Pin1 Catalytic and WW Domain Ligands

by

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Appendix-Spectra of Characterized Compounds

Should you have any questions, please contact Dr. Felicia Etzkorn at fetzkorn@vt.edu or Xingguo Chen at xgchen@vt.edu.
$^1$H NMR of 1-iodocyclohexene in CDCl$_3$ (500 MHz)
$^{13}$C NMR of 1-iodocyclohexene in CDCl$_3$ (125 MHz)
$^1$H NMR of (S)-2.2 in CDCl$_3$ (400 MHz)
$^1$H NMR of (S)-2.2 in CDCl$_3$ (100 MHz)
$^1$H NMR of the mixture of (2S,3R)- and (2S,3S)-2,3 in CDCl$_3$ (500 MHz)
\(^1\)H NMR of (2S,3R)-2.4 in CDCl\(_3\) (500 MHz)
$^{13}$C NMR of (2S,3R)-2.4 in CDCl$_3$ (100 MHz)
Analytical HPLC of (2S,3R)-2.4
Analytical HPLC of (2R,3S)-2.4
$^1$H NMR of (2R,3R)-2.4 in CDCl$_3$ (400 MHz)
$^{13}$C NMR of (2R,3R)-2.4 in CDCl$_3$ (100 MHz)
$^1$H NMR of (2S,3R)-2.5 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2$S$,3$R$)-2.5 in CDCl$_3$ (100 MHz)
$^1\text{H NMR of (2R,3R)-2.5}$ in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2$R$,3$R$)-2.5 in CDCl$_3$ (100 MHz)
$^{13}$C NMR of (2R,5S)-2.6 in CDCl$_3$ (100 MHz)
1D nOe of (2R,5S)-2.6 in CDCl₃ (100 MHz)
Analytic HPLC of (2R,5S)-2.6
$^1$H NMR of (2S,5S)-2,6 in CDCl₃ (500 MHz)
$^{13}$C NMR of (2S,5S)-2,6 in CDCl$_3$ (125 MHz)
COSY of (2S,5S)-2,6 in CDCl₃ (500 MHz)
1D nOe of (2S,5S)-2.6 in CDCl₃ (400 MHz)
$^1$H NMR of (2R,5S)-2.7 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2R,5S)-2.7 in CDCl$_3$ (125 MHz)
$^1$H NMR of (2S,5S)-2.7 in CDCl$_3$ (500 MHz)
$^1$H NMR of (2R,5S)-2.8 in CDCl$_3$ (500 MHz)
$^1$H NMR of (2R,5S)-2.8 in DMSO-d6 (500 MHz)
$^{13}$C NMR of (2R,5S)-2.8 in CDCl$_3$ (125 MHz)
Analytical HPLC of (2R,5S)-2.8
Analytical HPLC of \((2S,5R)\)-2.8
$^1$H NMR of (2S,5S)-2.8 in CDCl$_3$ (400 MHz)
$^{13}$C NMR of (2S,5S)-2.8 in CDCl$_3$ (100 MHz)
$^1$H NMR of (2R,5S)-2.9 in CDCl$_3$ (500 MHz)
Analytical HPLC of (2S,5R)-2.9
$^1$H NMR of (2S,5S)-2.9 in CDCl$_3$ (400 MHz)
$^{13}$C NMR of (2S,5S)-2.9 in CDCl$_3$ (100 MHz)
$^1$H NMR of (2R,5S)-2.10 in CD$_3$OD (500 MHz)
$^1$H NMR of (2R,5S)-2.10 in CD$_3$OD (125 MHz)
Analytical HPLC of (2R,5S)-2.10
$^1$H NMR of (2S,5S)-2.10 in CD$_3$OD (500 MHz)
$^{13}$C NMR of (2S,5S)-2.10 in CD$_3$OD (125 MHz)
$^1$H NMR of (2R,5S)-2.11 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2R,5S)-2.11 in CDCl₃ (125 MHz)
Analytical HPLC of (2S,5R)-2.11
$^1$H NMR of (2S,5S)-2.1 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2S,5S)-2.11 in CDCl$_3$ (125 MHz)
Analytical HPLC of (2S,5S)-2.11
$^1$H NMR of (2R,5S)-2.12 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2R,5S)-2.12 in CDCl$_3$ (125 MHz)
