Anhydrous tetrahydrofuran was freshly distilled from sodium-benzophenone. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography(TLC) using whatman precoated silica gel plates. Flash column chromatography was performed over silacyle silica gel (230-400 mesh). ^1H NMR and ^{13}C NMR spectra were recorded on Bruker DMX-500 spectrometers using residue solvent peaks as an internal standard. Infrared spectra were recorded with a Nicolet FTIR spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with a Varian Saturn 2000 GC-MS using EI method or an Agilent 1100 LCMS using APCI or ES methods.

Preparation of Enynes

Enyne 1. The title compound was prepared by using a procedure modified from that of Kende and co-workers.¹ To a solution of LDA in THF (10 mL), generated by the treatment of diisopropylamine (0.46 mL, 3.3 mmol) with 2.5 M n-BuLi in hexanes (1.32 mL, 3.3 mmol) and cooled in a dry ice-acetone bath, was added a solution of ethyl 2,4-dimethylpent-4-enoate (0.515 g, 3.3 mmol) in THF (2 mL). Upon completion, HMPA (0.574 mL, 3.3 mmol) was added. The enolate solution was stirred at the same temperature for 30 min before a solution of phenyl chloroacetylene (0.41 g, 3 mmol) in THF (2 mL) was added. The reaction was allowed to warm to room temperature overnight and then poured into water and extracted with Et₂O (3 x 20 mL). The combined organic layers were washed with H₂O and brine, dried (MgSO₄), and concentrated. The residue was purified through silica gel flash chromatography to yield the alkynyl ester. At 0°C, to a solution of the alkynyl ester obtained above in THF (30 mL) was added LiAlH₄ (0.152 g, 4 mmol). The reaction mixture was stirred at the same temperature for 2 h and worked up by treating it sequentially with H₂O (0.15 mL), aqueous NaOH (15%, 0.15 mL), and H₂O (0.45 mL) carefully. The resulting mixture was filtered and concentrated. The residue was purified by silica gel flash column chromatography to give enyne **1** in 63% overall yield. ^1H NMR (500 MHz, CDCl₃) δ

¹ Kende, A. S.; Fludzinski, P.; Hill, J. H.; Swenson, W.; Clardy, J. *JACS* **1984**, *106*, 3551-3562

7.41–7.37 (m, 2H), 7.23–7.16 (m, 3H), 4.93 (s, 1H), 4.84 (s, 1H), 3.57 (d, 1H, $J = 10.6$ Hz), 3.53 (d, 1H, $J = 10.6$ Hz), 2.43 (d, 1H, $J = 13.2$ Hz), 2.20 (d, 1H, $J = 13.2$ Hz), 1.97 (s, 3H), 1.29 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 142.5, 131.5, 128.2, 127.9, 123.3, 114.7, 93.7, 83.5, 70.6, 45.8, 37.8, 24.2, 23.6; IR (neat, cm^{-1}) 3362 (br), 3077, 2969, 2929, 1653, 1457; MS (EI) Calculated for $[\text{C}_{15}\text{H}_{18}\text{O}]^+$: 214.14; Found: 214.

Enyne 4. The title compound was obtained in 27% yield from ethyl 2-methyl-4-phenylpent-4-enoate following the same procedure as for enyne **1**. ^1H NMR (500 MHz, CDCl_3) δ 7.45 (d, 2H, $J = 7.1$ Hz), 7.30 (t, 2H, $J = 7.1$ Hz), 7.24–7.19 (m, 4H), 7.15–7.13 (m, 2H), 5.39 (s, 1H), 5.26 (s, 1H), 3.50–3.42 (m, 2H), 2.95 (d, 1H, $J = 13.4$ Hz), 2.72 (d, 1H, $J = 13.4$ Hz), 1.74 (t, 1H, $J = 7.8$ Hz), 1.20 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 145.3, 142.7, 131.6, 128.3, 128.0, 127.8, 127.3, 126.6, 123.1, 117.6, 93.0, 84.2, 70.0, 42.6, 39.0, 23.7; IR (neat, cm^{-1}) 3396 (br), 3080, 3055, 2925, 2852, 1623, 1598, 1491, 1443; MS (APCI) Calculated for $[\text{C}_{20}\text{H}_{21}\text{O}]^+$: 277.16; Found: 277.1.

Enyne 6. The title compound was obtained in 31% yield from methyl 3,5-dimethoxyphenylacetate in three steps through allylation of its enolate (generated by the treatment of LDA) with methallyl bromide followed by the the same procedure as for enyne **1**. ^1H NMR (500 MHz, CDCl_3) δ 7.50–7.47 (m, 2H), 7.34–7.32 (m, 3H), 6.78 (d, 2H, $J = 2.2$ Hz), 6.39 (t, 1H, $J = 2.2$ Hz), 4.82 (s, 1H), 4.75 (s, 1H), 3.84–3.78 (m, 8H), 2.79 (d, 1H, $J = 13.8$ Hz), 2.66 (d, 1H, $J = 13.8$ Hz), 1.91 (t, 1H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 160.7, 143.3, 141.6, 131.6, 128.3, 128.2, 123.1, 115.0, 105.8, 98.5, 91.1, 87.2, 71.1, 55.3, 48.7, 45.5, 24.1; IR (neat, cm^{-1}) 3405 (br), 2936, 1596, 1457; MS (APCI) Calculated for $[\text{C}_{22}\text{H}_{25}\text{O}]^+$: 337.18; Found: 337.1.

Enyne 8. To a solution of 1-trimethylsilylpropyne (2.24 g, 20 mmol) in THF (20 mL) cooled in an ice-water bath was added n-BuLi (2.5 M in hexanes, 8.4 mL, 21 mmol). The reaction mixture was stirred for 1h. Methallyl bromide (2.88 g, 21 mmol) was added dropwise and the reaction was allowed to warm to room temperature and stir for 1h. Then, the reaction mixture was cooled in a dry ice-acetone bath and treated with n-BuLi (2.5 M in hexanes, 8.4 mL, 21 mmol) and TMEDA (9.34 mL, 22 mmol). The resulting mixture was warmed to 0°C slowly in 1h before gaseous formaldehyde (generated by cracking excess paraformaldehyde at 150°C) was bubbled in. The reaction was diluted with H₂O, extracted with Et₂O (3 x 40 mL). The organic layers were combined, washed with H₂O, dried (MgSO₄), and concentrated. The residue was purified by silica gel flash column chromatography to give TMS-protected enyne as a clear liquid.

The TMS-protected enyne was converted into phenyl alkyne using Sonogashira reaction with TBAF as base.² The enyne (0.136 g, 0.7 mmol), phenyl iodide (0.169 g, 0.84 mmol), CuI (0.014 g, 0.07 mmol), and PdCl₂(PPh₃)₂ (0.025 g, 0.035 mmol) were added to THF (5 mL) in a round-bottom flask. The resulting mixture was treated with TBAF (1M in THF, 1.5 mL) and stirred for 2h. The reaction mixture was passed through a short celite pad and the filtrate was concentrated. The residue was purified through silica gel flash column chromatography to furnish enyne **8** (0.55 g; 21% yield from 1-trimethylsilylpropyne). ¹H NMR (500 MHz, CDCl₃) δ 7.41-7.39 (m, 2H), 7.30-7.28 (m, 3H), 4.86 (s, 2H), 3.76-3.71 (m, 1H), 3.69-3.64 (m, 1H), 3.02-2.96 (m, 1H), 2.33 (d, 2H, *J* = 7.4 Hz), 1.91 (br s, 1H), 1.81 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 142.6, 131.7, 128.2, 123.2, 112.8, 89.8, 83.6, 65.2, 39.8, 34.2, 22.4; IR (neat, cm⁻¹) 3364 (br), 3077, 2934, 1652, 1490, 1442; MS (EI) Calculated for [C₁₄H₁₆O]⁺: 200.12; Found: 200.

² Mori, A; Shimada, T; Kondo, T; Sekiguchi, A. *Synlett* **2001**, 649-651

Enyne 10. A solution of alcohol **1** (0.08 g, 0.4 mmol) in CH_2Cl_2 (2 mL) cooled in an ice-water bath was treated with Dess-Martin periodinane (15% solution in CH_2Cl_2 , 1.1 mL, 0.48 mmol). The resulting mixture was warmed to room temperature and stirred for 2h. The reaction mixture was passed through a short silica pad and the residue obtained after concentration was subjected to the next reaction without further purification.

The crude aldehyde was dissolved in THF (3 mL), *o*-Benzyl hydroxylamine hydrogen chloride (0.128 g, 0.8 mmol) and 4 Å molecular sieves (2 g) were added. The mixture was stirred overnight before filtration, concentration, and column purification (hexanes:ethyl acetate = 20:1).

To a solution of the *o*-benzyl oxime obtained above in THF (2 mL) was added LAH (0.046 g, 1.2 mmol). The reaction was stirred for 1h before being quenched with MeOH (1 mL). All solvents were removed under reduced pressure and the residue was partitioned between CHCl_3 (10 mL) and H_2O (10 mL). The organic layer was washed with saturated NH_4Cl and brine, dried (MgSO_4), and concentrated. The residue was dissolved in CH_2Cl_2 (2 mL). Et_3N (0.12 mL, 0.8 mmol) and TsCl (0.096 g, 0.5 mmol) were added. The reaction was stirred for 2h before being evaporated to dryness. The residue was purified through silica gel flash column chromatography to give the sulfonamide **10** (0.027 g, 18% overall yield). ^1H NMR (500 MHz, CDCl_3) δ 7.75 (d, 2H, J = 8.2 Hz), 7.34-7.28 (m, 7H), 4.90 (s, 1H), 4.78 (s, 1H), 4.76 (t, 1H, J = 6.4 Hz), 3.00 (dd, 1H, J = 6.4, 11.7 Hz), 2.93 (dd, 1H, J = 6.4, 11.7 Hz), 2.42 (s, 3H), 2.38 (d, 1H, J = 13.3 Hz), 2.16 (d, 1H, J = 13.3 Hz), 1.89 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 143.4, 141.8, 136.9, 131.5, 129.7, 128.3, 128.2, 127.0, 122.8, 115.4, 92.7, 83.9, 52.7, 46.9, 35.6, 24.7, 24.1, 21.5; IR (neat, cm^{-1}) 3283 (br), 3071, 2970, 2924, 1598, 1443; MS (APCI) Calculated for $[\text{C}_{22}\text{H}_{25}\text{NO}_2\text{S}]^+$: 368.17; Found: 368.1.

Enyne 12. At -78°C , to a solution of 3-methyl-1-triisopropylsilylbutyne ³(0.27 g, 1.2 mmol) in THF (20 mL) was added n-BuLi (2.5 M in hexanes, 0.48 mL) and TMEDA (0.18 mL, 1.2 mmol). The resulting mixture was warmed to 0°C and stirred for 2h before being cooled again to -78°C . 2-(4-bromomethylpent-4-enyloxy)tetrahydropyran ⁴ (0.263 g, 1.0 mmol) was added and the reaction mixture was allowed to warm to room temperature overnight. Silica gel (2 g) was added and the slurry was evaporated to dryness before being loaded onto a pre-packed wet column. Elution with hexanes/ethyl acetate gave the tips-protected enyne.

A mixture of the enyne obtained above, THF (5 mL), and TBAF (1M in THF, 2 mL) was heated at a water bath (bath temperature: 50°C) for 1h. The reaction was cooled to room temperature. Phenyl iodide (0.25 g, 1.2 mmol), CuI (0.023 g, 0.12 mmol), and $\text{PdCl}_2(\text{PPh}_3)_2$ (0.042 g, 0.06 mmol) were added and the reaction was stirred for 2h. The reaction mixture was passed through a short celite pad and the filtrate was concentrated. The residue was dissolved in methanol (5 mL) and TsOH (0.005 g) was added. The reaction was stirred for 2h at room temperature before being quenched with Et_3N (0.05 mL) and concentrated. The residue was purified through silica gel flash column chromatography to yield enyne **12** (0.11 g, 45% overall yield). ^1H NMR (500 MHz, CD_2Cl_2) δ 7.36-7.34 (m, 2H), 7.30-7.26 (m, 3H), 4.93 (s, 1H), 4.89 (s, 1H), 3.59 (q, 2H, $J = 6.0$ Hz), 2.35 (t, 2H, $J = 7.5$ Hz), 2.27 (s, 2H), 1.78-1.71 (m, 2H), 1.30 (s, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ 147.1, 131.6, 128.6, 127.9, 124.4, 113.6, 98.0, 80.9, 62.9, 49.0, 33.5, 31.5, 31.4, 29.9; IR (neat, cm^{-1}) 3334 (br), 3080, 2966, 2926, 2867, 2231, 1640, 1598, 1490, 1443; MS (APCI) Calculated for $[\text{C}_{17}\text{H}_{23}\text{O}]^+$: 243.17; Found: 243.1.

