SUPPORTING INFORMATION

Stereoselective Synthesis of Conjugated Fluoro Enynes

Rakesh Kumar and Barbara Zajc*

Department of Chemistry, The City College and The City University of New York, 160

Convent Avenue, New York, New York 10031

TABLE OF CONTENTS

Information	Page
¹ H NMR of 2-(3-(Trimethylsilyl)prop-2-ynylsulfanyl)benzo[<i>d</i>]thiazole (1)	3
¹³ C NMR of 2-(3-(Trimethylsilyl)prop-2-ynylsulfanyl)benzo[<i>d</i>]thiazole (1)	4
¹ H NMR of 2-[3-(Trimethylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (2)	5
¹³ C NMR of 2-[3-(Trimethylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (2)	6
¹ H NMR of 2-[1-Fluoro-3-(trimethylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (3)	7
¹³ C NMR of 2-[1-Fluoro-3-(trimethylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (3)	8
¹ H NMR of 4 : <i>E</i> / <i>Z</i> 88/12	9
¹³ C NMR of 4 : <i>E</i> / <i>Z</i> 74/26	10
¹ H NMR of 5 : <i>E/Z</i> 95/5	11
¹³ C NMR of 5 : <i>E/Z</i> 81/19	12
¹ H NMR of 6 : <i>E</i> / <i>Z</i> 78/22	13
¹³ C NMR of 6 : <i>E/Z</i> 90/10	14
¹ H NMR of 7 : <i>E/Z</i> 76/24	15
¹³ C NMR of 7 : <i>E</i> / <i>Z</i> 76/24	16
¹ H NMR of 8 : <i>E</i> / <i>Z</i> 70/30	17
¹³ C NMR of 8 : <i>E/Z</i> 70/30	18
¹ H NMR of 9 : <i>E/Z</i> 51/49	19
¹³ C NMR of 9 : <i>E/Z</i> 72/28	20
¹ H NMR of <i>E-</i> 9	21
¹³ C NMR of <i>E-</i> 9	22
¹ H NMR of 10 : <i>E</i> / <i>Z</i> 90/10	23
¹³ C NMR of 10 : <i>E/Z</i> 90/10	24
¹ H NMR of 11 : <i>E</i> / <i>Z</i> 91/9	25
¹³ C NMR of 11 : <i>E/Z</i> 91/9	26
¹ H NMR of 12 : <i>E</i> / <i>Z</i> 75/25	27
¹³ C NMR of 12 : <i>E/Z</i> 75/25	28

¹ H NMR of 13 : <i>E/Z</i> 72/28	29
¹³ C NMR of 13 : <i>E/Z</i> 72/28	30
¹ H NMR of 14 : <i>E</i> / <i>Z</i> 80/20	31
¹³ C NMR of 14 : <i>E</i> / <i>Z</i> 70/30	32
¹ H NMR of 15 : <i>E</i> / <i>Z</i> 85/15	33
¹³ C NMR of 15 : <i>E/Z</i> 85/15	34
¹ H NMR of 16	35
¹³ C NMR of 16	36
¹ H NMR of <i>E-</i> 17	37
¹³ C NMR of <i>E</i> - 17	38
¹ H NMR of 2-[3-(Triisopropylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (18)	39
¹³ C NMR of 2-[3-(Triisopropylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (18)	40
¹ H NMR of 2-[1-Fluoro-3-(triisopropylsilyl)prop-2-ynylsulfonyl]benzo[<i>d</i>]thiazole (19)	41
¹³ C NMR of 2-[1-Fluoro-3-(triisopropylsilyl)prop-2-ynylsulfonyl]benzo[d]thiazole (19)	42
¹ H NMR of 20 : <i>E</i> / <i>Z</i> 71/29	43
¹³ C NMR of 20 : <i>E</i> / <i>Z</i> 71/29	44
¹ H NMR of 21 : <i>E</i> / <i>Z</i> 76/24	45
¹³ C NMR of 21 : <i>E</i> / <i>Z</i> 76/24	46
¹ H NMR of 22 : <i>E</i> / <i>Z</i> 93/7	47
¹³ C NMR of 22 : <i>E</i> / <i>Z</i> 93/7	48
¹ H NMR of 23	49
¹³ C NMR of 23	50
¹ H NMR of 24	51
¹³ C NMR of 24	52
¹ H NMR of 25	53
¹³ C NMR of 25	54
¹ H NMR of 26	55
¹³ C NMR of 26	56
¹ H NMR of (<i>E</i>)-(3-Fluoropenta-2,4-dien-2-yl)benzene	57
NOESY of (E)-(3-Fluoropenta-2,4-dien-2-yl)benzene	58

