

Thiazole-fused Androstene and Ethisterone Derivatives: Potent β - and γ -Actin Cytoskeleton Inhibitors to Treat Melanoma Tumors

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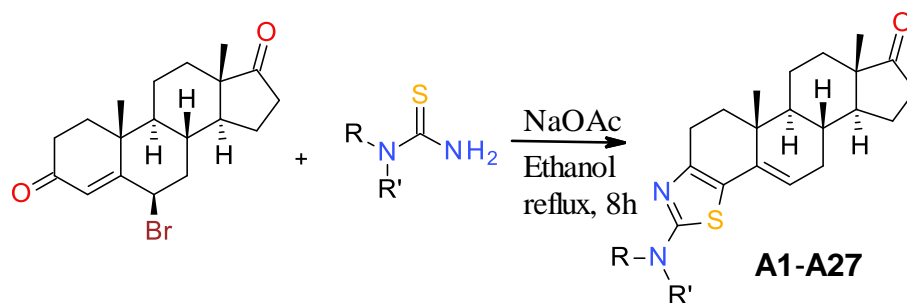
⁹Arkansas Biosciences Institute, Arkansas State University, Jonesboro, AR, 72467, USA

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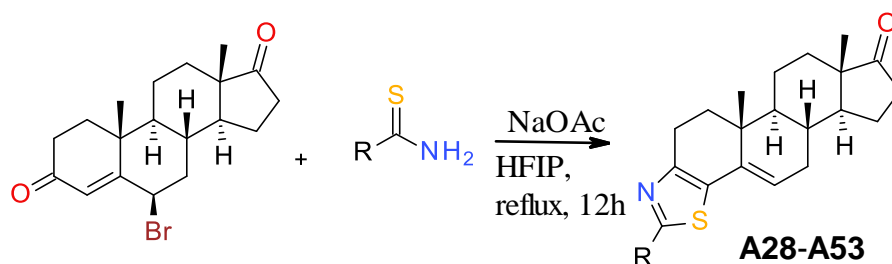
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Synthesis of fused-thiazolo androstenedione

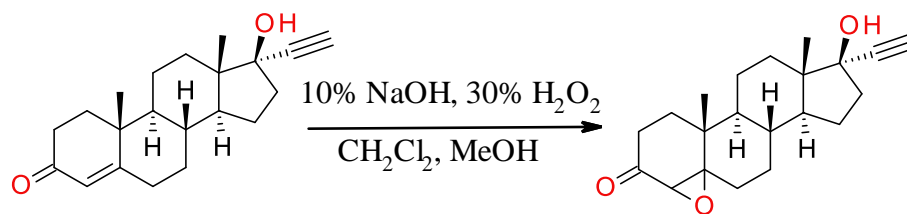


Scheme S1: Synthesis of fused aminothiazolo-androstenedione derivatives (A1-A27)



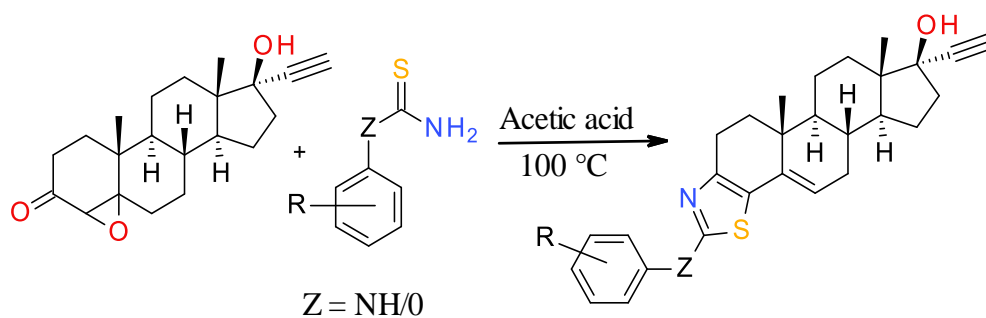
Scheme S2: Synthesis of fused thiazol-androstenedione derivatives (A1-A27)