³ it was prepared through the reaction of 3-methylbut-1-ynyl lithium generated from Corey-Fuchs reaction and TIPSOTf

⁴ The allyl bromide was obtained by following to a similar procedure: Hitchcock, S. A.; Houldsworth, S. J.; Pattenden, G.; Pryde, D. C.; Thomson, N. M.; Blake, A. J JCS Perk. 1 **1998**, 3181-3206

Enyne 18. At -78°C , to a solution of 3-methyl-1-triisopropylsilylbutyne³ (0.27 g, 1.2 mmol) in THF (20 mL) was added *n*-BuLi (2.5 M in hexanes, 0.48 mL) and TMEDA (0.18 mL, 1.2 mmol). The resulting mixture was warmed to 0°C and stirred for 2h before being cooled again to -78°C . (5-Bromo-4-methylpent-3-enyloxy)-*tert*-butyldimethylsilane⁵ (0.293 g, 1.0 mmol) was added and the reaction mixture was allowed to warm to room temperature overnight. Silica gel (2 g) was added and the slurry was evaporated to dryness before being loaded onto a pre-packed wet column. Elution with hexanes/ethyl acetate gave the tips-protected enyne.

A mixture of the enyne obtained above, THF (5 mL), and TBAF (1M in THF, 3 mL) was heated at a water bath (bath temperature: 50°C) for 1h. The reaction was cooled to room temperature. Phenyl iodide (0.25 g, 1.2 mmol), CuI (0.023 g, 0.12 mmol), and $\text{PdCl}_2(\text{PPh}_3)_2$ (0.042 g, 0.06 mmol) were added and the reaction was stirred for 2h. The reaction mixture was passed through a short celite pad and the filtrate was concentrated. The residue was purified through silica gel flash column chromatography to yield enyne **18** in 55% overall yield as a mixture of geometric isomers (*E/Z* = 9/1). For the *E*-isomer: ^1H NMR (500 MHz, CDCl_3) δ 7.31-7.28 (m, 2H), 7.21-7.19 (m, 3H), 5.19 (t, 1H, J = 7.2 Hz), 3.56 (t, 2H, J = 6.7 Hz), 2.27 (q, 2H, J = 6.7 Hz), 2.16 (s, 2H), 1.79 (s, 3H), 1.21 (s, 6H); ^{13}C NMR (125 MHz, CDCl_3) *E*-isomer: δ 136.3, 131.3, 128.2, 127.5, 124.4, 123.9, 97.7, 80.9, 62.3, 52.8, 31.68, 31.66, 29.8, 18.3; IR (neat, cm^{-1}) 3337, 3054, 2966, 2922, 2228, 1579, 1490, 1443, 1360; MS (APCI) Calculated for $[\text{C}_{17}\text{H}_{23}\text{O}]^+$: 243.17; Found: 243.1.

Enyne 20. The title compound was obtained in 60% overall yield as the *Z*-isomer only by using the same procedure as for enyne **18**. ^1H NMR (500 MHz, CDCl_3) δ 7.37-7.35 (m, 2H), 7.28-7.22 (m, 3H), 5.31 (t, 1H, J = 7.0 Hz), 3.62 (q, 2H, J = 6.0 Hz), 2.30 (s, 2H), 2.11 (q, 2H, J = 7.2 Hz), 1.94 (s, 3H), 1.60 (p, 2H, J = 6.8 Hz), 1.41 (t, 1H, J = 5.3 Hz), 1.30 (s, 6H); ^{13}C NMR (125 MHz,

⁵ As a mixture of isomers (*E/Z*=9/1).

CDCl₃): δ 133.4, 131.3, 128.11, 128.06, 127.4, 124.0, 98.2, 80.5, 62.6, 44.5, 32.8, 31.8, 30.0, 25.7, 24.9; IR (neat, cm⁻¹) 3339, 2964, 2933, 2867, 1598, 1491, 1443, 1479, 1360; MS (APCI) Calculated for [C₁₈H₂₅O]⁺: 257.19; Found: 257.1.

Enyne 22. The title compound was obtained from enyne **18** in 52% yield by using the same procedure as for enyne **14**. ¹H NMR (500 MHz, CDCl₃) δ 7.70 (d, 2H, *J* = 8.1 Hz), 7.35-7.33 (m, 2H), 7.27-7.25 (m, 5H), 5.07 (t, 1H, *J* = 7.2 Hz), 4.20 (t, 1H, *J* = 6.5 Hz), 2.97 (q, 2H, *J* = 6.5 Hz), 2.41 (s, 3H), 2.21 (dt, 2H, *J* = 6.5, 7.2 Hz), 2.16 (s, 2H), 1.77 (s, 3H), 1.25 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 143.3, 137.0, 136.7, 131.3, 129.6, 128.2, 127.5, 127.0, 124.0, 123.9, 97.6, 81.0, 52.6, 42.8, 31.5, 30.0, 29.7, 28.3, 21.5, 18.2; IR (neat, cm⁻¹) 3290 (br), 2969, 2925, 1684, 1598, 1491, 1442; MS (APCI) Calculated for [C₂₄H₃₀NO₂S]⁺: 396.57; Found: 396.1.

Enyne 24. The title compound was obtained in 45% overall yield as the *E*-isomer only by using the same procedure as for enyne **18**. ¹H NMR (500 MHz, CDCl₃) δ 7.37-7.35 (m, 2H), 7.28-7.24 (m, 3H), 5.25 (t, 1H, *J* = 7.1 Hz), 3.64 (t, 2H, *J* = 6.5 Hz), 2.20 (s, 2H), 2.12 (q, 2H, *J* = 7.1 Hz), 1.83 (s, 3H), 1.63 (p, 2H, *J* = 7.1 Hz), 1.27 (s, 6H); ¹³C NMR (125 MHz, CDCl₃): δ 133.3, 131.3, 128.3, 128.1, 127.3, 124.1, 98.0, 80.7, 62.6, 52.8, 32.6, 31.5, 29.7, 24.4, 18.0; IR (neat, cm⁻¹) 3330, 2965, 2927, 2229, 1598, 1491, 1443, 1380; MS (APCI) Calculated for [C₁₈H₂₅O]⁺: 257.19; Found: 257.1.

Gold-catalyzed Assembly of Heterobicyclic Systems

General Procedure A: To a solution of an alcohol (or sulfonamide **10**) in acetonitrile (0.05 M) at room temperature was added a solution of AuCl₃ in acetonitrile (5 mol%, 7.2 μ M; 10 mol% in the

cases of alcohols **18** and **20**). The reaction mixture was stirred for 1h and then treated with Et₃N (0.05 mL). Concentration and silica gel column chromatography yielded the cyclized product.

General Procedure B: A solution of [Au(PPh₃)]⁺ ClO₄⁻ in CH₂Cl₂ was prepared as following: AuCl(PPh₃) (70 mg, 0.2 mmol) was dissolved in CH₂Cl₂ (10 mL). The solution was treated with AgClO₄ (42 mg, 0.2 mmol) and stirred for 1h. AgCl precipitation formed gradually and the supernatant was used for the following reactions.

A solution of the alcohol in CH₂Cl₂ (0.05 M) at room temperature was treated with the [Au(PPh₃)]⁺ ClO₄⁻ solution (5 mol%) generated previously. The reaction mixture was stirred for 1h and then treated with Et₃N (0.05 mL). Concentration and silica gel column chromatography yielded the cyclized product.

Alkene **2** was obtained in 89% yield according to the general procedure A. ¹H NMR (500 MHz, CDCl₃) δ 7.40 (d, 2H, *J* = 7.6 Hz), 7.31 (t, 2H, *J* = 7.6 Hz), 7.23 (t, 1H, *J* = 7.6 Hz), 6.23 (s, 1H), 3.84 (d, 1H, *J* = 6.8 Hz), 3.64 (d, 1H, *J* = 6.8 Hz), 1.78 (d, 1H, *J* = 10.6 Hz), 1.72 (d, 1H, *J* = 10.6 Hz), 1.48 (s, 3H), 1.27 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 140.1, 135.2, 133.1, 128.2, 127.1, 124.9, 82.3, 81.1, 47.5, 43.6, 42.3, 26.0, 20.2; IR (neat, cm⁻¹) 3348, 3024, 2961, 2925, 2869, 1652, 1456, 1376; MS (EI) Calculated for [C₁₅H₁₉O]⁺: 214.15; Found: 214.

Alkene **5** was obtained in 90% yield according to the general procedure A. ¹H NMR (500 MHz, CDCl₃) δ 7.52 (d, 2H, *J* = 7.5 Hz), 7.43 (d, 2H, *J* = 7.5 Hz), 7.39 (t, 2H, *J* = 7.5 Hz), 7.33-7.28 (m,

3H), 7.25 (t, 1H, $J = 7.5$ Hz), 6.33 (s, 1H), 4.06 (d, 1H, $J = 6.8$ Hz), 3.77 (d, 1H, $J = 6.8$ Hz), 2.92 (d, 1H, $J = 6.8$ Hz), 2.85 (d, 1H, $J = 12.3$ Hz), 2.27 (d, 1H, $J = 10.6$ Hz), 2.04 (d, 1H, $J = 10.6$ Hz), 1.33 (s, 3H); ^{13}C NMR (125 MHz, acetone- d_6) δ 147.2, 141.0, 135.9, 133.9, 129.3, 129.1, 128.1, 127.8, 126.0, 125.8, 85.3, 83.1, 47.9, 45.5, 43.1, 19.9; IR (neat, cm^{-1}) 3057, 3026, 2958, 2925, 2852, 1600, 1495, 1447, 1357; MS (APCI) Calculated for $[\text{C}_{20}\text{H}_{21}\text{O}]^+$: 277.16; Found: 277.1.

Alkene **7** was obtained in 92% yield according to the general procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.41 (d, 2H, $J = 7.8$ Hz), 7.30 (t, 2H, $J = 7.8$ Hz), 7.24 (t, 1H, $J = 7.8$ Hz), 6.453 (s, 2H), 6.448 (s, 1H), 6.40 (s, 1H), 4.27 (d, 1H, $J = 6.7$ Hz), 4.03 (d, 1H, $J = 6.7$ Hz), 3.81 (s, 6H), 2.74 (d, 1H, $J = 17.3$ Hz), 2.66 (d, 1H, $J = 17.3$ Hz), 2.21 (d, 1H, $J = 10.4$ Hz), 2.15 (d, 1H, $J = 10.4$ Hz), 1.56 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 161.0, 145.7, 139.8, 135.1, 133.0, 128.3, 127.3, 125.1, 104.7, 98.2, 80.9, 80.8, 55.3, 51.0, 45.1, 43.5, 229.7, 26.1; IR (neat, cm^{-1}) 2962, 2928, 2855, 1597, 1457, 1424, 1358; MS (APCI) Calculated for $[\text{C}_{22}\text{H}_{25}\text{O}_3]^+$: 337.18; Found: 337.1.

Alkene **9** was obtained in 89% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.39 (d, 2H, $J = 7.8$ Hz), 7.31 (dd, 2H, $J = 7.2, 7.8$ Hz), 6.50 (d, 1H, $J = 6.8$ Hz), 3.96-3.92 (m, 2H), 2.87 (br s, 1H), 2.64-2.56 (m, 2H), 1.86 (d, 1H, $J = 5.5$ Hz), 1.82 (dd, 1H, $J = 3.4, 5.5$ Hz), 1.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 140.2, 135.5, 128.2, 128.1, 127.0, 124.9, 79.9, 76.8, 44.0, 40.3, 37.6, 25.8; IR (neat, cm^{-1}) 3054, 3031, 2965, 2925, 2858, 1598, 1494, 1446, 1376; MS (EI) Calculated for $[\text{C}_{14}\text{H}_{16}\text{O}]^+$: 200.12; Found: 200.

Alkene **11** was obtained in 82% yield according to the general procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.63 (d, 2H, $J = 8.3$ Hz), 7.26-7.20 (m, 3H), 7.14-7.10 (m, 2H), 7.03 (d, 2H, $J = 8.3$ Hz), 5.96 (s, 1H), 3.56 (d, 1H, $J = 8.7$ Hz), 3.25 (d, 1H, $J = 8.7$ Hz), 2.98 (d, 1H, $J = 17.5$ Hz), 2.46 (d, 1H, $J = 17.5$ Hz), 2.25 (s, 3H), 1.84 (d, 1H, $J = 10.7$ Hz), 1.73 (d, 1H, $J = 10.7$ Hz), 1.71 (s, 3H), 1.20 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 142.4, 139.4, 138.6, 135.3, 131.2, 129.2, 128.0, 127.2, 126.9, 124.9, 66.3, 63.7, 50.8, 41.3, 38.6, 29.7, 26.2, 21.3; IR (neat, cm^{-1}) 3026, 2958, 2926, 2871, 1598, 1446, 1337; MS (APCI) Calculated for $[\text{C}_{22}\text{H}_{25}\text{NO}_2\text{S}]^+$: 368.17; Found: 368.1.

Alkene **13** was obtained in 86% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.39 (d, 2H, $J = 8.0$ Hz), 7.31 (dd, 2H, $J = 7.4, 8.0$ Hz), 7.22 (t, 1H, $J = 7.4$ Hz), 5.86 (s, 1H), 3.92-3.82 (m, 2H), 2.48 (s, 2H), 1.98 (p, 2H, $J = 7.3$ Hz), 1.88-1.83 (m, 1H), 1.82 (d, 1H, $J = 13.5$ Hz), 1.78-1.73 (m, 1H), 1.56 (d, 1H, $J = 13.5$ Hz), 1.19 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 142.1, 134.4, 131.8, 128.1, 126.6, 125.3, 81.8, 66.4, 46.0, 38.7, 37.6, 34.1, 31.2, 30.6, 25.5; IR (neat, cm^{-1}) 2951, 1598, 1493, 1358; MS (EI) Calculated for $[\text{C}_{17}\text{H}_{22}\text{O}]^+$: 242.17; Found: 242.

