Supporting Information

Pd-Catalyzed Asymmetric Allylic Amination of Morita-Baylis-Hillman Adduct Derivatives Using Chiral Diaminophosphine Oxides: DIAPHOXs

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Supporting Information (2)

- 8. ^1H NMR and ^{13}C NMR charts for Purity Documentation**

F:\fukuyama\data\yk-mt-substrate_1.als
yk-mt-substrate

DFILE F:\fukuyama\data\yk-mt-subst
COMNT yk-mt-substrate
DATIM 15-MAR-2006 17:24:50
OBNUC 1H
EXMOD single pulse.exp
OBFRQ 399.00 MHz
OBSET 784.00 KHz
OBFIN 597.1 Hz
POINT 32768
FREQU 5998.8 Hz
SCANS 16
ACQTM 5.462 sec
PD 2.000 sec
PW1 6.8 us
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

F:\fukuyama\data\yk-mt-substrate-13c_1.als
yk-mt-substrate-13c

DFILE F:\fukuyama\data\yk-mt-subst
COMNT yk-mt-substrate-13c
DATIM 15-MAR-2006 17:30:13
OBNUC 13C
EXMOD single pulse dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 43
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 29

S-21

F:\07\YKBT-7-10P.NMF;1
YKBT-7-10P

DFILE F:\07\YKBT-7-10P.NMF;1
COMNT YKBT-7-10P
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 25
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 25.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

F:\07\YKBT-7-10PBCM.NMF;1
YKBT-7-10PBCM

DFILE F:\07\YKBT-7-10PBCM.NMF;1
COMNT YKBT-7-10PBCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 18
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 25.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-22

DFILE F:\04\YKBT-4-28PRO.NMF;1
COMNT YKBT-4-28PRO
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14

DFILE F:\04\YKBT-4-28PROBCM.NMF;1
COMNT YKBT-4-28PROBCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 49
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

F:\06\YKBT-6-56P.NMF;1
YKBT-6-56P

DFILE F:\06\YKBT-6-56P.NMF;1
COMNT YKBT-6-56P
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 24.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

F:\06\YKBT-6-56PBCM.NMF;1
YKBT-6-56PBCM

DFILE F:\06\YKBT-6-56PBCM.NMF;1
COMNT YKBT-6-56PBCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 41
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 24.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-24

F:\Data\YK-EY-DATA-WEIN-SM-1H.als
YK-EY-DATA-WEIN-SM-1H

DFILE F:\Data\YK-EY-DATA-WEIN-SM-1H
COMNT YK-EY-DATA-WEIN-SM-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 25.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

F:\Data\YK-EY-DATA-WEIN-SM-13C.als
YK-EY-DATA-WEIN-SM-13C

DFILE F:\Data\YK-EY-DATA-WEIN-SM-13C
COMNT YK-EY-DATA-WEIN-SM-13C
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 184
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 26.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

S-25

F:\Data\YK-EY-DATA-CN-SM-1H.als
YK-EY-DATA-CN-SM-1H

DFILE F:\Data\YK-EY-DATA-CN-SM-1H.als
COMNT YK-EY-DATA-CN-SM-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 25.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

F:\Data\YK-EY-DATA-CN-SM-13C.als
YK-EY-DATA-CN-SM-13C

DFILE F:\Data\YK-EY-DATA-CN-SM-13C.als
COMNT YK-EY-DATA-CN-SM-13C
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 171
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 26.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

S-26

F:\Data\YK-EY-DATA-L-CN-SM-1H-2.als
YK-EY-DATA-L-CN-SM-1H

DFILE F:\Data\YK-EY-DATA-L-CN-SM-1H
COMNT YK-EY-DATA-L-CN-SM-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFREQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

F:\Data\YK-EY-DATA-L-CN-SM-13C.als
YK-EY-DATA-L-CN-SM-13C

DFILE F:\Data\YK-EY-DATA-L-CN-SM-13C
COMNT YK-EY-DATA-L-CN-SM-13C
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFREQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 137
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

S-27

DFILE E:\03\YKBT-3-15P.als
COMNT YKBT-3-15P
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 2.500 sec
PW1 3.9 us
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

4aa

DFILE E:\03\YKBT-3-15PBCM.als
COMNT YKBT-3-15PBCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 64
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-28