Synthesis of ethisterone-epoxyketone



Scheme S3: Synthesis of epoxy ethisterone

Synthesis of fused thiazolo-ethisterone



Scheme S4: Synthesis of fused thiazolo-ethisterone derivatives

(1*S*,2*R*,13*R*,14*S*,18*S*)-7-(4-Fluoroanilino)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-one (A15)

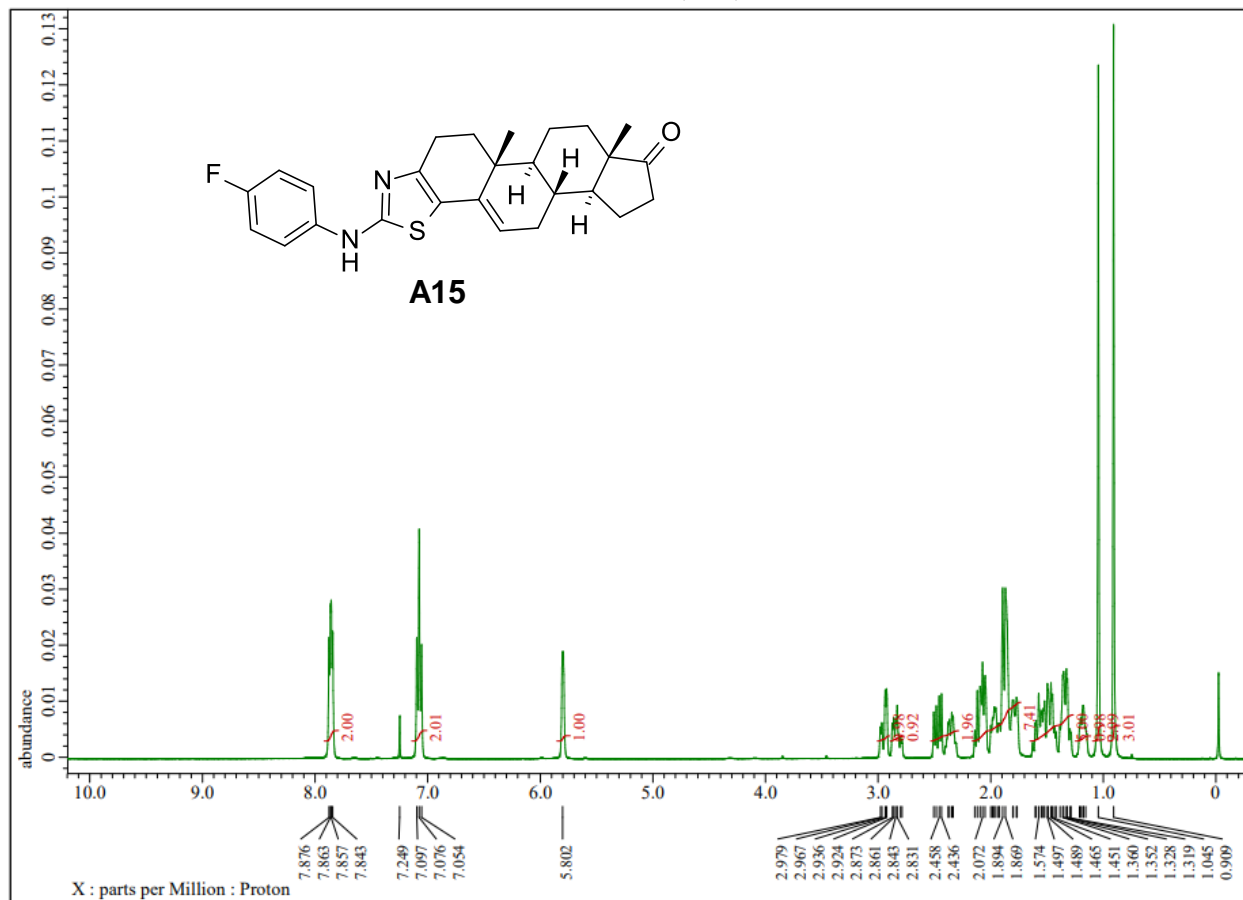


Figure S-1: ¹H NMR spectrum of compound A15 in CDCl₃

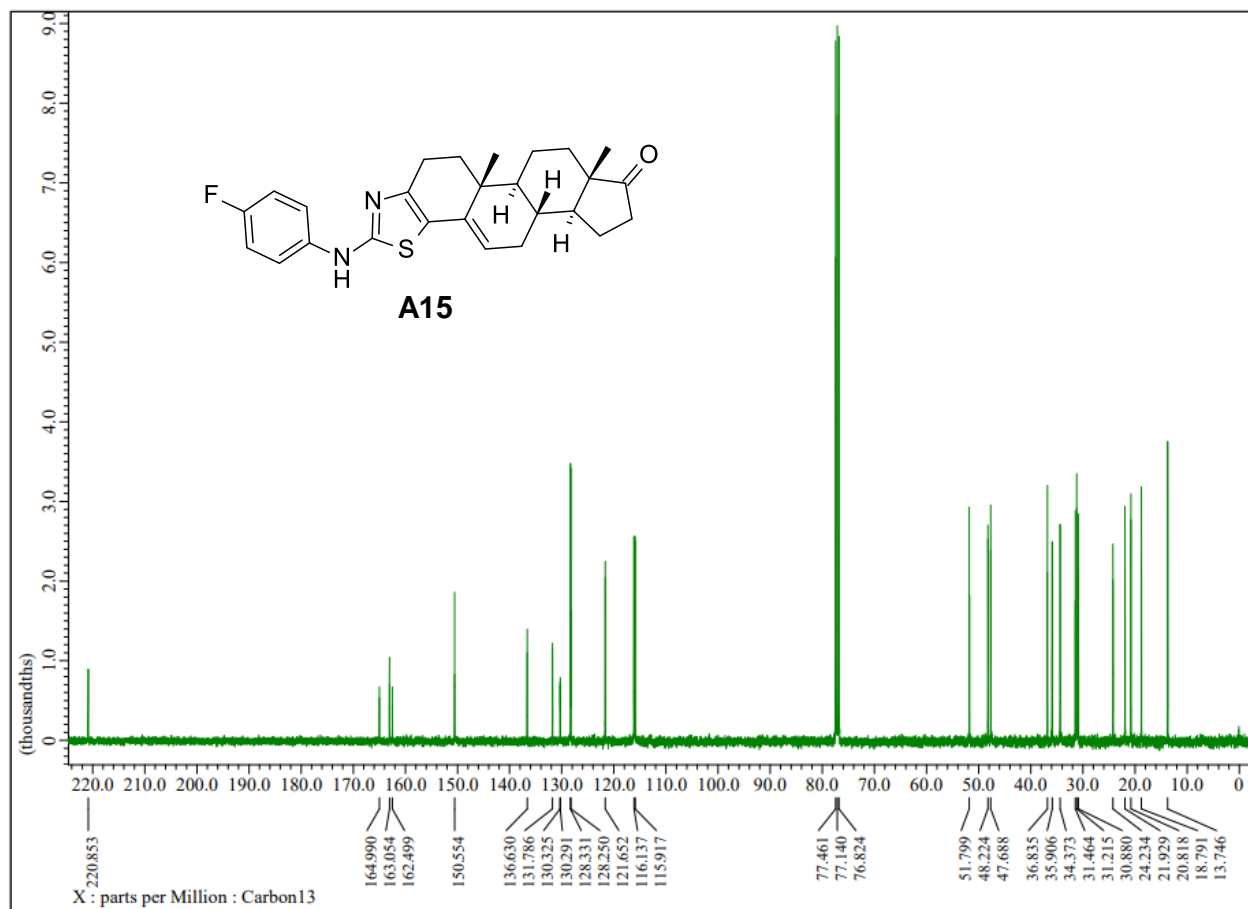


Figure S-2: ^{13}C NMR spectrum of compound **A15** in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-2
 Sample id#: 5180
 Instrument: Shimadzu IT-TOF