Alkene **15** was obtained in 87% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.77 (d, 2H, $J = 8.1$ Hz), 7.36-7.22 (m, 7H), 5.75 (s, 1H), 3.67-3.63 (m, 1H), 2.77 (d, 1H, $J = 12.9$ Hz), 2.44 (s, 3H), 2.36 (d, 1H, $J = 16.2$ Hz), 2.02-1.98 (m, 1H), 1.86-1.74 (m, 3H), 1.46

(d, 1H, $J = 12.9$ Hz), 1.14 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 142.6, 142.0, 139.2, 133.6, 132.8, 129.4, 128.2, 127.0, 126.8, 125.3, 69.0, 48.9, 45.5, 39.3, 38.4, 34.8, 33.3, 29.4, 23.1, 21.5; IR (neat, cm^{-1}) 2956, 2925, 2867, 1598, 1494, 1446; MS (APCI) Calculated for $[\text{C}_{24}\text{H}_{30}\text{NO}_2\text{S}]^+$: 396.57; Found: 396.1.

Alkene **17** was obtained in 96% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.41 (d, 2H, $J = 7.6$ Hz), 7.31 (t, 2H, $J = 7.6$ Hz), 7.22 (t, 2H, $J = 7.6$ Hz), 5.83 (s, 1H), 3.72-3.64 (m, 2H), 2.59 (d, 1H, $J = 16.9$ Hz), 2.42 (d, 1H, $J = 16.9$ Hz), 2.07 (d, 1H, $J = 14.1$ Hz), 1.71-1.52 (m, 6H), 1.38 (d, 1H, $J = 14.1$ Hz), 1.19 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 142.3, 134.0, 130.8, 128.1, 126.6, 125.4, 72.5, 61.4, 42.5, 38.4, 36.5, 33.2, 31.9, 30.0, 26.0, 19.4; IR (neat, cm^{-1}) 2928, 2860, 1598, 1493, 1443; MS (EI) Calculated for $[\text{C}_{18}\text{H}_{24}\text{O}]^+$: 256.18; Found: 256.

Starting from enyne **18** (E/Z = 9/1), A 9/1 mixture of **19** and its *cis*-fused isomer was formed in a combined yield of 86% according to the general procedure E (10 mol% AuCl_3). The diastereomers were separated using silica gel flash column chromatography.

5,6-*cis* diastereomer: ^1H NMR (500 MHz, CDCl_3) δ 7.37 (d, 2H, $J = 7.5$ Hz), 7.32 (dd, 2H, $J = 7.1$, 7.5 Hz), 7.24 (t, 1H, $J = 7.1$ Hz), 5.82 (s, 1H), 3.88-3.75 (m, 2H), 2.94 (dd, 1H, $J = 4.9$, 7.6 Hz), 2.33-2.26 (m, 1H), 1.87 (d, 1H, $J = 14.0$ Hz), 1.66-1.60 (m, 1H), 1.55 (d, 1H, $J = 14.0$ Hz), 1.35 (s, 3H), 1.17 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 141.8, 135.9, 135.2, 128.3, 126.8, 126.1, 81.6, 65.4, 45.34, 45.32, 32.7, 32.4, 31.6, 29.5, 28.9; IR (neat, cm^{-1}) 3055, 3021, 2953, 2923, 2861, 1598, 1444, 1358; MS (EI) Calculated for $[\text{C}_{17}\text{H}_{22}\text{O}]^+$: 242.17; Found: 242.

19

5,6-*trans* diastereomer **19**: ^1H NMR (500 MHz, CDCl_3) δ 7.33-7.22 (m, 5H), 5.49 (d, 1H, $J = 2.8$ Hz), 4.03-3.97 (m, 2H), 2.80 (ddd, 1H, $J = 2.8$, 7.3, 12.6 Hz), 2.23-2.17 (m, 1H), 1.91 (d, 1H, $J = 12.4$ Hz), 1.77 (d, 1H, $J = 12.4$ Hz), 1.73-1.64 (m, 1H), 1.19 (s, 3H), 1.16 (s, 3H), 1.05 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 141.3, 136.8, 128.1, 126.7, 126.6, 82.8, 66.0, 49.5, 46.9, 35.7, 33.1, 31.1, 27.0, 18.6; IR (neat, cm^{-1}) 3080, 3055, 2957, 2930, 2870, 1599, 1490, 1459, 1371; MS (EI) Calculated for $[\text{C}_{17}\text{H}_{22}\text{O}]^+$: 242.17; Found: 242.

20

21

Alkene **21** was formed in 90% yield according to the general procedure A (10 mol% AuCl_3). ^1H NMR (500 MHz, CDCl_3) δ 7.36-7.24 (m, 5H), 5.54 (s, 1H), 3.76-3.70 (m, 2H), 2.43 (dd, 1H, $J = 4.3$, 10.6 Hz), 2.26 (d, 1H, $J = 13.5$ Hz), 1.77-1.73 (m, 1H), 1.53-1.47 (m, 2H), 1.38 (s, 3H), 1.37-1.32 (m, 1H), 1.31 (d, 1H, $J = 13.5$ Hz), 1.19 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 141.7, 138.2, 128.2, 126.7, 126.3, 73.7, 60.9, 43.0, 40.3, 33.6, 32.9, 30.3, 28.5, 26.7; IR (neat,

cm⁻¹) 3055, 2935, 2860, 1599, 1493, 1468, 1444, 1375; MS (APCI) Calculated for [C₁₈H₂₄O]⁺: 256.18; Found: 256.

Alkene **23** was obtained in 81% yield according to the general procedure B. ¹H NMR (500 MHz, CDCl₃) δ 7.76 (d, 2H, *J* = 8.1 Hz), 7.30-7.26 (m, 3H), 7.22 (t, 1H, *J* = 7.2 Hz), 7.15 (d, 2H, *J* = 7.2 Hz), 5.46 (d, 1H, *J* = 2.6 Hz), 3.48 (t, 1H, *J* = 9.5 Hz), 3.39 (q, 1H, *J* = 8.8 Hz), 2.92 (1H, ddd, *J* = 2.6, 6.4, 13.5 Hz), 2.58 (d, 1H, *J* = 13.2 Hz), 2.42 (s, 3H), 2.10-2.04 (m, 1H), 1.91 (d, 1H, *J* = 13.5 Hz), 1.53-1.43 (m, 1H), 1.17 (s, 3H), 1.12 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 142.89, 140.9, 138.2, 137.3, 135.3, 129.4, 128.1, 127.4, m 127.0, 126.8, 68.0, 49.4, 48.8, 47.2, 35.0, 33.1, 31.0, 24.5, 21.5, 18.7; IR (neat, cm⁻¹) 2924, 1599, 1457, 1334; MS (APCI) Calculated for [C₂₄H₃₀NO₂S]⁺: 396.57; Found: 396.1.

Alkene **25** was formed in 98% yield according to the general procedure A (10 mol% AuCl₃). ¹H NMR (500 MHz, toluene-d₈) δ 7.40 (d, 2H, *J* = 8.3 Hz), 7.18 (d, 2H, *J* = 8.3 Hz), 7.11 (t, 1H, *J* = 8.3 Hz), 5.36 (s, 1H), 3.68-3.63 (m, 1H), 3.59 (dd, 1H, *J* = 5.9, 9.4 Hz), 3.54-3.51 (m, 1H), 2.06 (d, 1H, *J* = 12.7 Hz), 1.54-1.40 (m, 4H), 1.27-1.22 (m, 1H), 1.217 (s, 3H), 1.207 (s, 3H), 1.09 (s, 3H); ¹³C NMR (125 MHz, toluene-d₈) δ 147.9, 139.0, 138.8, 129.4, 127.9, 126.9, 82.9, 68.1, 55.2, 47.4, 42.5, 31.1, 30.2, 27.7, 26.3; IR (neat, cm⁻¹) 3020, 2956, 2925, 2860, 1598, 1462, 1441, 1371; MS (APCI) Calculated for [C₁₈H₂₄O]⁺: 256.18; Found: 256.

Tetrahydrofuran 3. To a NMR tube were added alcohol **1** (7.3 mg, 0.034 mmol), CD₃CN (0.5 mL) and HCl in Et₂O (1M, 17 μ L, 0.017 mmol). The resulting mixture was allow to stand for 2 days until all the starting material was consumed as indicated by ¹H NMR. The reaction mixture was neutralized with Et₃N (50 μ L) and concentrated under vacuum. Silica gel flash column chromatography gave compound **3** in 80% yield. ¹H NMR (500 MHz, CDCl₃) δ 7.40-7.38 (m, 2H), 7.29-7.27 (m, 3H), 4.03 (d, 1H, *J* = 8.5 Hz), 3.70 (d, 1H, *J* = 8.5 Hz), 2.24 (d, 1H, *J* = 12.6 Hz), 1.81 (d, 1H, *J* = 12.6 Hz), 1.45 (s, 3H), 1.39 (s, 3H), 1.33 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 131.5, 128.2, 127.7, 123.6, 95.4, 81.6, 80.7, 78.2, 53.5, 39.4, 29.4, 28.4, 26.5; IR (neat, cm⁻¹) 2970, 2930, 2869, 1599, 1492, 1445, 1366; MS (EI) Calculated for [C₁₅H₁₈O]⁺: 214.14; Found: 214.

Carbonate 26. Its structure was verified by X-Ray analysis, see page S-72. Alkene **25** (15.6 mg, 0.061 mmol) was mixed with pyridine (0.2 mL), H₂O (1.5 mL), ^tBuOH (4 mL) and OsO₄ (2.5 w% in ^tBuOH, 2 mL). The resulting solution was heated to reflux for 24 h before being cooled to room temperature and treated with saturated Na₂SO₃ aqueous solution (5 mL). ^tBuOH was removed under vacuum and the residue was saturated with NaCl and extracted with diethyl ether (3 x 10 mL). The combined organic extracts were dried (MgSO₄) and concentrated. Flash column chromatography yielded the diol as a clear liquid (13 mg).

The diol was then reacted with *p*-nitrophenyl isocyanate (7.5 mg) in refluxing CH₂Cl₂ (2 mL) for 4 h. The solvent was removed after the reaction and the residue was purified through flash column chromatography to yield carbonate **26** as a solid (5.2 mg, 27%). ¹H NMR (500 MHz, CDCl₃) δ

7.61-7.58 (m, 2H), 7.38-7.32 (m, 3H), 5.00 (s, 1H), 3.89 (dd, 1H, $J = 7.0, 15.0$ Hz), 3.51 (dd, 1H, $J = 7.3, 15.0$ Hz), 2.88 (dd, 1H, $J = 6.4, 9.3$ Hz), 2.05 (d, 1H, $J = 14.0$ Hz), 1.79 (d, 1H, $J = 14.0$ Hz), 1.73-1.69 (m, 1H), 1.57-1.53 (m, 1H), 1.45-1.34 (m, 2H), 1.34 (s, 3H), 1.20 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 154.5, 136.0, 128.5, 128.0, 126.6, 102.1, 93.6, 81.8, 67.6, 50.8, 48.9, 40.2, 29.6, 28.2, 27.0, 24.9, 18.6; IR (neat, cm^{-1}) 2962, 2873, 1795, 1446, 1340.

