

Supporting Information

Rec. Nat. Prod. 8:4 (2014) 422-425

Two New Scaralane-type Sesterterpenoids Isolated from the Marine Sponge *Hyrtios erectus*

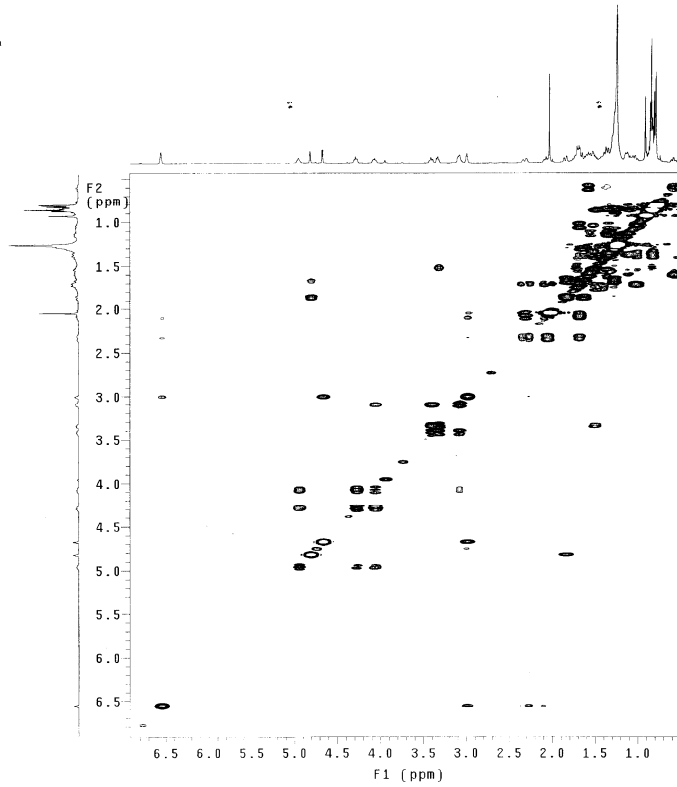
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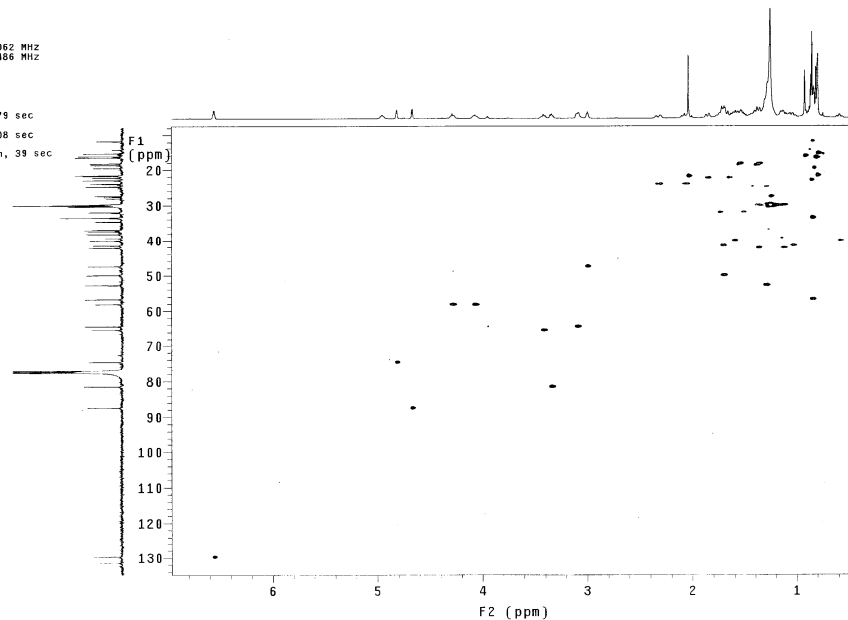
Table of Contents	Page
S1: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 1	2
S2: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of Compound 1	2
S3: COSY (500 MHz) Spectrum of Compound 1	3
S4: gHSQC (500 MHz) Spectrum of Compound 1	3
S5: HMBC (500 MHz) Spectrum of Compound 1	4
S6: 1D-GOSY (500 MHz) Spectrum of Compound 1	5
S7: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 2	6
S8: COSY (500 MHz) Spectrum of Compound 2	6
S9: HMQC (500 MHz) Spectrum of Compound 2	7
S10: HMBC (500 MHz) Spectrum of Compound 2	7
S11: HR-MS Spectrum of Compound 2	8
S12: Fundamental structural data for compounds 3 and 4	9