9/20/2023

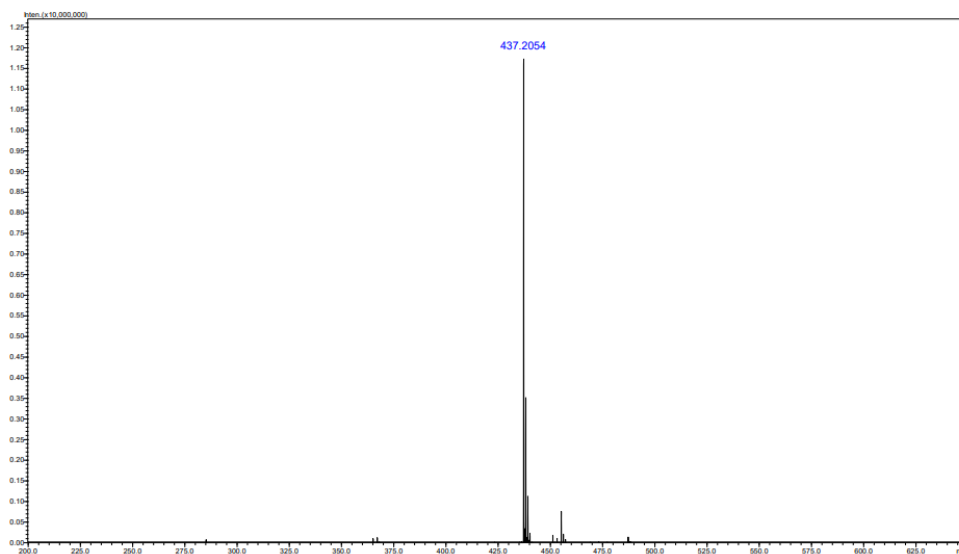


Figure S-3: High-resolution mass spectrum of compound **A15**

(1*S*,2*R*,13*R*,14*S*,18*S*)-7-(3,5-Dimethylanilino)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-one (A21)