Current Data Parameters
NAME: enyne-PhMeOH
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20040714
Time: 16.47
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zg
TO: 32768
SOLVENT: CDCl3
NS: 8
DS: 0
SWH: 5208.333 Hz
FIDRES: 0.158946 Hz
AQ: 3.145779 sec
RG: 32
DM: 96.000 usec
DE: 4.50 usec
TE: 300.0 K
D1: 2.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.132018 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1300139 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

10 NMR plot parameters
CX: 20.00 cm
F4P: 8.333 ppm
F4: 4187.59 Hz
FZP: 0.630 ppm
F2: 314.93 Hz
PPMCH: 0.36517 ppm/cm
HZCM: 192.63300 Hz/cm

Current Data Parameters
NAME: enyne-PhMe3OH
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20040714
Time: 16.52
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zgpg
TD: 238090
SOLVENT: Acetone
NS: 19
DS: 0
SWH: 39682.539 Hz
FIDRES: 0.166670 Hz
AQ: 2.9599840 sec
RG: 1024
DM: 12.600 USBC
DE: 7.50 USBC
TE: 300.0 K
D1: 4.00000000 sec
d11: 0.03000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.20 usec
PL1: 0.00 dB
SFO1: 125.7738214 MHz

===== CHANNEL f2 =====
CPOPRG2: waltz16
NUC2: 1H
PCPD2: 50.00 usec
PL2: 120.00 dB
PL12: 19.00 dB
SFO2: 500.138000 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577982 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 20.00 cm
F1P: 157.065 ppm
F1: 21009.74 Hz
F2P: 12.275 ppm
F2: 1543.66 Hz
PPMCH: 7.73951 ppm/cm
HZCM: 973.30365 Hz/cm

Current Data Parameters
NAME: enyne-Ph-2-OH
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20041021
Time: 15.35
INSTRUM: spect
PROBHD: 5 mm BNP 1H
PULPROG: zg
TD: 32768
SOLVENT: CDCl3
NS: 8
DS: 0
SWH: 5208.333 Hz
FIDRES: 0.158946 Hz
AQ: 3.1457779 sec
RG: 64
DM: 96.000 usec
DE: 4.50 usec
TE: 300.0 K
D1: 2.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.132018 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1300189 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CTP: 8.552 ppm
F1: 4278.94 Hz
F2P: -0.763 ppm
F2: -381.38 Hz
PPMCM: 0.46571 ppm/cm
HZCM: 232.91570 Hz/cm

Current Data Parameters
 NAME: enyne-Ph-OH
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20041021
 Time: 16.40
 INSTRUM: spect
 PULPROG: zgpg
 PULPROG: zgpg
 ID: 238090
 SOLVENT: Aceton
 NS: 38
 DS: 0
 SM: 39982.539 Hz
 FIDRES: 0.166670 Hz
 AQ: 2.9999840 sec
 RG: 1024
 DW: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.00000000 sec
 d11: 0.03000000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SF01: 125.7730214 MHz

===== CHANNEL f2 =====
 CPOPRG2: waltz16
 NUC2: 1H
 PCPO2: 50.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SF02: 500.1360000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577958 MHz
 WDM: EN
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 165.961000 MHz
 F1: 20995.65 Hz
 F2P: 14.078000 MHz
 F2: 1770.44 Hz
 PPMCH: 7.54414 ppm/cm
 HZCH: 961.31067 Hz/cm

Current Data Parameters
NAME enyne-OMe-OMe
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041020
Time 14.22
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 128
DM 56.000 USFC
DE 4.50 USFC
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 USFC
PL4 0.00 dB
SFO1 500.1320118 MHz

F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3D NMR plot parameters
CX 20.00 cm
FLP 8.094 ppm
F1 4046.31 Hz
F2P -0.303 ppm
F2 -151.45 Hz
PPMCM 0.41967 ppm/cm
HZCM 209.88805 Hz/cm

Current Data Parameters
NAME: enyne-07-4602P
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20041020
Time: 14.26
INSTRUM: spect
PROBHD: 5 mm BNP 1H
PULPROG: zgpg
TD: 26850
SOLVENT: Aceton
NS: 77
DS: 0
SWH: 30632.539 Hz
FIDRES: 0.165670 Hz
AQ: 2.9599840 sec
RG: 2048
DM: 12.600 USRC
DE: 7.50 USRC
TE: 300.0 K
D1: 4.00000000 sec
d11: 0.03000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.20 usec
PL1: 0.00 dB
SFO1: 125.770214 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 90.00 usec
PL2: 120.00 dB
PL12: 19.00 dB
SFO2: 500.132800 MHz

F2 - Processing parameters
SI: 32768
SF: 125.757394 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 20.00 cm
F1P: 191.253 00a
F1: 24051.57 Hz
F2P: 16.996 00a
F2: 2137.34 Hz
PPMCH: 8.71288 ppm/cm
HZCH: 1035.7151 Hz/cm

Current Data Parameters
NAME: enyne-PhMe-OH
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20041028
Time: 15.35
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zg
TO: 32768
SOLVENT: CDCl3
NS: 8
DS: 0
SWH: 5208.332 Hz
FIDRES: 0.199946 Hz
AQ: 3.165779 sec
RG: 128
DM: 96.000 usec
DE: 4.50 usec
TE: 300.0 K
D1: 2.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.1320118 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1301139 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
F1P: 8.217 ppm
F1: 4109.66 Hz
F2P: -0.274 ppm
F2: -136.96 Hz
PRGM: 0.46493 ppm/cm
HZCM: 212.35081 Hz/cm

Current Data Parameters
NAME: enyne-PhMe-OH
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20041028
Time: 15.39
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zgpg
TO: 238050
SOLVENT: Aceton
NS: 28
DS: 0
SWH: 39582.539 Hz
FIDRES: 0.16670 Hz
AQ: 2.9959840 sec
RG: 1024
DM: 12.600 usec
DE: 7.50 usec
TE: 300.0 K
D1: 4.00000000 sec
d11: 0.03000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.20 usec
PL1: 0.00 dB
SFO1: 125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 50.00 usec
PL2: 120.00 dB
PL12: 19.00 dB
SFO2: 500.1380000 MHz

F2 - Processing parameters
SI: 32768
SF: 125.757946 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

10 NMR plot parameters
CX: 20.00 cm
F1P: 169.561 ppm
F1: 21322.35 Hz
F2P: 8.443 ppm
F2: 1061.74 Hz
PPHMM: 8.05541 ppm/cm
HZCM: 1013.03046 Hz/cm

S-26

Current Data Parameters
 NAME: enyn-N1S
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20041018
 Time: 13.37
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H
 PULPROG: zgpg
 ID: 238090
 SOLVENT: Aceton
 NS: 114
 DS: 0
 SMA: 39982.539 Hz
 FIDRES: 0.165670 Hz
 AQ: 2.9999840 sec
 RG: 512
 DW: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.00000000 sec
 d11: 0.03000000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SFO1: 125.7736214 MHz

===== CHANNEL f2 =====
 CPOPRG2: waltz16
 NUC2: 1H
 PCPD2: 50.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SFO2: 500.1360000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.757946 MHz
 NQW: EN
 SSF: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 164.435 ppm
 F1: 20678.95 Hz
 F2P: 13.001 ppm
 F2: 1634.97 Hz
 PPMCN: 7.57169 ppm/cm
 HZCN: 952.19973 Hz/cm

Current Data Parameters
 NAME: enyn-pmk2-3
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20041217
 Time: 14.03
 INSTRUM: spect
 PROBD: 5 mm QNP 1H
 PULPROG: zg
 TO: 32768
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SWH: 10000.000 Hz
 FIDRES: 0.306178 Hz
 AQ: 1.6384600 sec
 RG: 256
 DM: 50.000 usec
 DE: 4.50 usec
 TE: 300.0 K
 D1: 2.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.00 usec
 PL1: 0.00 dB
 SFO1: 500.130018 MHz

F2 - Processing parameters
 SI: 16384
 SF: 500.1300213 MHz
 WDW: EM
 SSF: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 20.00 cm
 F1P: 8.028 ppm
 F1: 4014.84 Hz
 F2P: -0.182 ppm
 F2: -90.88 Hz
 FPMCM: 0.41047 ppm/cm
 HZCM: 205.28592 Hz/cm

Current Data Parameters
 NAME: enm-ph2-3
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20041217
 Time: 14.08
 INSTRUM: spect
 PULPROG: zgpg
 PULPROG: zgpg
 TO: 230000
 SOLVENT: Aceton
 NS: 258
 DS: 0
 SM: 39882.539 Hz
 FIDRES: 0.166670 Hz
 AQ: 2.9999840 sec
 RG: 512
 DW: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.00000000 sec
 d11: 0.03000000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SFO1: 125.773214 MHz

===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SFO2: 500.138000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.757452 MHz
 NQ: EN
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

10 NMR plot parameters
 CX: 20.00 cm
 FIP: 159.251 ppm
 F1: 20027.04 Hz
 F2P: 15.475 ppm
 F2: 156.06 Hz
 PPM01: 7.18981 ppm/cm
 MZ01: 504.04501 Hz/cm

Current Data Parameters
 NAME AU-NH-55-splro
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050329
 Time 15.02
 INSTRUM spect
 PULPROG 5 mm QNP 1H
 TD 29
 SOLVENT DMSO
 NS 8
 DS 0
 SMH 7002.801 Hz
 FIDRES 0.336156 Hz
 AQ 1.4874548 sec
 RG 128
 CW 71.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.130008 MHz

F2 - Processing Parameters
 SI 16384
 SF 500.1300135 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 MHz plot parameters
 CK 20.00 cm
 F1P 6.373 DPM
 F1 4187.62 Hz
 F2P 0.659 DPM
 F2 329.56 Hz
 PPMCK 0.38571 DPM/cm
 HZCK 192.90298 Hz/cm

Current Data Parameters
 NAME: Au-MH-56-spr
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050329
 Time: 15:08
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H
 PULPROG: zgpg
 TO: 230090
 SOLVENT: Aceton
 NS: 39
 DS: 0
 SWH: 39682.539 Hz
 FIDRES: 0.155570 Hz
 AQ: 2.9939840 sec
 RG: 1024
 DW: 12.500 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.00000000 sec
 d11: 0.03000000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SFO1: 125.7736214 MHz

===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 PCPD2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SFO2: 500.1338000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577958 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 160.522 ppm
 F1: 20237.21 Hz
 F2P: 8.160 ppm
 F2: 1026.16 Hz
 FREQM: 7.63811 ppm/cm
 HZCM: 960.55212 Hz/cm

2.0000000 sec

Current Data Parameters
 NAME: eny-fine2-4
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20041220
 Time: 12.13
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: Acetone
 NS: 22
 DS: 0
 SM: 39992.539 Hz
 FIDRES: 0.166670 Hz
 AQ: 2.9999840 sec
 RG: 8192
 DW: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.0000000 sec
 d11: 0.0300000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SFO1: 125.7735214 MHz

===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SFO2: 500.138000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577954 MHz
 WDW: EM
 SSF: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

10 NMR plot parameters
 CX: 20.00 cm
 F1P: 159.856 ppm
 F1: 20.003.18 Hz
 F2P: 45.043 ppm
 F2: 1591.81 Hz
 PPMCM: 7.24065 ppm/cm
 HZCM: 910.56660 Hz/cm

Current Data Parameters
 NAME: eny-PhMe3-66
 EXPRNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050120
 Time: 22.59
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H
 PULPROG: zg
 TD: 32768
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SWH: 8012.820 Hz
 FIDRES: 0.24632 Hz
 AQ: 2.0447731 sec
 RG: 64
 DM: 62.400 uSec
 DE: 4.50 uSec
 TE: 300.0 K
 D1: 2.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.00 uSec
 PL1: 0.00 dB
 SFO1: 500.1320118 MHz

F2 - Processing parameters
 SI: 16384
 SF: 500.1300511 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 8.193 pps
 F1: 4097.70 Hz
 F2P: -0.212 pps
 F2: -105.18 Hz
 PHA0: 0.42026 pps/cm
 HZCM: 210.15391 Hz/cm

Current Data Parameters
 NAME: ethyl-1163-66
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20050120
 Time: 23.11
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H
 PULPROG: zgpg30
 TD: 32768
 SOLVENT: Acetone
 NS: 96
 DS: 0
 SWH: 39692.539 Hz
 FIDRES: 0.165670 Hz
 AQ: 2.9999840 sec
 RG: 4096
 CW: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.0000000 sec
 d11: 0.0300000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SF01: 125.7736214 MHz

===== CHANNEL f2 =====
 GPCPRG2: waltz16
 NUC2: 1H
 PCPD2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SF02: 500.136000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577359 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR Plot Parameters
 CX: 20.00 cm
 F1P: 156.775 ppm
 F1: 19715.64 Hz
 F2P: 6.432 ppm
 F2: 808.65 Hz
 PPBCH: 7.5175 ppm/cm
 HZCM: 945.33978 Hz/cm

Current Data Parameters
 NAME: enjre-M3-56
 EXPNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050121
 Time: 19.37
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H
 PULPROG: zg
 TO: 20832
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SM: 5208.333 Hz
 FIDRES: 0.250016 Hz
 AQ: 1.5995220 sec
 RG: 64
 DM: 95.000 USAC
 DE: 4.50 USAC
 TE: 300.0 K
 D1: 2.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.00 USAC
 PL1: 0.00 dB
 SFO1: 500.1320118 MHz

F2 - Processing parameters
 SI: 16384
 SF: 500.1300142 MHz
 MDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 7.678 GDM
 F1: 3940.05 Hz
 F2P: 0.464 GDM
 F2: 232.03 Hz
 PPM0H: 0.37070 ppm/cm
 HZCM: 185.40068 Hz/cm

Current Data Parameters
 NAME: enyne-Me3-56
 EXPNO: 4
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050121
 Time: 19.46
 INSTRUM: spect
 PROBRD: 5 mm BBO 1H
 PULPROG: zgpg30
 TD: 288096
 SOLVENT: Acetone
 NS: 42
 DS: 0
 SWH: 39682.539 Hz
 FIDRES: 0.166770 Hz
 AQ: 2.9999840 sec
 RG: 4096
 DW: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.0000000 sec
 d11: 0.0300000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SF01: 125.7736214 MHz

===== CHANNEL f2 =====
 CPOPRG2: waltz16
 NUC2: 1H
 P2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SF02: 500.1360000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577958 MHz
 NCM: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CY: 20.00 cm
 F1P: 154.355 ppm
 F1: 19411.39 Hz
 F2P: 5.049 ppm
 F2: 634.99 Hz
 PPMCM: 7.46530 ppm/cm
 HZCM: 538.82019 Hz/cm