E:\fukuyama\data\yk-mt-PMB_1.als
yk-mt-PMB

DFILE E:\fukuyama\data\yk-mt-PMB_1
COMNT yk-mt-PMB
DATIM 16-MAR-2006 15:26:54
OBNUC 1H
EXMOD single pulse.exp
OBFRQ 399.00 MHz
OBSET 784.00 KHz
OBFIN 597.1 Hz
POINT 32768
FREQU 5998.8 Hz
SCANS 6
ACQTM 5.462 sec
PD 2.000 sec
PW1 6.8 us
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14

E:\fukuyama\data\yk-mt-PMB-13c_1.als
yk-mt-PMB-13c

DFILE E:\fukuyama\data\yk-mt-PMB-1-
COMNT yk-mt-PMB-13c
DATIM 16-MAR-2006 15:32:18
OBNUC 13C
EXMOD single pulse_dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 41
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 29

S-29

E:\03\YKBT-3-44P.als
YKBT-3-44P

DFILE E:\03\YKBT-3-44P.als
COMNT YKBT-3-44P
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 2.500 sec
PW1 3.9 us
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

E:\03\YKBT-3-44BCM.NMF;1
YKBT-3-44BCM

DFILE E:\03\YKBT-3-44BCM.NMF;1
COMNT YKBT-3-44BCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 34
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-30

F:\07\YKBT-7-37P.NMF;1
YKBT-7-37P

DFILE F:\07\YKBT-7-37P.NMF;1
COMNT YKBT-7-37P

1H
SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 9
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 26.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

F:\07\YKBT-7-37PBCM.NMF;1
YKBT-7-37PBCM

DFILE F:\07\YKBT-7-37PBCM.NMF;1
COMNT YKBT-7-37PBCM

13C
SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 121
ACQTM 1.209 sec
PD 2.500 sec
PW1 4.9 us
IRNUC 1H
CTEMP 27.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-31

DFILE E:\03\YKBT-3-46P.als
COMNT YKBT-3-46P
DATIM
OBNUC
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 19.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

DFILE E:\03\YKBT-3-46PBCM.NMF;1
COMNT YKBT-3-46PBCM
DATIM
OBNUC
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 64
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-32

E:\03\YKBT-3-51P.als
YKBT-3-51P

DFILE E:\03\YKBT-3-51P.als
COMNT YKBT-3-51P
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 20.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

E:\03\YKBT-3-51PBCM.als
YKBT-3-51PBCM

DFILE E:\03\YKBT-3-51PBCM.als
COMNT YKBT-3-51PBCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 64
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-33

E:\fukuyama\data\yk-mt-mor_1.als
yk-mt-mor

DFILE E:\fukuyama\data\yk-mt-mor_1
COMNT yk-mt-mor
DATIM 16-MAR-2006 15:36:32
OBNUC 1H
EXMOD single pulse.exp
OBFRQ 399.00 MHz
OBSET 784.00 KHz
OBFIN 597.1 Hz
POINT 32768
FREQU 5998.8 Hz
SCANS 16
ACQTM 5.462 sec
PD 2.000 sec
PW1 6.8 us
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14

4ag

E:\fukuyama\data\yk-mt-mor-13c_1.als
yk-mt-mor-13c

DFILE E:\fukuyama\data\yk-mt-mor-1
COMNT yk-mt-mor-13c
DATIM 16-MAR-2006 15:40:09
OBNUC 13C
EXMOD single pulse dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 22
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 28

S-34

E:\data\YK-TN-061231-data_1.als
YK-TN-061231-data

DFILE E:\data\YK-TN-061231-data_1.als
COMPT YK-TN-061231-data
DATIM 31-DEC-2006 18:16:39
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.00 MHz
OBSET 734.00 KHz
OBFIN 597.1 Hz
POINT 32763
FREQU 5993.3 Hz
SCANS 3
ACQTM 5.462 sec
PD 2.300 sec
PWL 6.7 us
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 3.00 ppm
BF 3.12 Hz
RGAIN 21

4ah

E:\data\YK-TN-061231-data-13C_1.als
YK-TN-061231-data-13C

DFILE E:\data\YK-TN-061231-data-13C
COMPT YK-TN-061231-data-13C
DATIM 31-DEC-2006 19:26:21
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 1000
ACQTM 2.602 sec
PD 1.500 sec
PWL 3.5 us
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 29