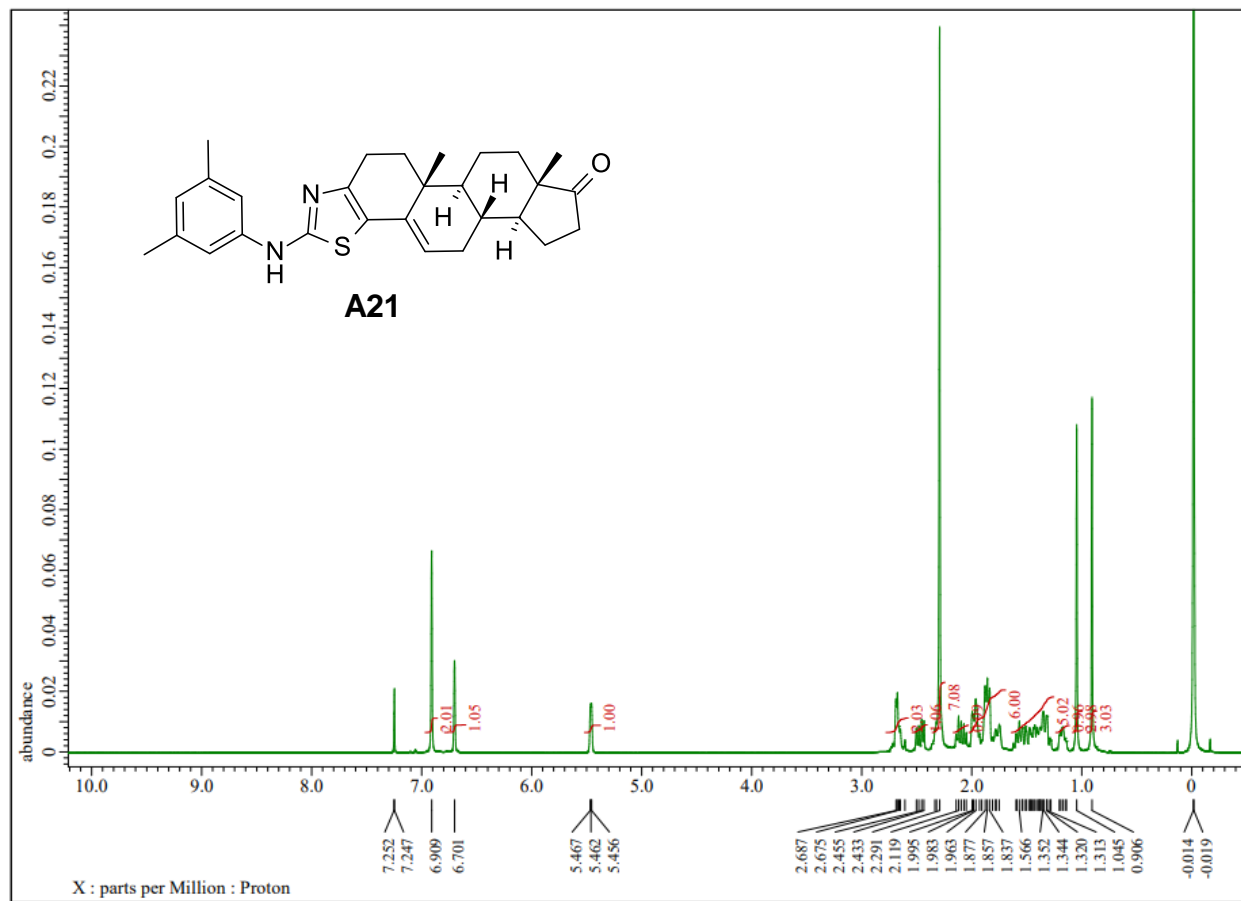


Figure S-4: ¹H NMR spectrum of compound A21 in CDCl₃

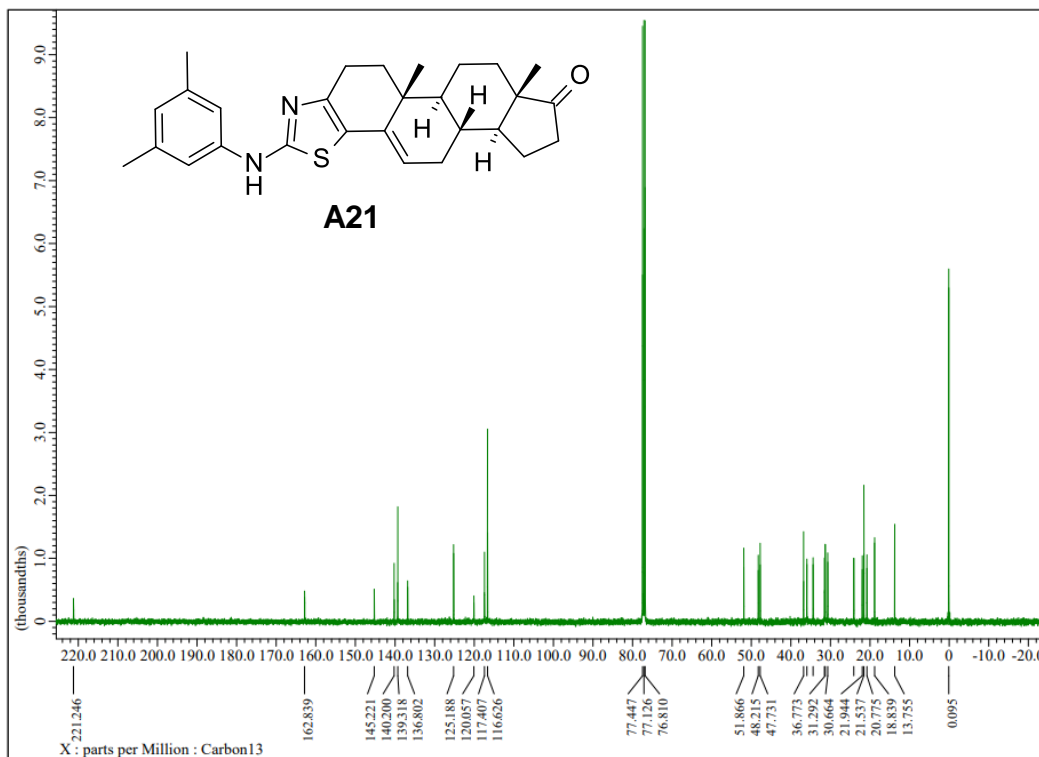


Figure S-5: ^{13}C NMR spectrum of compound **A21** in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI Mass Spectrum