Current Data Parameters
NAME: enyne-2-56
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20050209
Time: 16.33
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zg
TD: 32768
SOLVENT: CDCl3
NS: 8
DS: 0
SWH: 5208.333 Hz
FIDRES: 0.158946 Hz
AQ: 3.1457779 sec
RG: 32
DM: 96.000 usec
DE: 4.50 usec
TE: 300.0 K
D1: 2.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.1320118 MHz

F2 - Processing parameters
SI: 16384
SF: 500.130181 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

10 NMR plot parameters
CX: 20.00 cm
F1P: 7.836 ppm
F1: 3919.04 Hz
F2P: 0.000 ppm
F2: -0.04 Hz
PPMCH: 0.39181 ppm/cm
HZCH: 195.85427 Hz/cm

Current Data Parameters
 NAME: enyne-Z-66
 EXNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050209
 Time: 16:38
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H
 PULPROG: zgpg
 TO: 236090
 SOLVENT: CDCl3
 NS: 33
 DS: 0
 SWH: 39682.539 Hz
 FIDRES: 0.166670 Hz
 AQ: 2.9999840 sec
 RG: 1024
 DM: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 U1: 4.00000000 sec
 U11: 0.03000000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SFO1: 125.7735214 MHz

===== CHANNEL f2 =====
 CPDPRG2: mltzt16
 NUC2: 1H
 PCPD2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SFO2: 500.1338000 MHz

F2 - Processing parameters
 S1: 32768
 SF: 125.7577982 MHz
 KW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 155.027 DPM
 F1: 19495.89 Hz
 F2P: 2.956 DPM
 F2: 371.78 Hz
 PPMCM: 7.60355 DPM/cm
 HZCM: 956.20581 Hz/cm

Current Data Parameters
NAME Au-NH-56-Fuse
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050329
Time 18.35
INSTRUM spect
PROBHD 5 mm QNP 3H
PULPROG zg
TD 26832
SOLVENT CDCl3
NS 8
DS 0
SWH 7002.801 Hz
FIDRES 0.336156 Hz
AQ 1.4874548 sec
RG 128
DM 71.400 usec
DE 4.50 usec
TE 300.0 K
D1 2.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 500.1300008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CY 20.00 cm
FIP 8.618 ppm
F1 4309.92 Hz
F2P -0.170 ppm
F2 -85.05 Hz
PPMCM 0.43938 ppm/cm
HZCM 219.74835 Hz/cm

Current Data Parameters

NAME	VALUE
NAME	AU-NH-56-fuse
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Time	Value
Date_	20050329
Time	18.40
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zgpg
TD	238000
SOLVENT	CDCl3
NS	73
DS	0
SMH	39682.539 Hz
FTIDEC	0.166670 Hz
AQ	2.9999640 sec
RG	2048
DM	12.600 usec
DE	7.50 usec
TE	300.0 K
D1	4.00000000 sec
cl1	0.03000000 sec

===== CHANNEL f1 =====

NUC1	13C
P1	8.20 usec
PL1	0.00 dB
SFO1	125.7736214 MHz

===== CHANNEL f2 =====

CPDPRG2	NAME	VALUE
NUC2	1H	
PCPD2	90.00 usec	
PL2	120.00 dB	
PL12	19.00 dB	
SFO2	500.1338000 MHz	

F2 - Processing parameters

SI	Value
SF	125.7577946 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

Parameter	Value
CX	20.00 cm
F1P	157.072 ppm
F1	19753.05 Hz
F2P	8.112 ppm
F2	1020.11 Hz
PRACH	7.44802 ppm/cm
HZCM	936.64657 Hz/cm

Current Data Parameters
NAME: enyne-PhMeOme
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20040715
Time: 15.07
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zg
TD: 32768
SOLVENT: CDCl3
NS: 8
DS: 0
SWH: 5208.333 Hz
FIDRES: 0.158946 Hz
AQ: 3.1457779 sec
RG: 128
DM: 96.000 usec
DE: 4.50 usec
TE: 300.0 K
D1: 2.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.130018 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1300182 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
F1P: 8.552 DPM
F1: 4276.94 Hz
F2P: 0.763 DPM
F2: -381.38 Hz
PPHOM: 0.46571 DPM/cm
HZCM: 232.91570 HZ/cm

Current Data Parameters
NAME: enyne-PhMeDme
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20040715
Time: 15.11
INSTRUM: spect
PROBHD: 5 mm QNP 3H
PULPROG: zgpg
TO: 23000
SOLVENT: Aceton
NS: 30
DS: 0
SWH: 36982.539 Hz
FIDRES: 0.16670 Hz
AQ: 2.9999640 sec
RG: 2048
DM: 12.600 usec
DE: 7.50 usec
TE: 300.0 K
D1: 4.00000000 sec
d11: 0.03000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.20 usec
PL1: 0.00 dB
SFO1: 125.7736214 MHz

===== CHANNEL f2 =====
GPRPG2: waltz16
NUC2: 1H
PCPD2: 90.00 usec
PL2: 120.00 dB
PL12: 19.00 dB
SFO2: 500.1338000 MHz

F2 - Processing parameters
SI: 32768
SF: 125.757946 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 20.00 cm
F1P: 154.809 ppm
F1: 19468.44 Hz
F2P: 8.794 ppm
F2: 1105.89 Hz
PNUC1: 7.30076 ppm/cm
HZCN: 918.12775 Hz/cm

Current Data Parameters
NAME Au-enrjdh-ph2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041022
Time 23.35
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TO 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5208.323 Hz
FIDRES 0.158946 Hz
AQ 3.145779 sec
RG 64
GB 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 500.1320118 MHz

F2 - Processing parameters
SI 16384
SF 500.1300159 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FIP 7.922 DPM
FI 3962.27 Hz
FZP -0.136 DPM
F2 -68.06 Hz
PPMCH 0.40253 DPM/cm
HZCH 201.51643 Hz/cm

Current Data Parameters

NAME	Value
NAME	Au-enyph-Ph2
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20041025	10.46

INSTRUM spect

PROBHD 5 mm QNP 1H

PULPROG zgpg

TO 230090

SOLVENT Aceton

NS 42

DS 0

SWH 39682.539 Hz

FIDRES 0.166670 Hz

AQ 2.999840 sec

RG 1024

DM 12.600 usec

DE 7.50 usec

TE 300.0 K

D1 4.00000000 sec

d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1	13C
P1	8.20 usec
PL1	0.00 dB
SFO1	125.776214 MHz

===== CHANNEL f2 =====

CPDPRG2	WALTZ16
NUC2	1H
PCPD2	90.00 usec
PL2	120.00 dB
PL12	19.00 dB
SFO2	500.1338000 MHz

F2 - Processing parameters

SI	32768
SF	125.7515739 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CX	20.00 cm
F1P	160.129 ppm
F1	20137.43 Hz
F2P	-6.283 ppm
F2	-790.12 Hz
PPMCM	8.3059 ppm/cm
HZCM	1046.3755 Hz/cm

Current Data Parameters
 NAME Au-enyem-Me02
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041031
 Time 11.26
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.156946 Hz
 AQ 3.1457779 sec
 RG 64
 DB 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 500.1320148 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1320142 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.084 DPM
 F1 404.3 05 Hz
 F2P -0.163 DPM
 F2 -81.40 Hz
 FPMCM 0.41234 DPM/cm
 HZCM 206.22261 Hz/cm

Current Data Parameters
 NAME Au-enver-Me02
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041031
 Time 11.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TO 230050
 SOLVENT Aceton
 NS 39
 DS 0
 SM 39682.539 Hz
 FIDRES 0.166370 Hz
 AQ 2.9959640 sec
 RG 1024
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7738214 MHz

===== CHANNEL f2 =====
 GPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PLP2 19.00 dB
 SFO2 500.1338000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577958 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR p10t parameters
 CX 20.00 cm
 F1P 184.283 ppm
 F1 23175.05 Hz
 F2P 12.645 ppm
 F2 1590.22 Hz
 PPMCH 8.58191 ppm/cm
 HZCH 1079.24146 Hz/cm

Current Data Parameters
 NAME Au-enV-Me-Ph
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041102
 Time 12.23
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.159346 Hz
 AQ 3.1457779 sec
 RG 64
 DB 0
 DE 95.000 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1301139 MHz
 WDW EN
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

3D NMR plot parameters
 CX 20.00 cm
 F1P 8.220 ppm
 F1 410.87 Hz
 F2P -19.29 ppm
 F2 0.41291 ppm/cm
 FPMCM 206.50784 Hz/cm

Current Data Parameters

NAME	Value
NAME	4-methyl-4-phenyl-2,3-dihydro-2H-pyran
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	SOLVENT	NS	DS	SWH	FIDRES	RG	OR	DE	TE	D1
20041102	12:28	5 mm QNP 3H	zgpg	Aceton	38	0	3968.539 Hz	0.16670 Hz	2.9999840 sec	512	12.600 usec	7.50 usec	300.0 K	0.03000000 sec

===== CHANNEL f1 =====

NUC1	P1	PL1	SFO1
13C	8.20 usec	0.00 dB	125.7736214 MHz

===== CHANNEL f2 =====

CPDPRG2	NUC2	PCPD2	PL2	SFO2
zgpg	1H	90.00 usec	120.00 dB	500.136000 MHz

F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
32768	125.7577958 MHz	EM	0	1.00 Hz	0	1.40

10 NMR data parameters

CK	F1P	F2P	PPMCM	HZCM
20.00 cm	157.256 ppm	19776.21 Hz	11.943 ppm	7.26566 ppm/cm
				913.71369 Hz/cm

Current Data Parameters

NAME: Au-ene-N1s

EXPNO: 1

PROCNO: 1

F2 - Acquisition Parameters

Date_: 20041018

Time: 15.34

INSTRUM: spect

PROBHD: 5 mm QNP 1H

PULPROG: zg

TD: 32768

SOLVENT: CDCl3

NS: 8

DS: 0

SWH: 5208.333 Hz

FIDRES: 0.158946 Hz

AQ: 3.1457779 sec

RG: 128

DM: 95.000 usec

DE: 4.50 usec

TE: 300.0 K

D1: 2.00000000 sec

===== CHANNEL f1 =====

NUC1: 1H

P1: 10.00 usec

PL1: 0.00 dB

SFO1: 500.1320148 MHz

F2 - Processing parameters

SI: 16384

SF: 500.130039 MHz

WDW: EM

SSB: 0

LB: 0.30 Hz

GB: 0

PC: 1.00

1D NMR plot parameters

CX: 20.00 cm

F1P: 8.562 ppm

F1: 4276.94 Hz

F2P: -0.763 ppm

F2: -881.38 Hz

PCPCH: 0.46571 ppm/cm

HZCM: 232.91570 Hz/cm

Current Data Parameters

NAME	Ac-enyne-N1S
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20041018
Time	15.41
INSTRUM	spect
PROBHD	5 mm DNP 1H
PULPROG	zgpg
TO	238090
SOLVENT	Aceton
NS	52
DS	0
SWH	39682.539 Hz
FIDRES	0.166670 Hz
AQ	2.9595940 sec
RG	512
DM	12.600 usec
DE	7.50 usec
TE	300.0 K
D1	4.00000000 sec
d11	0.03000000 sec

===== CHANNEL f1 =====

NUC1	13C
P1	8.20 usec
PL1	0.00 dB
SFO1	125.7736214 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2 <td>1H</td>	1H
PCPD2 <td>90.00 usec</td>	90.00 usec
PL2	120.00 dB
PL12	19.00 dB
SFO2	500.136000 MHz

F2 - Processing parameters

SI	32768
SF	125.7577946 MHz
WDM	EN
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR Plot parameters

CK	20.00 cm
F1P	150.327 ppm
F1	18904.79 Hz
F2P	13.276 ppm
F2	1669.51 Hz
PPMCM	5.85257 use/cm
HZCM	861.76416 Hz/cm

Current Data Parameters
NAME Spino-56-Me2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041221
Time 17.17
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TO 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5208.333 Hz
FIDRES 0.138946 Hz
AQ 3.145779 sec
RG 64
DM 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 500.1320118 MHz

F2 - Processing parameters
SI 16384
SF 500.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FLP 7.798 ppm
F1 3800.11 Hz
F2P 0.544 ppm
F2 271.96 Hz
PPM0M 0.36272 ppm/cm
HZCM 181.40744 Hz/cm

Current Data Parameters

NAME	Spiro-56-Me2
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20041221
Time	17:22
INSTRUM	spect
PROBHD	5 mm QNP 3H
PULPROG	zgpg
TD	238090
SOLVENT	Aceton
NS	34
DS	0
SWH	36882.539 Hz
FIDRES	0.166370 Hz
AQ	2.8999840 sec
RG	1024
OW	12.600 usec
DE	7.50 usec
TE	300.0 K
D1	4.00000000 sec
d11	0.03000000 sec

===== CHANNEL f1 =====

NUC1	13C
P1	8.20 usec
PL1	0.00 dB
SFO1	125.7735214 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	120.00 dB
PL12	19.00 dB
SFO2	500.1339900 MHz

F2 - Processing parameters

SI	32768
SF	125.7577970 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CX	20.00 cm
FAP	157.456 ppm
F1	19801.35 Hz
FAP	17.482 ppm
F2	2198.47 Hz
PPMCH	5.98872 ppm/cm
HZCH	880.14398 Hz/cm