HSyan21
 Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory: auto_130ct2004
 Pulse Sequence: gCOSY
 Solvent: cdc13
 Ambient temperature
 User: 1-14-97
 File: yun.0187
 INOVA-500 "unknown"
 Relax. delay 1.000 sec
 Acq. time 0.171 sec
 Width 6000.6 Hz
 2D Width 6000.6 Hz
 16 repetitions
 256 increments
 OBSERVE F1: 499.5727062 MHz
 DATA PROCESSING
 Sg. sine bell 0.085 sec
 F1 DATA PROCESSING
 Sg. sine bell 0.021 sec
 FT Size 4096 x 4096
 Total time 1 hr, 22 min, 34 sec



S3: COSY (500 MHz) Spectrum of Compound

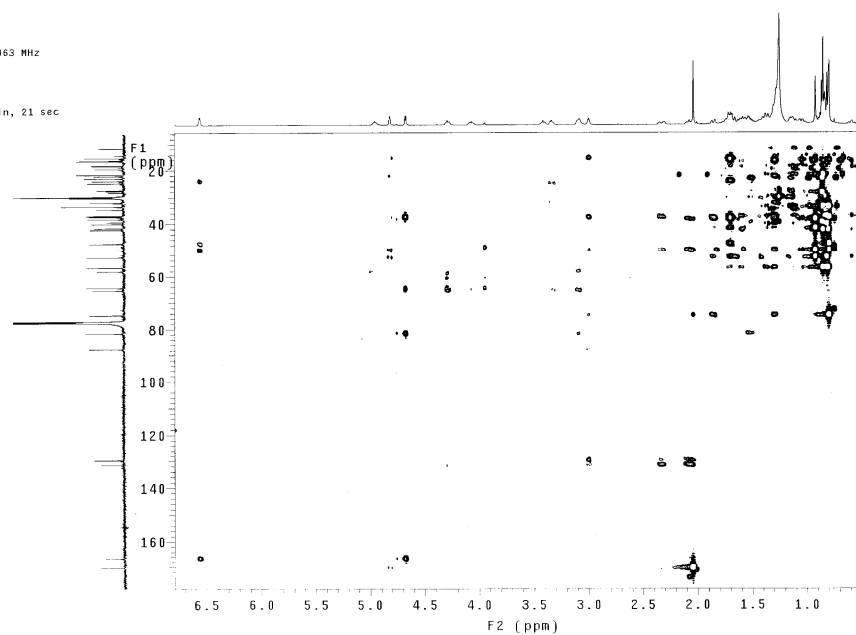
HSyan21
 Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory: auto_130ct2004
 Pulse Sequence: gHSQC
 Solvent: cdc13
 Ambient temperature
 User: 1-14-97
 File: yun.0188
 INOVA-500 "unknown"
 Relax. delay 1.000 sec
 Acq. time 0.171 sec
 Width 4900.0 Hz
 2D Width 21356.1 Hz
 16 repetitions
 2 x 256 increments
 OBSERVE F1: 499.5727062 MHz
 DECOUPLE C13: 125.6270486 MHz
 Power 40 dB
 on during acquisition
 off during delay
 GMRP-1 modulated
 DATA PROCESSING
 Gauss apodization 0.079 sec
 F1 DATA PROCESSING
 Gauss apodization 0.008 sec
 FT size 2048 x 4096
 Total time 2 hr, 50 min, 39 sec