Sample Name: A1
 Sample id#: 5253
 Instrument: Shimadzu IT-TOF

11/8/2023

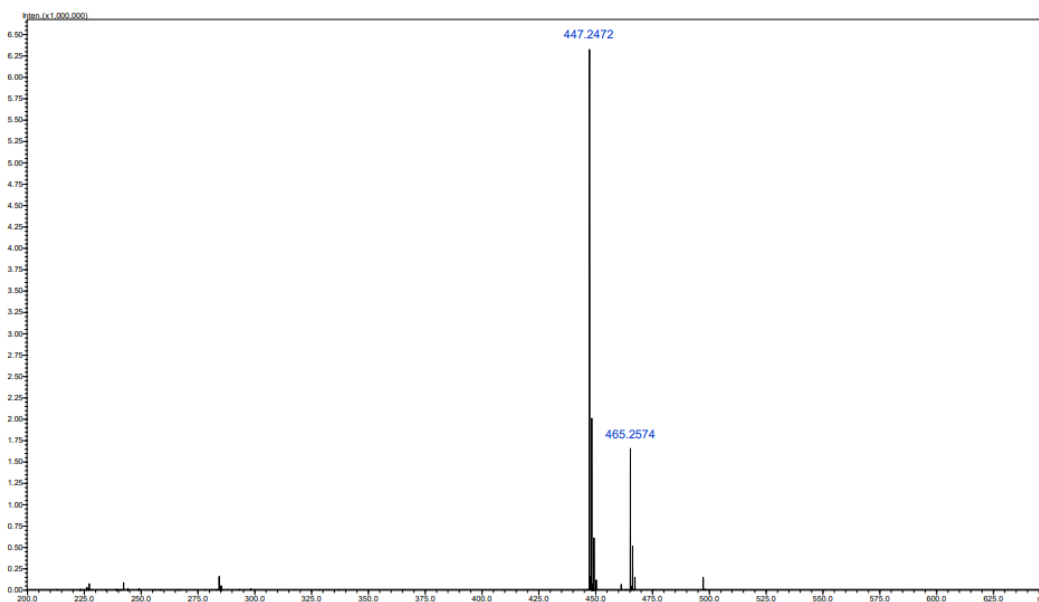


Figure S-6: High-resolution mass spectrum of compound **A21**

3-[[*(1S,2R,13R,14S,17R,18S)*-17-Ethynyl-17-hydroxy-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-7-yl]amino]benzoic acid (**E4**)