Current Data Parameters
 NAME: AUC-56-spr
 EXPNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050330
 Time: 13:52
 INSTRUM: spect
 PROBNM: 5 mm QNP 1H
 PULPROG: zg
 TD: 20832
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SWH: 7002.801 Hz
 FIDRES: 0.336156 Hz
 AQ: 1.4874548 sec
 RG: 128
 DW: 71.400 usec
 DE: 4.50 usec
 TE: 300.0 K
 D1: 2.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.00 usec
 PL1: 0.00 dB
 SF01: 500.1350008 MHz

F2 - Processing parameters
 SI: 16384
 SF: 500.1300135 MHz
 NCH: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 20.00 cm
 CY: 8.373 ppm
 F1P: 4187.62 Hz
 F2P: 0.628 ppm
 F2: 314.22 Hz
 PPMCH: 0.38724 ppm/cm
 HZCH: 159.67000 Hz/cm

Current Data Parameters
NAME AUNC-5b-5p1r
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050320
Time 13.58
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 238090
SOLVENT Aceton
NS 47
DS 0
SMH 39682.539 Hz
FIDRES 0.166570 Hz
AQ 2.9999840 sec
RG 2048
DM 12.600 uSFC
DE 7.50 uSFC
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.20 uSFC
PL1 0.00 dB
SF01 125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 50.00 uSFC
PL2 120.00 dB
PL12 19.00 dB
SF02 500.1360000 MHz

F2 - Processing parameters
SI 32768
SF 125.7577946 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 152.291 ppm
F1 19151.82 Hz
F2P 14.045 ppm
F2 1756.26 Hz
PPMCH 6.91232 ppm/cm
HZCM 869.27735 Hz/cm

Current Data Parameters

NAME	Soliro-55-Me2
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20041221
Time	17.33
INSTRUM	5 mm GNP 1H
PROBHD	zgpg
PULPROG	zgpg
TD	238090
SOLVENT	Aceton
NS	31
DS	0
SWH	39682.539 Hz
FIDRES	0.168670 Hz
AQ	2.999840 sec
RG	1024
DM	12.600 usec
DE	7.50 usec
TE	300.0 K
D1	4.00000000 sec
d11	0.03000000 sec

===== CHANNEL f1 =====

NUC1	13C
P1	8.20 usec
PL1	0.00 dB
SFO1	125.7736214 MHz

===== CHANNEL f2 =====

CPDPRG2	WALTZ16
NUC2	1H
POPD2	90.00 usec
PL2	120.00 dB
PL12	19.00 dB
SFO2	500.1338000 MHz

F2 - Processing parameters

SI	32768
SF	125.7577958 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	159.885 ppm
F1	20106.82 Hz
F2P	9.197 ppm
F2	1156.56 Hz
PPMCM	7.53443 ppm/cm
HZCM	947.51294 Hz/cm

Current Data Parameters
 NAME fus65-463-mj
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041229
 Time 11.11
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SMH 5206.323 Hz
 FIDRES 0.158946 Hz
 AQ 3.145779 sec
 RB 64
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300142 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FAP 7.718 DPM
 F1 3860.18 Hz
 F2P -0.106 DPM
 F2 -53.20 Hz
 FPMCH 0.59124 DPM/cm
 HZCH 195.66504 Hz/cm

Current Data Parameters
 NAME tune56-m3-m3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041229
 Time 11.39
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TO 238090
 SOLVENT CDCl3
 NS 62
 DS 0
 SWH 39582.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.5958940 sec
 RG 8192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

===== CHANNEL f2 =====
 CDPFR02 wa12z16
 NUC2 1H
 P2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1338000 MHz

F2 - Processing Parameters
 SI 32768
 SF 125.757958 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 157.120 ppm
 F1 19759.10 Hz
 F2P -2.554 ppm
 F2 -321.22 Hz
 PRCKM 7.98373 ppm/cm
 HZCM 1004.01593 Hz/cm

Current Data Parameters
 NAME: fues6-463-411
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20041228
 Time: 17.45
 INSTRUM: spect
 PROBD: 5 mm QNP 1H
 PULPROG: zg
 TO: 32768
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SWH: 5208.332 Hz
 FIDRES: 0.189546 Hz
 AQ: 3.1457779 sec
 RB: 128
 DM: 96.000 usac
 DE: 4.50 usac
 TE: 300.0 K
 D1: 2.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.00 usac
 PL1: 0.00 dB
 SFO1: 500.1320118 MHz

F2 - Processing parameters
 SI: 16384
 SF: 500.1300139 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 C1P: 8.552 ppm
 F1: 4275.94 Hz
 F2P: -0.763 ppm
 F2: -381.38 Hz
 PPM0H: 0.46571 ppm/cm
 HZ0H: 232.91570 Hz/cm

Current Data Parameters
 NAME: tu056-M63-M1
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20041228
 Time: 17.50
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H
 PULPROG: zgpg
 TO: 238090
 SOLVENT: Aceton
 NS: 264
 DS: 0
 SWH: 39682.539 Hz
 FIDRES: 0.165670 Hz
 AQ: 2.5995840 sec
 RG: 8192
 DN: 12.600 usec
 DE: 7.50 usec
 TE: 300.0 K
 D1: 4.00000000 sec
 d11: 0.03000000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 8.20 usec
 PL1: 0.00 dB
 SF01: 125.7735214 MHz

===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 90.00 usec
 PL2: 120.00 dB
 PL12: 19.00 dB
 SF02: 500.1338000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.757946 MHz
 WDM: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR Plot Parameters
 CX: 20.00 cm
 FIP: 166.116 ppm
 F1: 20890.37 Hz
 F2: 12.662 ppm
 F2: 1592.40 Hz
 PPMCH: 7.67267 ppm/cm
 HZCH: 964.89856 Hz/cm

Current Data Parameters
NAME fuse66-Me3
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041229
Time 17.49
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 238050
SOLVENT Aceton
NS 110
DS 0
SWH 39682.539 Hz
FIDRES 0.165670 Hz
AQ 2.9593840 sec
RG 4086
DM 12.500 usec
DE 7.50 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.20 usec
PL1 0.00 dB
SFO1 125.7735214 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPRG2 90.00 usec
PL2 120.00 dB
PL12 19.00 dB
SFO2 500.1339000 MHz

F2 - Processing parameters
SI 32768
SF 125.7577481 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 151.647 ppm
F1 20328.35 Hz
F2P 10.613 ppm
F2 1334.63 Hz
PPMCH 7.55171 ppm/cm
HZCH 949.69616 Hz/cm

Current Data Parameters
NAME fuse6-Me3
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041229
Time 17.43
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT TOL
NS 8
DS 0
SWH 5208.333 Hz
FIDRES 0.159946 Hz
AQ 3.1457779 sec
RG 64
DS 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 2.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 500.130118 MHz

F2 - Processing parameters
SI 16384
SF 500.130198 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 20.00 cm
FIP 8.552 ppm
F1 4275.94 Hz
F2P -0.763 ppm
F2 -381.38 Hz
PPMCM 0.46571 ppm/cm
HZCM 232.91570 Hz/cm

Current Data Parameters
 NAME fused-66-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050210
 Time 11:55
 INSTRUM spect
 PROBD 5 mm QNP 3H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DN 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 500.1300118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300142 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.346 ppm
 F1 3974.27 Hz
 F2P -53.20 ppm
 F2 -53.20 Hz
 PRNCH 0.40264 ppm/cm
 HZCM 201.37389 Hz/cm

Current Data Parameters
 NAME fused-65-2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050210
 Time 12.00
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 238090
 SOLVENT Aceton
 NS 34
 DS 0
 SWH 39682.539 Hz
 FIDRES 0.166570 Hz
 AQ 2.9959840 sec
 RG 512
 DM 12.600 usec
 DE 77.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.775214 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.135000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577970 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 F1P 152.678 dB
 F1 15200.43 Hz
 F2P 19.814 dB
 F2 2491.82 Hz
 PPMCM 6.64317 ppm/cm
 HZCM 835.43036 Hz/cm

Current Data Parameters

NAME	VALUE
NAME	AUC-56-1use
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

NAME	VALUE
Date_	20050330
Time	13.32
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zg
TD	20332
SOLVENT	CDCl3
NS	8
DS	0
SWH	7002.801 Hz
FIDRES	0.36156 Hz
AQ	1.4874548 sec
RG	128
DW	71.400 usec
DE	4.50 usec
TE	300.0 K
D1	2.0000000 sec

CHANNEL f1

NAME	VALUE
NUC1	1H
P1	10.00 usec
PL1	0.00 dB
SFO1	500.1330008 MHz

F2 - Processing parameters

NAME	VALUE
SI	16384
SF	500.1300135 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

NAME	VALUE
CX	20.00 cm
FLP	8.567 ppm
F1	4279.67 Hz
F2P	0.393 ppm
F2	191.50 Hz
PPMCH	0.40871 ppm/cm
HZCM	204.40814 Hz/cm

Current Data Parameters

NAME	AuNC-5b-Tuse
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20050330
Time	13:37
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zgpg
TD	238090
SOLVENT	CDCl3
NS	32
DS	0
SMH	39682.539 Hz
FTIDRES	0.166670 Hz
AQ	2.9999840 sec
RG	2048
DM	12.600 usec
DE	7.50 usec
TE	300.0 K
D1	4.00000000 sec
d11	0.03000000 sec

===== CHANNEL f1 =====

MUFG1	13C
PC1	8.20 usec
PL1	0.00 dB
SFO1	125.7735214 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
MUFG2	1H
PCPD2	90.00 usec
PL2	120.00 dB
PL12	19.00 dB
SFO2	500.1338000 MHz

F2 - Processing parameters

SI	32768
SF	125.7577934 MHz
KOM	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	150.536 ppm
F1	20196.16 Hz
F2P	5.760 ppm
F2	724.33 Hz
PRNCH	7.74180 ppm/cm
HZCM	973.59137 Hz/cm

Current Data Parameters
NAME enyne-1T0H-PMe
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041107
Time 14.50
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TO 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5206.333 Hz
FIDRES 0.158946 Hz
AQ 3.145779 sec
RG 64
DM 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 500.132018 MHz

F2 - Processing parameters
SI 16384
SF 500.130042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 20.00 cm
F1P 7.939 ppm
F1 3970.30 Hz
F2P -0.101 ppm
F2 -50.38 Hz
PPM0H 0.40195 ppm/cm
HZ0H 201.03354 Hz/cm

Current Data Parameters
 NAME fused-66-012-C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050211
 Time 12.46
 INSTRUM spect
 PROBO 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 128
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300135 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.119 ppm
 F1 4060.48 Hz
 F2P -0.333 ppm
 F2 -166.66 Hz
 PPMCM 0.42260 ppm/cm
 HZCM 211.35680 Hz/cm

Current Data Parameters
 NAME fused-66-OH2-C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050211
 Time 13.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 238930
 SOLVENT CDCl3
 NS 82
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 512
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1338000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577934 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 179.259 ppm
 F1 22543.21 Hz
 F2P 7.833 ppm
 F2 985.12 Hz
 PPMCM 8.57128 ppm/cm
 HZCM 1077.90479 Hz/cm

Crystallographic Analysis of Carbonate 26

Data Collection

An irregular broken fragment (0.45 x 0.30 x 0.05 mm) was selected under a stereo-microscope while immersed in Fluorolube oil to avoid possible reaction with air. The crystal was removed from the oil using a tapered glass fiber that also served to hold the crystal for data collection. The crystal was mounted and centered on a Bruker SMART APEX system at 100 K. Rotation and still images showed the diffractions to be sharp. Frames separated in reciprocal space were obtained and provided an orientation matrix and initial cell parameters. Final cell parameters were obtained from the full data set.

A “full sphere” data set was obtained which samples approximately all of reciprocal space to a resolution of 0.84 Å using 0.3° steps in ω using 10 second integration times for each frame. Data collection was made at 100 K. Integration of intensities and refinement of cell parameters were done using SAINT [1]. Absorption corrections were applied using SADABS [1] based on redundant diffractions.

Structure solution and refinement

The space group was determined as P2(1) based on systematic absences and intensity statistics. Direct methods were used to locate all non-hydrogen atoms from the E-map. Repeated difference Fourier maps allowed recognition of all expected C and O atoms. Final refinement was anisotropic for non-hydrogen atoms and isotropic for H atoms. No anomalous bond lengths or thermal parameters were noted. The unit cell is appropriately described as monoclinic (b), despite the small β angle of 90.07°. All ORTEP diagrams have been drawn with 50% probability ellipsoids.

Equations of interest:

$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

$$wR2 = [\Sigma [w (F_o^2 - F_c^2)^2] / \Sigma [w (F_o^2)^2]]^{1/2}$$

$$\text{GooF} = S = [\Sigma [w (F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$$

$$\text{where: } w = q / \sigma^2 (F_o^2) + (aP)^2 + bP;$$

$$n = \text{number of independent reflections};$$

$$q, a, b, P \text{ as defined in [1]}$$

$$p = \text{number of parameters refined.}$$

References

[1] All software and sources of scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-ray Systems, Madison, WI).

Table 1. Crystal and structure refinement for Liming1.