Due to volatility of some products, removal of solvent traces was difficult, therefore some spectra may contain traces of hexanes used in chromatography.











1222-RK-02-144-13C

Pulse Sequence: s2pul

Solvent: CDC13 Temp. 25.0 C / 298.1 K Operatori barbara File: 1222-RK-02-144-13C INOVA-500 "riga" Relar. delary 4.000 sec Pulse 52.1 degrees Acq. time 1.000 sec Midth 29996.3 Hz 100 repetitions 0BSENVE C13, 125.6674411 NHz 0 during acquisition MALTP-16 modulated DATA PROCESSING Line broadening 1.0 Hz 1 rise 111072 Total time 9 min, 12 sec















Archive directory: /export/home/mkl/vnmrsys/data	
Sample directory: auto_13Dec2004	
Pulse Sequence: s2pul	
Solvent: cdcl3	
Temp. 25.0 C / 298.1 K	<u> </u>
Operator: barbara	Ξ
File: 1222-RK-03-187-pure	6 : <i>E</i> / <i>Z</i> 78/22
INOVA-500 "riga"	500 MHz. CDCIa
Relax. delay 1.000 sec	
Pulse 45.0 degrees	
Acq. time 1.892 sec	
Width 7544.3 Mrz	
32 repetitions	
OBSERVE H1, 499.7707212 NHz	
DATA PROCESSING	
Line broadening 0.5 Hz	
FT size 32768	
Total time 1 min, 32 sec	
-	

mqq

H

2

ŝ

4

ĿO

9

œ

















Fulse Sequence: s2pul











1222-RK-03-223-pure

Archive directory: /export/home/mkl/vnmrsys/data Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solventi cdcl3 Temp. 25.0 C / 298.1 K Operator: barbara File: 1222-RK-03-223-pure INOVA-500 "riga" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.092 sec Width 7544.3 Mz 20 repetitions OBSERVE H1, 499.7707207 NHz DATA PROCESSING Line broadening 2.0 Hz T size 32768 Total time 1 min, 32 sec



















Pulse Sequence: s2pul Solvent: CDC13 Temp. 25.0 C / 298.1 K Operator: barbara File: 1222-RK-10-750 INOVA-500 "riga" Relar. delay 3.000 sec Pulse 57.9 degrees Acq. time 1.892 sec Width 8000.0 Hz 16 repetitions OMSERVE H1, 499.7707212 NHz DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 16 min, 20 sec







1231-8K-10-750-13C

1231-RK-14-43-pure-rxn2

Archive directory: /export/home/mkl/vnmrsys/data Sample directory: auto_13Dec2004

Pulse Sequence: s2pul

Solvent: cdcl3 Temp. 24.0 C / 297.1 K Operator: barbara File: 1231-RK-14-43-pure-rxn2 INOVA-500 "riga" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.892 sec Width 7544.3 Hz 32 repetitions OBSERVE H1, 499.7707216 MHz DATA PROCESSING Line broadening 0.1 Hz FI size 3768 Total time 9 min, 40 sec

























mqq











1231-RK-15-21-pure

Archive directory: /export/home/mkl/vnmrsys/data Sample directory: auto_13Dec2004 File: 1231-RK-15-21-pure

Pulse Sequence: s2pul

Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: barbara File: 1231-RK-15-21-pure INOVA-500 "capella500" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.892 sec Width 7544.3 Hz 24 repetitions OBSERVE H1, 499.7707216 MHz OBSERVE H1, 499.7707216 MHz DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 9 min, 40 sec



















































CH₃ NOESY correlation