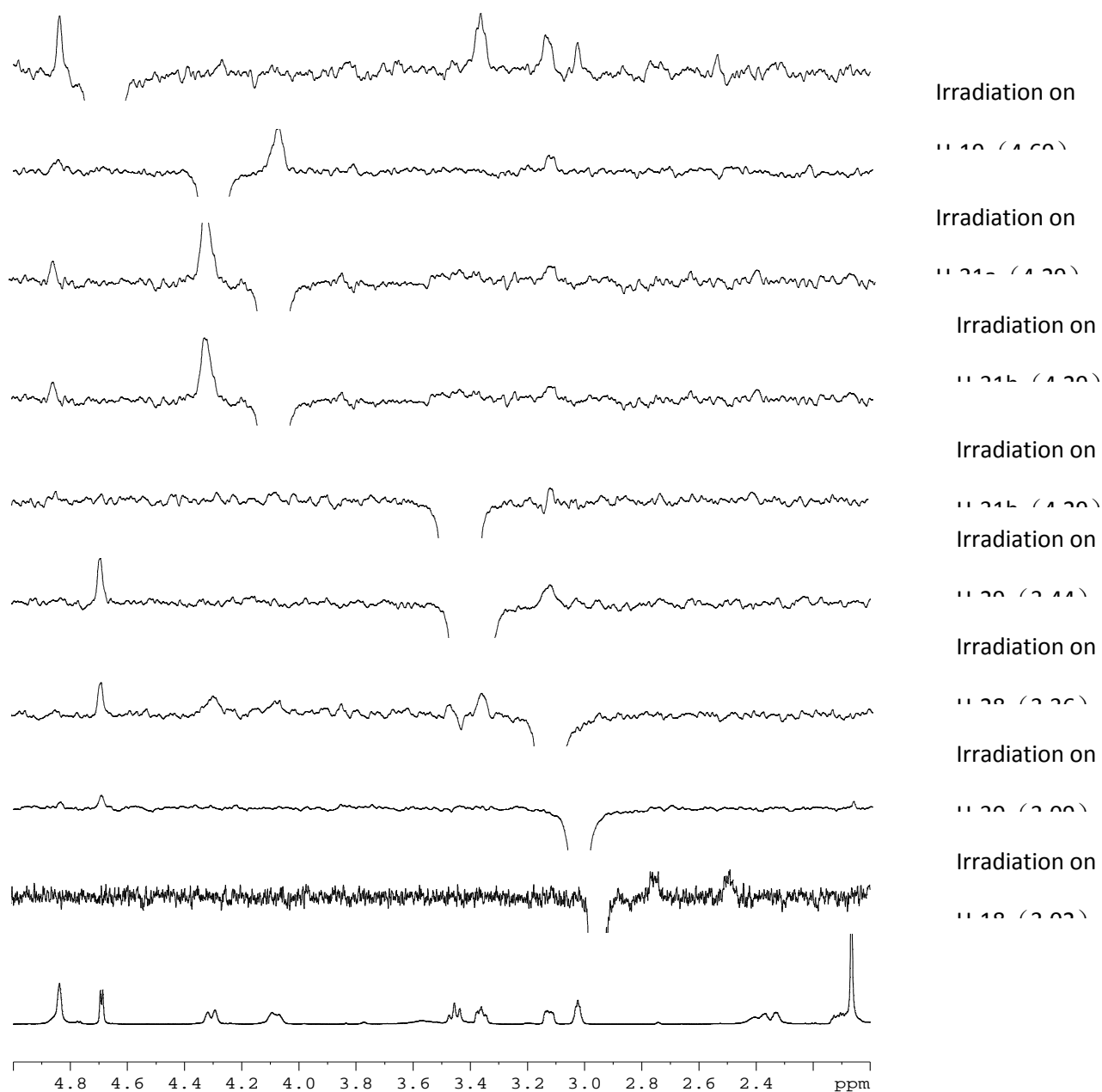
1

S4: gHSQC (500 MHz) Spectrum of Compound 1

hsyan-21
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: auto_13Oct2004
Pulse Sequence: gHMBC
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: yun_0287
INOVA-500 "unknown"
Relax. delay 1.000 sec
Acq. time 0.171 sec
Width 6000.6 Hz
F0 Width 30143.2 Hz
128 repetitions
256 increments
OBSERVE F1 499.5661863 MHz
DATA PROCESSING
Sine bell 0.005 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 4096
Total time 11 hr, 38 min, 21 sec