$^{31}$P NMR of (2R,5S)-2.12 in CDCl$_3$ (202 MHz)
$^{31}P$ NMR of (2R,5S)-2.12 in CDCl$_3$ (202 MHz)
$^1$H NMR of (2S,5S)-2.12 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2S,5S)-2.12 in CDCl$_3$ (125 MHz)
Analytical HPLC of (2S,5S)-2.12
$^1$H NMR of (2R,5S)-2,1 in CD$_3$OD (500 MHz)
$^{13}$C NMR of (2R,5S)-2.1 in CD$_3$OD (125 MHz)
$^{31}$P NMR of (2R,5S)-2.1 in CD$_3$OD (202 MHz)
Analytic HPLC of $(2R,5S)\cdot 2.1$
Analytic HPLC of ($2S,5R$)-2.1
$^1$H NMR of (2S,S)-2.1 in CD$_3$OD (500 MHz)
$^{13}$C NMR of (2S,5S)-2,1 in DMSO-d$_6$ (125 MHz)
$^3$P NMR of (2S,5S)-2.1 in DMSO-d$_6$ (162 MHz)
$^{31}$P NMR of (2S,5S)-2.1 in DMSO-d6 (162 MHz)
Analytical HPLC of (2S,5S)-2.1
$^{1}H$ NMR of the mixture of $(2R,3R)$- and $(2R,3S)$-2,13 in CDCl$_3$ (500 MHz)
\( ^1H \) NMR of \((2S,5S)-2.14\) in CDCl\(_3\) (500 MHz)
$^{13}$C NMR of \((2S, 5S)-2.14\) in CDCl$_3$ (125 MHz)
COSY of (2S,5S)-2.14 in CDCl3 (500 MHz)
NOESY of (2S,5S)-2.14 in CDCl$_3$ (400 MHz)
$^1$H NMR of (2S,5S)-2.14 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of (2S,5R)-2.14 in CDCl$_3$ (125 MHz)
COSY of (2S,5R)-2.14 in CDCl₃ (500 MHz)
1D nOe of (2S,5R)-2.14 in CDCl₃ (400 MHz)
$^1$H NMR of the mixture of 2-cyanoethyl phosphite and $i$Pr$_2$NH · TFA salt in CDCl$_3$ (400 MHz)
$^1$H NMR of 4.4 in CDCl$_3$ (500 MHz)
$^{13}$C NMR of 4.4 in CDCl$_3$ (125 MHz)
$^{1}$H NMR of 4.5 in DMSO-d6 (500 MHz)
$^1$H NMR of 4.5 in DMSO-d6 (125 MHz)
$^1$H NMR of 4.6 in CDCl$_3$ (500 MHz)
$^1$H NMR of 4.10a{21} in CD$_3$OD (500 MHz)
$^1$H NMR of 4.1{21, l} in CD$_3$OD (500 MHz)
$^{31}$P NMR of 4.1(21, l) in CD$_3$OD (202 MHz)
$^1$H NMR of crude product of 4.1(2, d) in CD$_3$OD (500 MHz)
$^1$H NMR of cis-4.1{2, d} in DMSO-d6 (500 MHz)
$^{13}$C NMR of cis-4.1\{2, d\} in DMSO-d6 (125 MHz)
$^3$P NMR of cis-4,l (2, d) in DMSO-d$_6$ (202 MHz)
$^{31}$P NMR of cis-4.1{2, d} in DMSO-d6 (202 MHz)
$^1$H NMR of trans-4.1{2, d} in DMSO-d6 (500 MHz)
$^{13}$C NMR of trans-4.1 2, d in DMSO-d$_6$ (125 MHz)
$^{31}$P NMR of trans-4.1{2, d} in DMSO-d6 (202 MHz)
$^{31}$P NMR of trans-4.1{2, d} in DMSO-d6 (202 MHz)
$^1$H NMR of 4.1{2, o} in DMSO-d6 (500 MHz)
$^{13}$C NMR of 4.1{2, o} in DMSO-d6 (125 MHz)
$^{31}$P NMR of 4.1{2, o} in DMSO-d6 (202 MHz)
$^{31}$P NMR of 4.1{2, o} in DMSO-d6 (202 MHz)
$^1$H NMR of 4.1{18, m} in CD$_3$OD (500 MHz)
$^{13}$C NMR of 4.1\{18, m\} in CD$_3$OD (125 MHz)
$^{31}\text{P}$ NMR of 4.1{18, m} in CD$_3$OD (202 MHz)
$^{31}$P NMR of 4.1\{18, m\} in CD$_3$OD (202 MHz)
$^1$H NMR of (2S,5R)-2.1 in CD$_3$OD (500 MHz), peaks for DBU are marked with *