

NMR data – file names for compound numbers/names

Compound 2: ASC004

¹H-NMR: 30

Compound 3: WKU180

¹H-NMR: 10

¹³C-NMR: 11

Compound S2: WKU166

¹H-NMR: 20

¹³C-NMR: 21

Compound 4: WKU168

¹H-NMR: 1

¹³C-NMR: 21

Compound 5: WKU185

¹H-NMR: 10

¹³C-NMR: 13

Compound 6: WKU188

¹H-NMR: 20

¹³C-NMR: 21

Compound ax-7: WKU189

¹H-NMR: 30

¹³C-NMR: 13

Compound equ-7: WKU189

¹H-NMR: 20

¹³C-NMR: 23

Compound S3: WKU194

¹H-NMR: 10

¹³C-NMR: 11

Compound 14: WKU283

¹H-NMR: 30

¹³C-NMR: 31

Compound NMe-13: ASC242

¹H-NMR: 190

¹³C-NMR: 194

Compound 9: WKU309

¹H-NMR: 20

Compound 16: WKU253

¹H-NMR: 10

¹³C-NMR: 11

iTCO-MMAE: ASC055

¹H-NMR: 50

¹³C-NMR: 54

iTCO-Dox: ASC227

¹H-NMR: 50

¹³C-NMR: 54

iTCO-CA4: SCS081

¹H-NMR: 14

¹³C-NMR: 11

Compound S4: HES736

¹H-NMR: 1

¹³C-NMR: 5

Compound S5: MST026

¹H-NMR: 4

Compound S7: MST031

¹H-NMR: 1

4,5-DHP formed after reaction of **NMe-13** and Pyr₂ (**1**): ASC242

¹H-NMR: 40

Oxidized cyclic elimination product P_{io} with DMT: WKU285

¹H-NMR: 10

¹³C-NMR: 11

HMBC: 14

Aromatic elimination product P_a with DMT: WKU285

¹H-NMR: 20

¹³C-NMR: 41

HMBC: 43

Cyclic elimination product P_i with Pyr₂: WKU299

¹H-NMR: 10

HMBC: 16

Oxidized cyclic elimination product P_{io} with Pyr₂: WKU285

¹H-NMR: 10

¹³C-NMR: 51

HMBC: 58