S-35

DFILE F:\03\YKBT-3-27PRODUCT.NMF;1
COMNT YKBT-3-27PRODUCT
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 15
ACQTM 4.099 sec
PD 2.500 sec
PW1 3.9 us
IRNUC 1H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

DFILE F:\03\YKBT-3-27BCM.NMF;1
COMNT YKBT-3-27BCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 29
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

F:\04\YKBT-4-44PRODUCT.NMF;1
YKBT-4-44PRODUCT

DFILE F:\04\YKBT-4-44PRODUCT.NMF;1
COMNT YKBT-4-44PRODUCT
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 3.000 sec
PW1 3.9 us
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

F:\04\YKBT-4-44BCM.NMF;1
YKBT-4-44BCM

DFILE F:\04\YKBT-4-44BCM.NMF;1
COMNT YKBT-4-44BCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 49
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 24.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-37

F:\06\YKBT-6-62P.NMF;1
YKBT-6-62P

DFILE F:\06\YKBT-6-62P.NMF;1
COMNT YKBT-6-62P
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 24.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

F:\06\YKBT-6-72BCM.NMF;1
13C-COM

DFILE F:\06\YKBT-6-72BCM.NMF;1
COMNT 13C-COM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 41
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 26.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-38

F:\Data\YK-EY-DATA-WEIN-BN-1H.als
YK-EY-DATA-WEIN-BN-1H

DFILE F:\Data\YK-EY-DATA-WEIN-BN-1H
COMNT YK-EY-DATA-WEIN-BN-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 25.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

F:\Data\YK-EY-DATA-WEIN-BN-13C.als
YK-EY-DATA-WEIN-BN-13C

DFILE F:\Data\YK-EY-DATA-WEIN-BN-13C
COMNT YK-EY-DATA-WEIN-BN-13C
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 96
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 26.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

S-39

DFILE F:\Data\YK-EY-DATA-CN-BN-1H.als
COMNT YK-EY-DATA-CN-BN-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 26.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19

4fa

DFILE F:\Data\YK-EY-DATA-CN-BN-13C.als
COMNT YK-EY-DATA-CN-BN-13C
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 138
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 26.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-40

F:\Data\YK-EY-DATA-L-CN-BN-1H-2.als
YK-EY-DATA-L-CN-BN-1H-2

DFILE F:\Data\YK-EY-DATA-L-CN-BN-1H-2.als
COMNT YK-EY-DATA-L-CN-BN-1H-2
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 23

4ga

F:\Data\YK-EY-DATA-L-CN-BN-13C.als
YK-EY-DATA-L-CN-BN-13C

DFILE F:\Data\YK-EY-DATA-L-CN-BN-13C.als
COMNT YK-EY-DATA-L-CN-BN-13C
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 188
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

S-41

DFILE F:\No.15\YK-TN-15-26-1H_1.als
COMNT YK-TN-15-26-1H
DATIM 14-AUG-2006 21:10:00
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.00 MHz
OBSET 784.00 KHz
OBFIN 597.1 Hz
POINT 32768
FREQU 5998.8 Hz
SCANS 16
ACQTM 5.462 sec
PD 2.000 sec
PW1 6.8 us
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

DFILE F:\No.15\YK-TN-15-26-13C_1.als
COMNT YK-TN-15-26-13C
DATIM 14-AUG-2006 21:27:03
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 200
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 29

S-42

DFILE F:\07\YKBT-7-34-PRODUCT.NMF;1
COMNT YKBT-7-34-PRODUCT
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFREQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 26.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

DFILE F:\07\YKBT-7-34PBCM.NMF;1
COMNT YKBT-7-34PBCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFREQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 19
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 24.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-43

F:\07\YKBT-7-4P.NMF;1
YKBT-7-4P

DFILE F:\07\YKBT-7-4P.NMF;1
COMNT YKBT-7-4P
DATIM
OBNUC
EXMOD
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 24.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

7

F:\07\ykbt-7-4p-bcm_1.als
ykbt-7-4p-bcm

DFILE F:\07\ykbt-7-4p-bcm_1.als
COMNT ykbt-7-4p-bcm
DATIM 27-JUL-2006 00:13:12
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 152
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 29

S-44

F:\07\YKBT-7-50-1.NMF;1
YKBT-7-50-1

DFILE F:\07\YKBT-7-50-1.NMF;1
COMNT YKBT-7-50-1
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 16
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 26.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