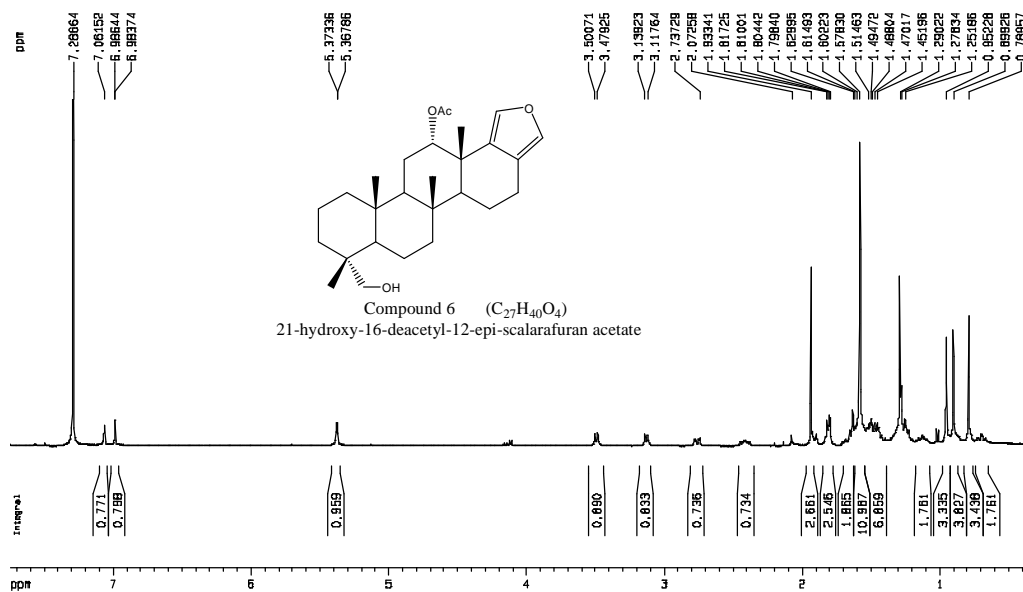


S5: HMBC (500 MHz) Spectrum of Compound 1



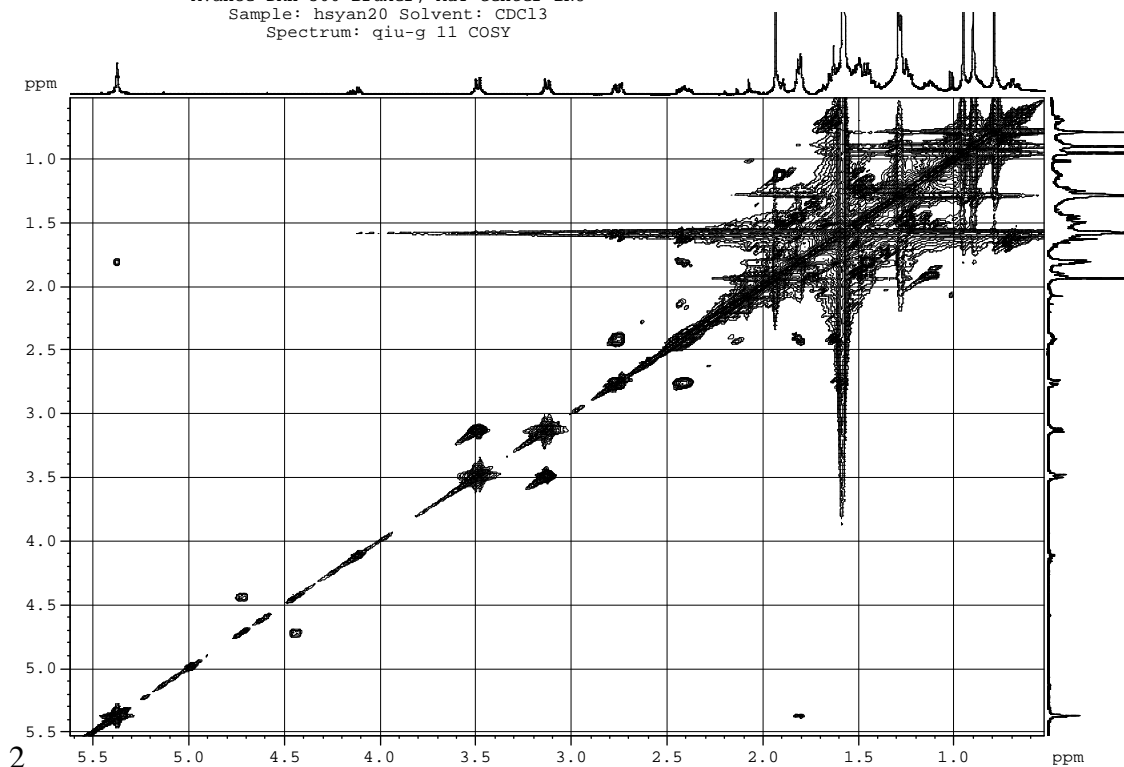
S6: 1D-GOSY (500 MHz) Spectrum of Compound 1