Identification Code	Liming1	
Empirical formula	C ₁₉ O ₄ H ₂₄	
Formula weight	366.38	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic (b)	
Space Group	P2(1)	
Unit cell dimensions	$a = 8.124(2)$ Å	$\alpha = 90.00^\circ$
	$b = 12.920(3)$ Å	$\beta = 90.069(4)^\circ$
	$c = 15.721(4)$ Å	$\gamma = 90.00^\circ$
Volume	1650.0(7) Å ³	
Z	4	
Density (calculated)	1.274 Mg/m ³	
Absorption coefficient	0.088 mm ⁻¹	
F(000)	680	
Crystal size, color, habit	0.45 x 0.30 x 0.05 mm, transparent, plate	
Theta range for data collection	1.30 – 28.82°	
Index ranges	-11 ≤ h ≤ 10, -17 ≤ k ≤ 17, -21 ≤ l ≤ 20	
Reflections collected	19819	
Independent reflections	7989 (R _{int} = 0.0333)	
Reflections with I > 4σ(F _o)	6613	
Flack parameter		
Absorption correction	SADABS based on redundant diffractions	
Max. and min. transmission	1.0, 0.833317	
Refinement method	Full-matrix least squares on F ²	
Weighting scheme	w = q [σ ² (F _o ²) + (aP) ² + bP] ⁻¹ where: P = (F _o ² + 2F _c ²)/3, a = 0.0292, b = 0.0, q = 1	
Data / restraints / parameters	7989 / 1 / 421	
Goodness-of-fit on F ²	1.005	
Final R indices [I > 2 sigma(I)]	R1 = 0.0497, wR2 = 0.0801	
R indices (all data)	R1 = 0.0647, wR2 = 0.0844	
Largest diff. peak and hole	0.230, -0.250 eÅ ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Liming1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$	SOF
C(1)	1954(2)	5721(2)	4806(1)	25(1)	
C(2)	1355(2)	6072(2)	4033(1)	30(1)	
C(3)	1117(2)	7115(2)	3905(1)	29(1)	
C(4)	1491(2)	7808(2)	4541(1)	26(1)	
C(5)	2125(2)	7463(2)	5311(1)	23(1)	
C(6)	2346(2)	6413(2)	5457(1)	21(1)	
C(7)	3019(2)	6002(2)	6294(1)	21(1)	
C(8)	2440(2)	6536(2)	7107(1)	21(1)	
C(9)	911(3)	5095(2)	6922(1)	28(1)	
C(10)	4921(2)	5891(2)	6360(1)	22(1)	
C(11)	5538(3)	4912(2)	5911(1)	30(1)	
C(12)	5777(2)	6817(2)	5949(1)	23(1)	
C(13)	7657(2)	6812(2)	5970(1)	30(1)	
C(14)	8058(2)	7955(2)	5956(2)	37(1)	
C(15)	6701(2)	8416(2)	6493(2)	35(1)	
C(16)	5213(2)	5836(2)	7329(1)	30(1)	
C(17)	3715(2)	6304(2)	7817(1)	26(1)	
C(18)	4141(3)	7303(2)	8286(1)	36(1)	
C(19)	3091(3)	5519(2)	8469(1)	34(1)	
C(20)	2122(2)	2463(2)	9687(1)	23(1)	
C(21)	1491(2)	2806(2)	10457(1)	26(1)	
C(22)	1117(2)	2116(2)	11095(1)	29(1)	
C(23)	1354(2)	1072(2)	10968(1)	29(1)	
C(24)	1954(2)	722(2)	10196(1)	26(1)	
C(25)	2346(2)	1413(2)	9544(1)	22(1)	
C(26)	3019(2)	999(2)	8707(1)	21(1)	
C(27)	909(3)	96(2)	8080(1)	28(1)	
C(28)	2439(2)	1533(2)	7893(1)	22(1)	
C(29)	4921(2)	891(2)	8641(1)	22(1)	
C(30)	5540(3)	-89(2)	9091(1)	29(1)	
C(31)	5776(2)	1816(2)	9049(1)	23(1)	
C(32)	7657(2)	1813(2)	9029(1)	30(1)	
C(33)	8059(3)	2956(2)	9043(2)	37(1)	
C(34)	6704(2)	3417(2)	8507(2)	35(1)	
C(35)	5217(2)	835(2)	7669(1)	29(1)	
C(36)	3716(2)	1304(2)	7184(1)	25(1)	
C(37)	4142(3)	2300(2)	6715(1)	35(1)	
C(38)	3092(3)	515(2)	6532(1)	35(1)	
O(1)	863(1)	6045(1)	7261(1)	25(1)	
O(2)	-99(2)	4444(1)	7030(1)	41(1)	
O(3)	2275(2)	4974(1)	6433(1)	26(1)	
O(4)	5296(2)	7751(1)	6384(1)	27(1)	
O(5)	2274(2)	-26(1)	8566(1)	26(1)	
O(6)	-97(2)	-557(1)	7970(1)	42(1)	
O(7)	862(1)	1045(1)	7738(1)	26(1)	
O(8)	5296(2)	2751(1)	8617(1)	26(1)	

Table 3. Bond lengths [Å] and angles [°] for Liming1.

C(1)–C(2)	1.385(3)
C(1)–C(6)	1.395(3)
C(2)–C(3)	1.376(3)
C(3)–C(4)	1.376(3)
C(4)–C(5)	1.389(3)
C(5)–C(6)	1.387(3)
C(6)–C(7)	1.520(3)
C(7)–O(3)	1.476(2)
C(7)–C(8)	1.528(2)
C(7)–C(10)	1.555(2)
C(8)–O(1)	1.450(2)
C(8)–C(17)	1.551(3)
C(9)–O(2)	1.188(2)
C(9)–O(1)	1.339(2)
C(9)–O(3)	1.358(2)
C(10)–C(12)	1.528(3)
C(10)–C(11)	1.533(3)
C(10)–C(16)	1.543(2)
C(12)–O(4)	1.441(2)
C(12)–C(13)	1.528(3)
C(13)–C(14)	1.512(3)
C(14)–C(15)	1.512(3)
C(15)–O(4)	1.439(2)
C(16)–C(17)	1.561(3)
C(17)–C(18)	1.526(3)
C(17)–C(19)	1.528(3)
C(20)–C(25)	1.387(3)
C(20)–C(21)	1.388(3)
C(21)–C(22)	1.376(3)
C(22)–C(23)	1.377(3)
C(23)–C(24)	1.383(3)
C(24)–C(25)	1.396(3)
C(25)–C(26)	1.521(3)
C(26)–O(5)	1.473(2)
C(26)–C(28)	1.527(2)
C(26)–C(29)	1.555(2)
C(27)–O(6)	1.187(2)
C(27)–O(7)	1.339(2)
C(27)–O(5)	1.355(2)
C(28)–O(7)	1.449(2)
C(28)–C(36)	1.552(3)
C(29)–C(31)	1.524(3)
C(29)–C(30)	1.534(3)
C(29)–C(35)	1.548(2)
C(31)–O(8)	1.439(2)
C(31)–C(32)	1.529(3)
C(32)–C(33)	1.513(3)
C(33)–C(34)	1.509(3)
C(34)–O(8)	1.443(2)
C(35)–C(36)	1.560(3)
C(36)–C(37)	1.523(3)
C(36)–C(38)	1.532(3)

C(2)-C(1)-C(6)	120.9(2)
C(3)-C(2)-C(1)	119.93(19)
C(4)-C(3)-C(2)	119.94(18)
C(3)-C(4)-C(5)	120.4(2)
C(6)-C(5)-C(4)	120.33(19)
C(5)-C(6)-C(1)	118.44(18)
C(5)-C(6)-C(7)	122.01(17)
C(1)-C(6)-C(7)	119.54(17)
O(3)-C(7)-C(6)	107.19(14)
O(3)-C(7)-C(8)	98.93(14)
C(6)-C(7)-C(8)	117.16(16)
O(3)-C(7)-C(10)	108.29(14)
C(6)-C(7)-C(10)	116.55(14)
C(8)-C(7)-C(10)	107.01(14)
O(1)-C(8)-C(7)	102.42(14)
O(1)-C(8)-C(17)	112.68(15)
C(7)-C(8)-C(17)	107.98(15)
O(2)-C(9)-O(1)	124.92(19)
O(2)-C(9)-O(3)	124.3(2)
O(1)-C(9)-O(3)	110.78(17)
C(12)-C(10)-C(11)	107.58(15)
C(12)-C(10)-C(16)	112.58(16)
C(11)-C(10)-C(16)	111.49(16)
C(12)-C(10)-C(7)	110.60(15)
C(11)-C(10)-C(7)	111.79(15)
C(16)-C(10)-C(7)	102.85(13)
O(4)-C(12)-C(13)	105.37(15)
O(4)-C(12)-C(10)	109.33(14)
C(13)-C(12)-C(10)	116.32(16)
C(14)-C(13)-C(12)	102.19(16)
C(15)-C(14)-C(13)	102.69(17)
O(4)-C(15)-C(14)	106.10(17)
C(10)-C(16)-C(17)	110.36(15)
C(18)-C(17)-C(19)	108.24(17)
C(18)-C(17)-C(8)	109.54(16)
C(19)-C(17)-C(8)	112.85(16)
C(18)-C(17)-C(16)	112.85(17)
C(19)-C(17)-C(16)	109.39(17)
C(8)-C(17)-C(16)	104.01(15)
C(25)-C(20)-C(21)	120.21(19)
C(22)-C(21)-C(20)	120.7(2)
C(21)-C(22)-C(23)	119.84(18)
C(22)-C(23)-C(24)	119.78(19)
C(23)-C(24)-C(25)	121.1(2)
C(20)-C(25)-C(24)	118.34(18)
C(20)-C(25)-C(26)	122.08(17)
C(24)-C(25)-C(26)	119.57(18)
O(5)-C(26)-C(25)	107.34(14)
O(5)-C(26)-C(28)	98.82(14)
C(25)-C(26)-C(28)	117.06(16)
O(5)-C(26)-C(29)	108.45(14)
C(25)-C(26)-C(29)	116.61(14)
C(28)-C(26)-C(29)	106.85(14)
O(6)-C(27)-O(7)	124.97(19)
O(6)-C(27)-O(5)	124.2(2)
O(7)-C(27)-O(5)	110.82(17)
O(7)-C(28)-C(26)	102.49(14)

O(7)-C(28)-C(36)	112.79(15)
C(26)-C(28)-C(36)	108.07(15)
C(31)-C(29)-C(30)	107.66(15)
C(31)-C(29)-C(35)	112.35(16)
C(30)-C(29)-C(35)	111.45(16)
C(31)-C(29)-C(26)	110.68(14)
C(30)-C(29)-C(26)	111.65(15)
C(35)-C(29)-C(26)	103.08(13)
O(8)-C(31)-C(29)	109.68(14)
O(8)-C(31)-C(32)	105.22(15)
C(29)-C(31)-C(32)	116.42(16)
C(33)-C(32)-C(31)	102.33(16)
C(34)-C(33)-C(32)	102.67(17)
O(8)-C(34)-C(33)	105.99(17)
C(29)-C(35)-C(36)	110.00(15)
C(37)-C(36)-C(38)	108.23(17)
C(37)-C(36)-C(28)	109.85(16)
C(38)-C(36)-C(28)	112.79(16)
C(37)-C(36)-C(35)	112.75(17)
C(38)-C(36)-C(35)	109.06(16)
C(28)-C(36)-C(35)	104.21(15)
C(9)-O(1)-C(8)	107.97(15)
C(9)-O(3)-C(7)	108.38(14)
C(15)-O(4)-C(12)	109.94(14)
C(27)-O(5)-C(26)	108.46(14)
C(27)-O(7)-C(28)	107.84(15)
C(31)-O(8)-C(34)	110.07(14)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Liming1.
The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	24(1)	29(1)	22(1)	-2(1)	-1(1)	1(1)
C(2)	26(1)	44(1)	20(1)	-6(1)	-3(1)	-1(1)
C(3)	20(1)	48(1)	19(1)	8(1)	-3(1)	3(1)
C(4)	18(1)	32(1)	29(1)	9(1)	3(1)	1(1)
C(5)	17(1)	29(1)	25(1)	-1(1)	0(1)	-2(1)
C(6)	17(1)	29(1)	18(1)	-2(1)	2(1)	1(1)
C(7)	25(1)	19(1)	19(1)	0(1)	-1(1)	-1(1)
C(8)	19(1)	27(1)	18(1)	-2(1)	0(1)	0(1)
C(9)	34(1)	34(1)	17(1)	4(1)	-1(1)	-6(1)
C(10)	22(1)	27(1)	18(1)	1(1)	-2(1)	7(1)
C(11)	34(1)	29(1)	27(1)	1(1)	5(1)	9(1)
C(12)	20(1)	28(1)	22(1)	-2(1)	0(1)	5(1)
C(13)	24(1)	38(1)	29(1)	-3(1)	2(1)	7(1)
C(14)	22(1)	42(2)	48(1)	-7(1)	8(1)	-3(1)
C(15)	27(1)	33(1)	44(1)	-9(1)	7(1)	-6(1)
C(16)	27(1)	40(1)	22(1)	0(1)	-1(1)	8(1)
C(17)	27(1)	35(1)	16(1)	1(1)	-2(1)	3(1)
C(18)	29(1)	54(2)	24(1)	-10(1)	-3(1)	-1(1)
C(19)	34(1)	52(2)	17(1)	5(1)	-2(1)	7(1)
C(20)	18(1)	27(1)	24(1)	0(1)	-1(1)	-3(1)
C(21)	18(1)	32(1)	28(1)	-10(1)	-4(1)	1(1)
C(22)	20(1)	49(2)	19(1)	-6(1)	2(1)	2(1)
C(23)	24(1)	44(1)	19(1)	6(1)	2(1)	0(1)
C(24)	24(1)	31(1)	24(1)	0(1)	0(1)	3(1)
C(25)	17(1)	30(1)	19(1)	2(1)	-2(1)	0(1)
C(26)	24(1)	19(1)	20(1)	2(1)	-1(1)	1(1)
C(27)	32(1)	34(1)	17(1)	-4(1)	1(1)	-4(1)
C(28)	20(1)	25(1)	20(1)	2(1)	-2(1)	0(1)
C(29)	21(1)	28(1)	18(1)	0(1)	1(1)	7(1)
C(30)	35(1)	27(1)	27(1)	-1(1)	-7(1)	9(1)
C(31)	20(1)	26(1)	24(1)	2(1)	0(1)	7(1)
C(32)	24(1)	36(1)	31(1)	3(1)	-3(1)	6(1)
C(33)	23(1)	39(2)	49(1)	7(1)	-8(1)	-3(1)
C(34)	28(1)	34(1)	44(1)	6(1)	-10(1)	-6(1)
C(35)	28(1)	39(1)	20(1)	-1(1)	2(1)	8(1)
C(36)	27(1)	32(1)	17(1)	0(1)	0(1)	3(1)
C(37)	28(1)	53(2)	24(1)	10(1)	2(1)	-2(1)
C(38)	34(1)	52(2)	20(1)	-6(1)	2(1)	6(1)
O(1)	22(1)	34(1)	20(1)	-2(1)	0(1)	-4(1)
O(2)	44(1)	43(1)	36(1)	-2(1)	6(1)	-20(1)
O(3)	32(1)	24(1)	21(1)	0(1)	3(1)	-3(1)
O(4)	20(1)	28(1)	32(1)	-8(1)	2(1)	0(1)
O(5)	32(1)	24(1)	21(1)	-1(1)	-3(1)	-2(1)
O(6)	45(1)	45(1)	35(1)	2(1)	-7(1)	-21(1)
O(7)	22(1)	34(1)	21(1)	2(1)	-1(1)	-4(1)
O(8)	19(1)	27(1)	33(1)	8(1)	-2(1)	1(1)

Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Liming1.

	x	y	z	U(eq)
H(1)	2101	5000	4894	30
H(2)	1108	5594	3592	36
H(3)	695	7356	3377	35
H(4)	1314	8527	4453	31
H(5)	2410	7948	5741	28
H(8)	2310	7298	7019	26
H(11A)	4918	4311	6116	45
H(11B)	6711	4814	6035	45
H(11C)	5382	4984	5296	45
H(12)	5409	6867	5343	28
H(13A)	8078	6478	6493	37
H(13B)	8118	6454	5467	37
H(14A)	9154	8092	6208	45
H(14B)	8031	8233	5369	45
H(15A)	7036	8442	7098	42
H(15B)	6442	9128	6301	42
H(16A)	6224	6225	7477	35
H(16B)	5372	5106	7502	35
H(18A)	3159	7566	8575	54
H(18B)	4533	7820	7877	54
H(18C)	5005	7165	8706	54
H(19A)	3951	5389	8893	52
H(19B)	2812	4870	8180	52
H(19C)	2110	5795	8751	52
H(20)	2401	2948	9257	27
H(21)	1315	3525	10545	31
H(22)	696	2359	11622	35
H(23)	1107	593	11408	35
H(24)	2101	1	10109	31
H(28)	2310	2295	7983	26
H(30A)	6715	-182	8973	44
H(30B)	4927	-690	8882	44
H(30C)	5374	-18	9706	44
H(31)	5412	1865	9655	28
H(32A)	8120	1455	9532	36
H(32B)	8077	1479	8505	36
H(33A)	8033	3233	9630	45
H(33B)	9155	3093	8792	45
H(34A)	6447	4129	8697	42
H(34B)	7035	3440	7901	42
H(35A)	5375	105	7496	35
H(35B)	6227	1224	7523	35
H(37A)	4997	2158	6291	53
H(37B)	4547	2815	7122	53
H(37C)	3157	2567	6429	53
H(38A)	2109	788	6249	53

H (38B)	2818	-134	6822	53
H (38C)	3952	386	6108	53

Table 6. Torsion angles [$^{\circ}$] for Liming1.

C(6)-C(1)-C(2)-C(3)	-0.9(3)
C(1)-C(2)-C(3)-C(4)	0.7(3)
C(2)-C(3)-C(4)-C(5)	0.7(3)
C(3)-C(4)-C(5)-C(6)	-1.8(3)
C(4)-C(5)-C(6)-C(1)	1.5(3)
C(4)-C(5)-C(6)-C(7)	-179.35(16)
C(2)-C(1)-C(6)-C(5)	-0.2(3)
C(2)-C(1)-C(6)-C(7)	-179.31(17)
C(5)-C(6)-C(7)-O(3)	149.10(16)
C(1)-C(6)-C(7)-O(3)	-31.8(2)
C(5)-C(6)-C(7)-C(8)	39.1(2)
C(1)-C(6)-C(7)-C(8)	-141.75(17)
C(5)-C(6)-C(7)-C(10)	-89.5(2)
C(1)-C(6)-C(7)-C(10)	89.7(2)
O(3)-C(7)-C(8)-O(1)	-32.49(16)
C(6)-C(7)-C(8)-O(1)	82.14(19)
C(10)-C(7)-C(8)-O(1)	-144.84(15)
O(3)-C(7)-C(8)-C(17)	86.62(16)
C(6)-C(7)-C(8)-C(17)	-158.75(16)
C(10)-C(7)-C(8)-C(17)	-25.7(2)
O(3)-C(7)-C(10)-C(12)	161.75(14)
C(6)-C(7)-C(10)-C(12)	40.9(2)
C(8)-C(7)-C(10)-C(12)	-92.47(17)
O(3)-C(7)-C(10)-C(11)	41.90(19)
C(6)-C(7)-C(10)-C(11)	-79.0(2)
C(8)-C(7)-C(10)-C(11)	147.68(16)
O(3)-C(7)-C(10)-C(16)	-77.83(17)
C(6)-C(7)-C(10)-C(16)	161.30(17)
C(8)-C(7)-C(10)-C(16)	28.0(2)
C(11)-C(10)-C(12)-O(4)	-176.93(15)
C(16)-C(10)-C(12)-O(4)	-53.70(19)
C(7)-C(10)-C(12)-O(4)	60.73(18)
C(11)-C(10)-C(12)-C(13)	-57.8(2)
C(16)-C(10)-C(12)-C(13)	65.4(2)
C(7)-C(10)-C(12)-C(13)	179.86(15)
O(4)-C(12)-C(13)-C(14)	-30.99(19)
C(10)-C(12)-C(13)-C(14)	-152.25(17)
C(12)-C(13)-C(14)-C(15)	36.6(2)
C(13)-C(14)-C(15)-O(4)	-29.8(2)
C(12)-C(10)-C(16)-C(17)	98.40(19)
C(11)-C(10)-C(16)-C(17)	-140.59(17)
C(7)-C(10)-C(16)-C(17)	-20.7(2)
O(1)-C(8)-C(17)-C(18)	-114.50(18)
C(7)-C(8)-C(17)-C(18)	133.12(17)
O(1)-C(8)-C(17)-C(19)	6.2(2)
C(7)-C(8)-C(17)-C(19)	-106.22(18)
O(1)-C(8)-C(17)-C(16)	124.62(17)
C(7)-C(8)-C(17)-C(16)	12.2(2)
C(10)-C(16)-C(17)-C(18)	-112.96(19)
C(10)-C(16)-C(17)-C(19)	126.48(18)
C(10)-C(16)-C(17)-C(8)	5.7(2)
C(25)-C(20)-C(21)-C(22)	1.6(3)
C(20)-C(21)-C(22)-C(23)	-0.7(3)

C(21)-C(22)-C(23)-C(24)	-0.6(3)
C(22)-C(23)-C(24)-C(25)	0.8(3)
C(21)-C(20)-C(25)-C(24)	-1.3(3)
C(21)-C(20)-C(25)-C(26)	179.43(16)
C(23)-C(24)-C(25)-C(20)	0.1(3)
C(23)-C(24)-C(25)-C(26)	179.38(17)
C(20)-C(25)-C(26)-O(5)	-148.78(16)
C(24)-C(25)-C(26)-O(5)	32.0(2)
C(20)-C(25)-C(26)-C(28)	-38.9(2)
C(24)-C(25)-C(26)-C(28)	141.82(17)
C(20)-C(25)-C(26)-C(29)	89.4(2)
C(24)-C(25)-C(26)-C(29)	-89.9(2)
O(5)-C(26)-C(28)-O(7)	32.52(16)
C(25)-C(26)-C(28)-O(7)	-82.18(19)
C(29)-C(26)-C(28)-O(7)	144.96(15)
O(5)-C(26)-C(28)-C(36)	-86.78(16)
C(25)-C(26)-C(28)-C(36)	158.52(16)
C(29)-C(26)-C(28)-C(36)	25.7(2)
O(5)-C(26)-C(29)-C(31)	-162.03(14)
C(25)-C(26)-C(29)-C(31)	-40.8(2)
C(28)-C(26)-C(29)-C(31)	92.31(17)
O(5)-C(26)-C(29)-C(30)	-42.11(19)
C(25)-C(26)-C(29)-C(30)	79.1(2)
C(28)-C(26)-C(29)-C(30)	-147.77(16)
O(5)-C(26)-C(29)-C(35)	77.64(17)
C(25)-C(26)-C(29)-C(35)	-161.13(17)
C(28)-C(26)-C(29)-C(35)	-28.0(2)
C(30)-C(29)-C(31)-O(8)	177.07(15)
C(35)-C(29)-C(31)-O(8)	53.98(19)
C(26)-C(29)-C(31)-O(8)	-60.65(18)
C(30)-C(29)-C(31)-C(32)	57.8(2)
C(35)-C(29)-C(31)-C(32)	-65.3(2)
C(26)-C(29)-C(31)-C(32)	-179.92(15)
O(8)-C(31)-C(32)-C(33)	30.77(19)
C(29)-C(31)-C(32)-C(33)	152.43(17)
C(31)-C(32)-C(33)-C(34)	-36.6(2)
C(32)-C(33)-C(34)-O(8)	30.0(2)
C(31)-C(29)-C(35)-C(36)	-98.39(18)
C(30)-C(29)-C(35)-C(36)	140.67(17)
C(26)-C(29)-C(35)-C(36)	20.8(2)
O(7)-C(28)-C(36)-C(37)	114.26(18)
C(26)-C(28)-C(36)-C(37)	-133.18(17)
O(7)-C(28)-C(36)-C(38)	-6.6(2)
C(26)-C(28)-C(36)-C(38)	106.00(18)
O(7)-C(28)-C(36)-C(35)	-124.70(17)
C(26)-C(28)-C(36)-C(35)	-12.1(2)
C(29)-C(35)-C(36)-C(37)	113.28(19)
C(29)-C(35)-C(36)-C(38)	-126.48(18)
C(29)-C(35)-C(36)-C(28)	-5.8(2)
O(2)-C(9)-O(1)-C(8)	169.87(19)
O(3)-C(9)-O(1)-C(8)	-10.4(2)
C(7)-C(8)-O(1)-C(9)	27.75(18)
C(17)-C(8)-O(1)-C(9)	-88.01(17)
O(2)-C(9)-O(3)-C(7)	167.16(19)
O(1)-C(9)-O(3)-C(7)	-12.6(2)
C(6)-C(7)-O(3)-C(9)	-94.05(17)
C(8)-C(7)-O(3)-C(9)	28.10(17)

C(10)-C(7)-O(3)-C(9)	139.44(14)
C(14)-C(15)-O(4)-C(12)	10.6(2)
C(13)-C(12)-O(4)-C(15)	13.0(2)
C(10)-C(12)-O(4)-C(15)	138.70(16)
O(6)-C(27)-O(5)-C(26)	-167.43(19)
O(7)-C(27)-O(5)-C(26)	13.0(2)
C(25)-C(26)-O(5)-C(27)	93.69(16)
C(28)-C(26)-O(5)-C(27)	-28.37(17)
C(29)-C(26)-O(5)-C(27)	-139.53(14)
O(6)-C(27)-O(7)-C(28)	-169.56(19)
O(5)-C(27)-O(7)-C(28)	10.0(2)
C(26)-C(28)-O(7)-C(27)	-27.53(18)
C(36)-C(28)-O(7)-C(27)	88.42(17)
C(29)-C(31)-O(8)-C(34)	-138.57(16)
C(32)-C(31)-O(8)-C(34)	-12.6(2)
C(33)-C(34)-O(8)-C(31)	-10.9(2)