F:\07\YKBT-7-50-1BCM.NMF;1
YKBT-7-50-1BCM

DFILE F:\07\YKBT-7-50-1BCM.NMF;1
COMNT YKBT-7-50-1BCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 700
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 26.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-45

DFILE F:\09\YKBT-9-13-1H.als
COMNT YKBT-9-13-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22

DFILE F:\DATA\YKBT-KETONE-DATA-BCM.
COMNT YKBT-KETONE-DATA-BCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 64
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-46

F:\08\YKBT-8-1PRO.NMF;1
YKBT-8-1PRO

DFILE F:\08\YKBT-8-1PRO.NMF;1
COMNT YKBT-8-1PRO
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 9
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 28.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

10

F:\08\ykbt-8-1bcm.als
13C-COM

DFILE F:\08\ykbt-8-1bcm.als
COMNT 13C-COM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 64
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 29.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-47

F:\09\YKBT-9-62PRO-1H.NMF;1
YKBT-9-62PRO-1H

DFILE F:\09\YKBT-9-62PRO-1H.NMF;1
COMNT YKBT-9-62PRO-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 17
ACQTM 4.099 sec
PD 3.000 sec
PW1 3.9 us
IRNUC 1H
CTEMP 23.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

F:\09\YKBT-9-62PROBCM.NMF;1
13C-COM

DFILE F:\09\YKBT-9-62PROBCM.NMF;1
COMNT 13C-COM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 18
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 23.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

S-48

F:\DATA\YKBT-DIELS-1H.NMF;1
YKBT-DIELS-1H

DFILE F:\DATA\YKBT-DIELS-1H.NMF;1
COMNT YKBT-DIELS-1H
DATIM
OBNUC 1H
EXMOD SINGL-NON
OBFRQ 399.65 MHz
OBSET 130.00 KHz
OBFIN 4500.0 Hz
POINT 32768
FREQU 7993.6 Hz
SCANS 33
ACQTM 4.099 sec
PD 2.500 sec
PW1 4.0 us
IRNUC 1H
CTEMP 49.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

F:\07\YKBT-7-57P2BCM.NMF;1
YKBT-7-57P2BCM

DFILE F:\07\YKBT-7-57P2BCM.NMF;1
COMNT YKBT-7-57P2BCM
DATIM
OBNUC 13C
EXMOD SINGL-BCM
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.0 Hz
POINT 32768
FREQU 27100.3 Hz
SCANS 4910
ACQTM 1.209 sec
PD 3.700 sec
PW1 4.9 us
IRNUC 1H
CTEMP 28.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 24

S-49

F:\fukuyama\data\yk-mt-lig_1.als
yk-mt-lig

DFILE F:\fukuyama\data\yk-mt-lig_1.
COMNT yk-mt-lig
DATIM 17-MAR-2006 14:44:31
OBNUC 1H
EXMOD single pulse.exp
OBFRQ 399.00 MHz
OBSET 784.00 KHz
OBFIN 597.1 Hz
POINT 32768
FREQU 5998.8 Hz
SCANS 6
ACQTM 5.462 sec
PD 2.000 sec
PW1 6.8 us
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

F:\fukuyama\data\yk-mt-lig-13c_1.als
yk-mt-lig-13c

DFILE F:\fukuyama\data\yk-mt-lig-13c
COMNT yk-mt-lig-13c
DATIM 17-MAR-2006 15:00:35
OBNUC 13C
EXMOD single pulse dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 200
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 29

S-50

DFILE F:\No.12\YK-TN-12-46-product_1.als
COMNT YK-TN-12-46-product
DATIM 4-OCT-2005 16:16:12
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.00 MHz
OBSET 784.00 KHz
OBFIN 597.1 Hz
POINT 32768
FREQU 5998.8 Hz
SCANS 4
ACQTM 5.462 sec
PD 2.000 sec
PW1 6.8 us
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 21

DFILE F:\data\YK-TN-060825-CF3-ligand-13C_1.als
COMNT YK-TN-060825-CF3-ligand-13C
DATIM 25-AUG-2006 21:51:47
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.00 MHz
OBSET 536.00 KHz
OBFIN 361.1 Hz
POINT 65536
FREQU 25188.9 Hz
SCANS 699
ACQTM 2.602 sec
PD 1.500 sec
PW1 3.5 us
IRNUC 1H
CTEMP 25.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 28

S-51