Avance 500 Bruker, A&T Center BNU
Sample: hsyam-20 Solvent: cdcl3
Spectrum: qiu-c 3

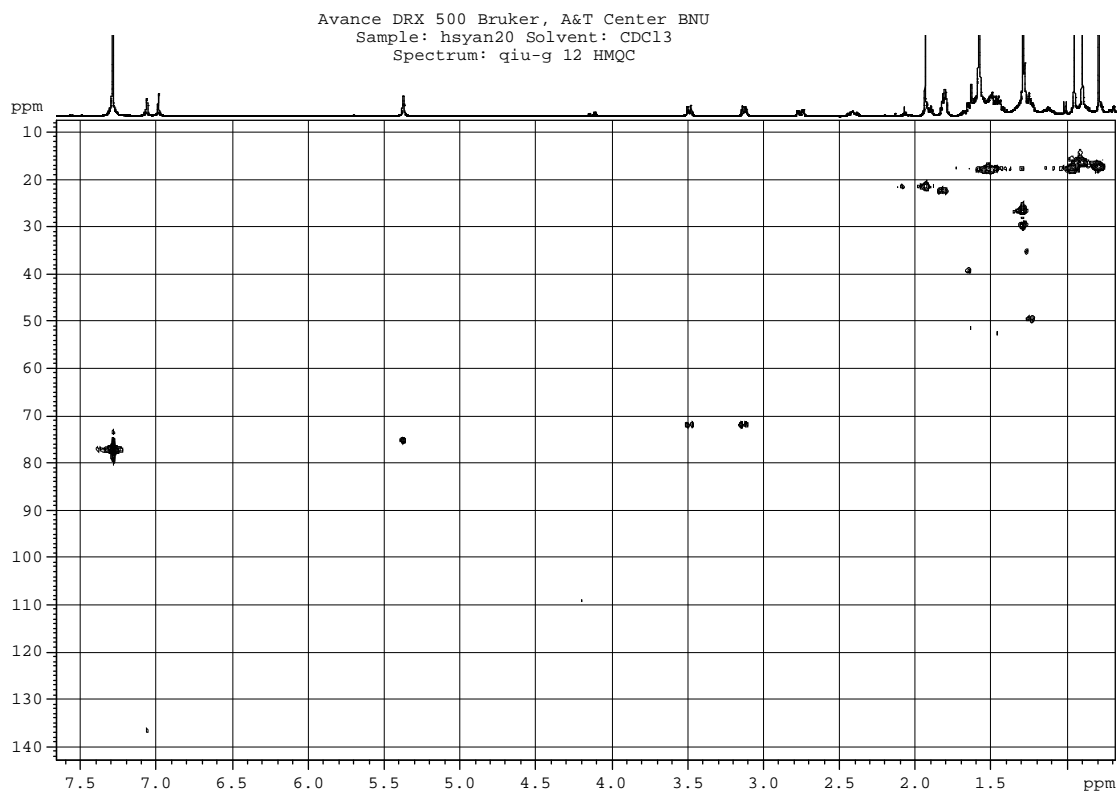


S7: ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound

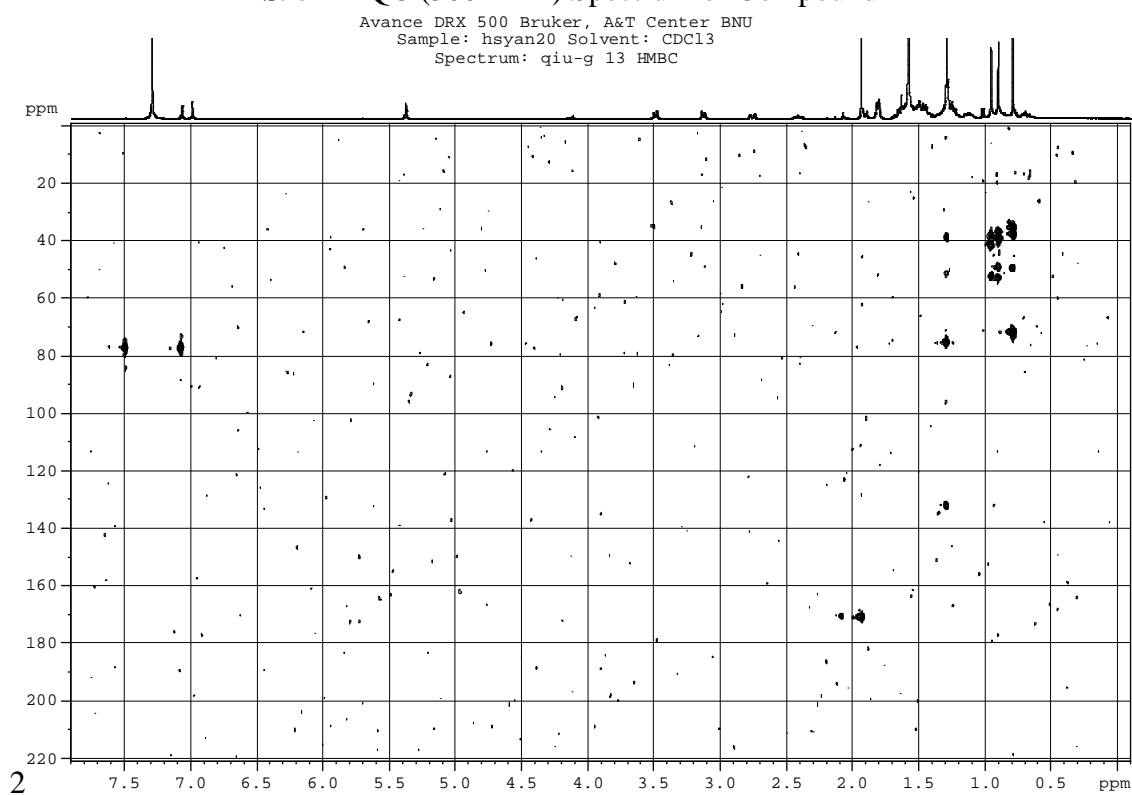
Avance DRX 500 Bruker, A&T Center BNU
Sample: hsyam20 Solvent: CDCl₃
Spectrum: qiu-g 11 COSY



S8: COSY (500 MHz) Spectrum of Compound 2

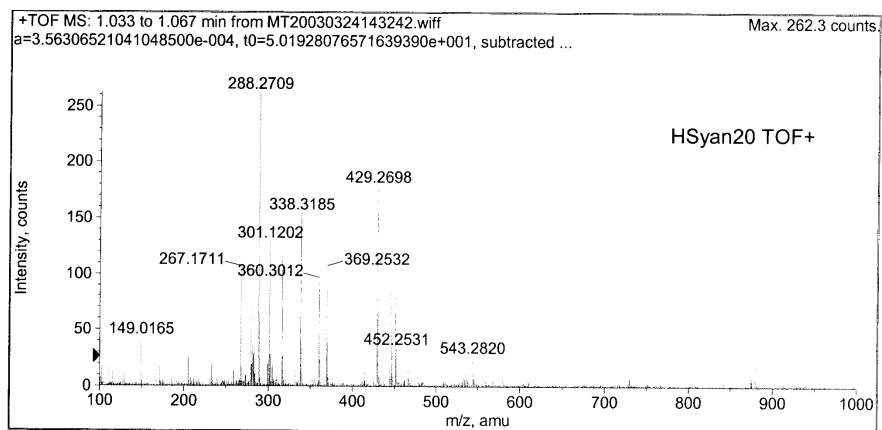


S9: HMQC (500 MHz) Spectrum of Compound

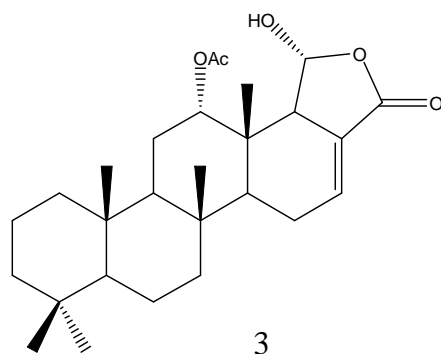


S10: HMBC (500 MHz) Spectrum of Compound 2

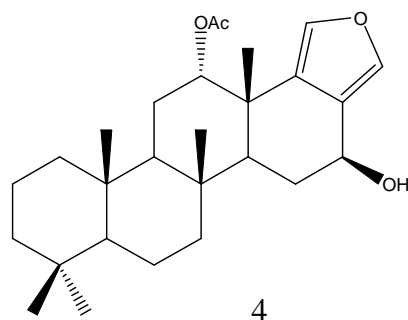
Workstation: QSTAR



S11: HR-MS Spectrum of Compound 2



Compound **3**, white amorphous, $[\alpha]_D^{25} = +43.2$ ($c=0.60$, CHCl_3); ESI-MS: m/z : 445 $[\text{M}+\text{H}]^+$. $^1\text{H-NMR}$ (CDCl_3): δ_{H} 6.82 (1H, br s, H-16), 5.69 (1H, d, $J = 5.5\text{Hz}$, H-19), 4.91 (1H, br s, H-12), 2.11 (3H, s, COCH_3), 0.95 (3H, s, CH_3 -24), 0.88 (3H, s, CH_3 -21), 0.87 (3H, s, CH_3 -23), 0.84 (3H, s, CH_3 -22), 0.82 (3H, s, CH_3 -25); $^{13}\text{C-NMR}$ (CDCl_3): δ_{C} 171.3 (s, CO), 167.8 (s, C-20), 135.2 (d, C-16), 128.1 (s, C-17), 98.3 (d, C-19), 74.6 (d, C-12), 56.4 (d, C-5), 52.4 (d, C-9), 50.6 (d, C-18), 49.8 (d, C-14), 41.9 (t, C-7), 41.4 (t, C-3), 39.7 (t, C-1), 37.8 (s, C-8), 37.2 (s, C-10), 36.8 (s, C-13), 33.28 (s, C-4), 33.25 (q, C-21), 24.2 (t, C-15), 22.3 (t, C-11), 26.7 (q, C-25), 22.3 (t, C-15), 21.4 (q, C-22), 21.3 (q, COCH_3), 18.4 (t, C-6), 18.0 (t, C-2), 16.3 (q, C-23), 16.0 (t, C-24), 15.0 (q, C-25).



Compound **4**, white amorphous, $[\alpha]_D^{25} = +52.0$ ($c=0.40$, CHCl_3); ESI-MS: m/z : 446 $[\text{M}+\text{NH}_4]^+$, 429 $[\text{M}+\text{H}]^+$. $^1\text{H-NMR}$ (CDCl_3): δ_{H} 7.38 (1H, s, H-19), 7.00 (1H, s, H-20), 5.38 (1H, br s, H-12), 4.74 (1H, dd, $J = 10.0, 7.0\text{ Hz}$, H-16), 1.92 (3H, s, COCH_3), 1.33 (3H, s, CH_3 -25), 0.95 (3H, s, CH_3 -24), 0.88 (3H, s, CH_3 -21), 0.85 (3H, s, CH_3 -23), 0.84 (3H, s, CH_3 -22). $^{13}\text{C-NMR}$ (CDCl_3): δ_{C} 170.7 (s, CO), 138.5 (d, C-19), 135.5 (d, C-20), 131.7 (s, C-18), 125.9 (s, C-17), 74.9 (d, C-12), 66.8 (d, C-16), 56.7 (d, C-5), 52.8 (d, C-14), 49.9 (d, C-9), 41.9 (t, C-7), 41.5 (t, C-3), 39.7 (t, C-1), 38.8 (s, C-13), 37.6 (s, C-10), 36.9 (s, C-8), 33.3 (s, C-4), 33.2 (q, C-21), 29.7 (t, C-11), 26.7 (q, C-25), 22.2 (t, C-15), 21.3 (q, COCH_3), 21.3 (q, C-22), 18.5 (t, C-6), 18.1 (t, C-2), 17.5 (q, C-24), 16.0 (q, C-23).

S12: Fundamental structural data for compounds 3 and 4