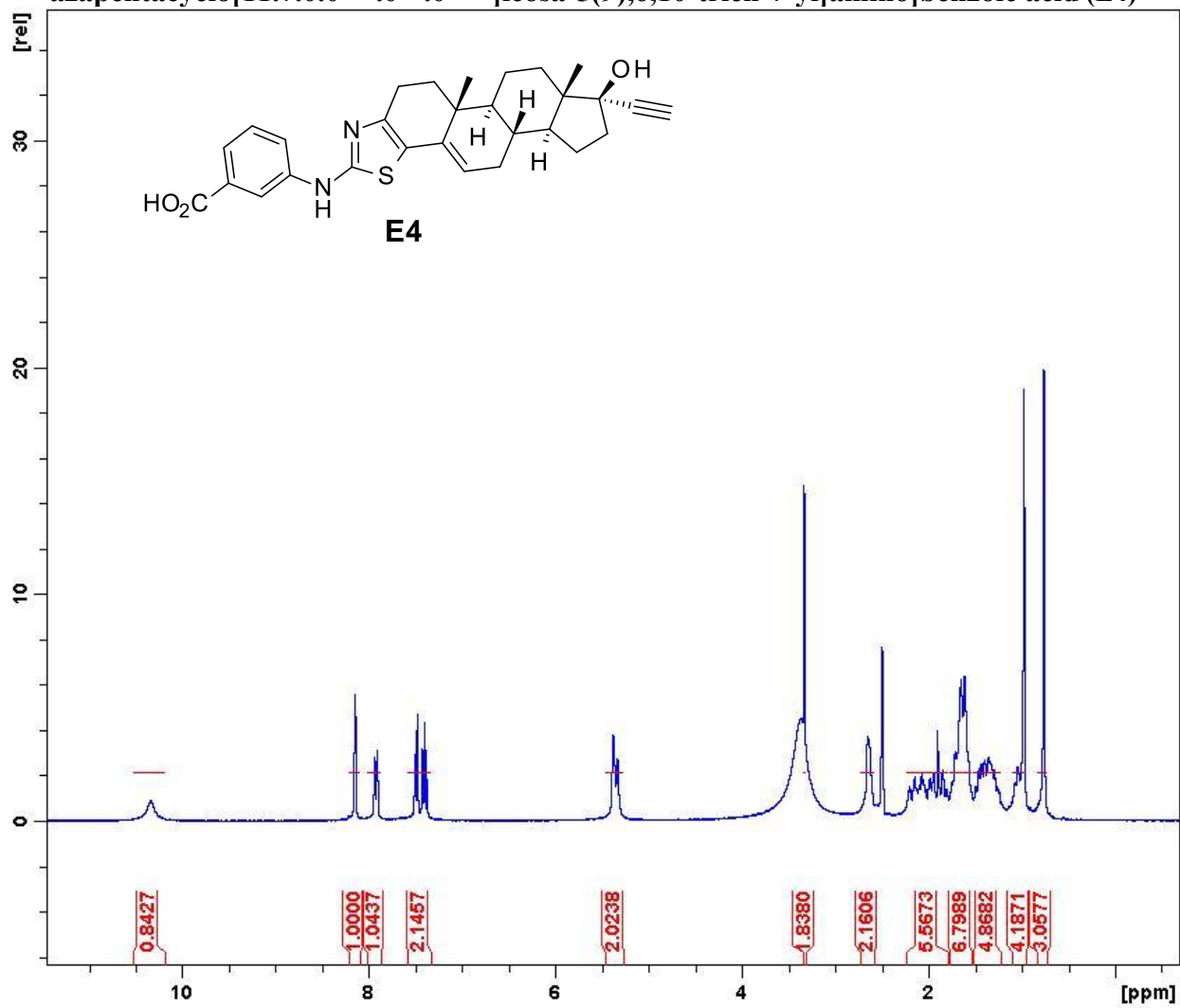


Figure S-7: ¹H NMR spectrum of compound **E4** in DMSO-*d*₆

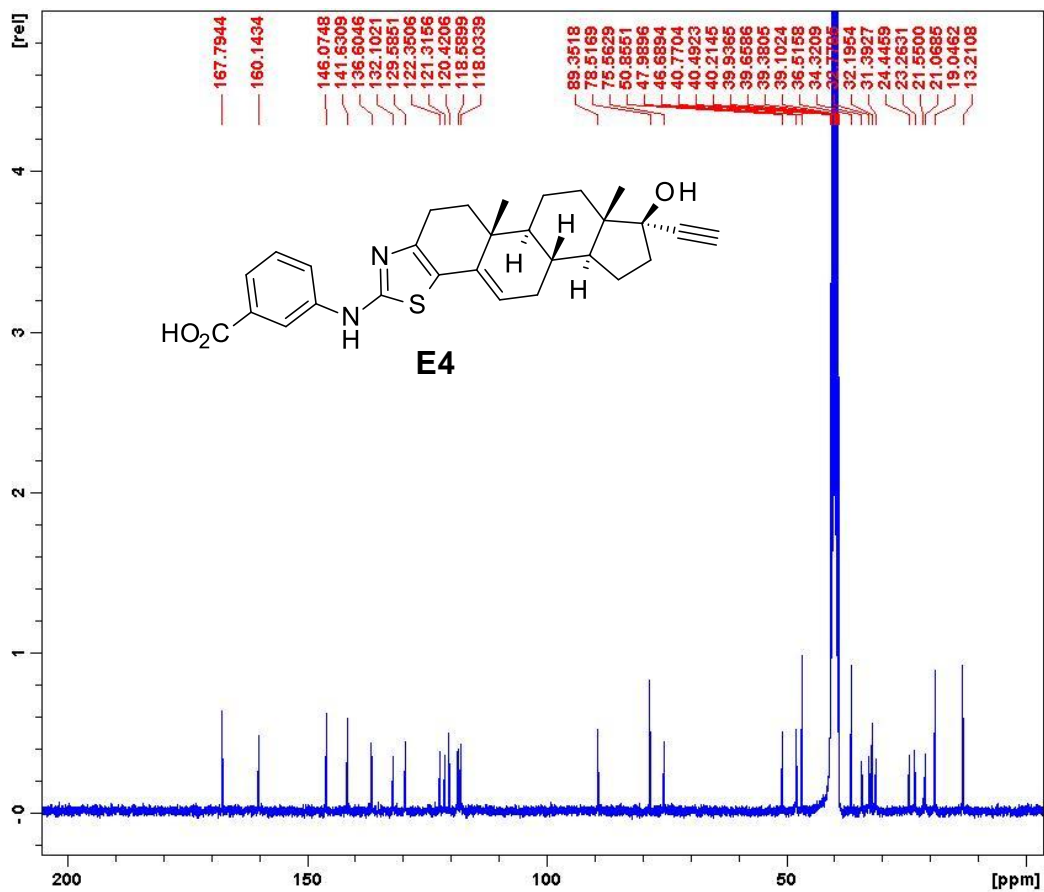


Figure S-8: ^{13}C NMR spectrum of compound E4 in DMSO- d_6

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-3
 Sample id#: 5181
 Instrument: Shimadzu IT-TOF

9/20/2023

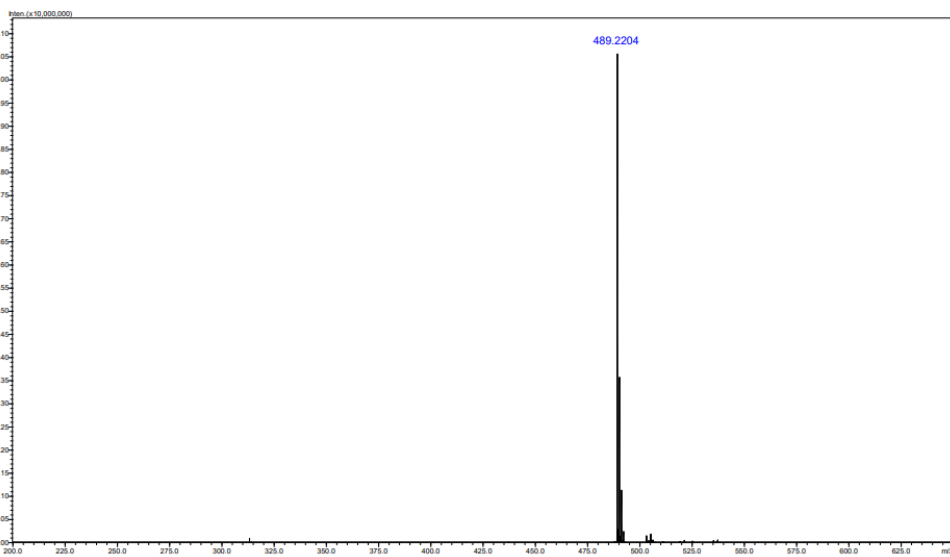


Figure S-9: High-resolution mass spectrum of compound E4

4-[[*(1S,2R,13R,14S,17R,18S)*-17-Ethynyl-17-hydroxy-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-7-yl]amino]benzoic acid (**E5**)

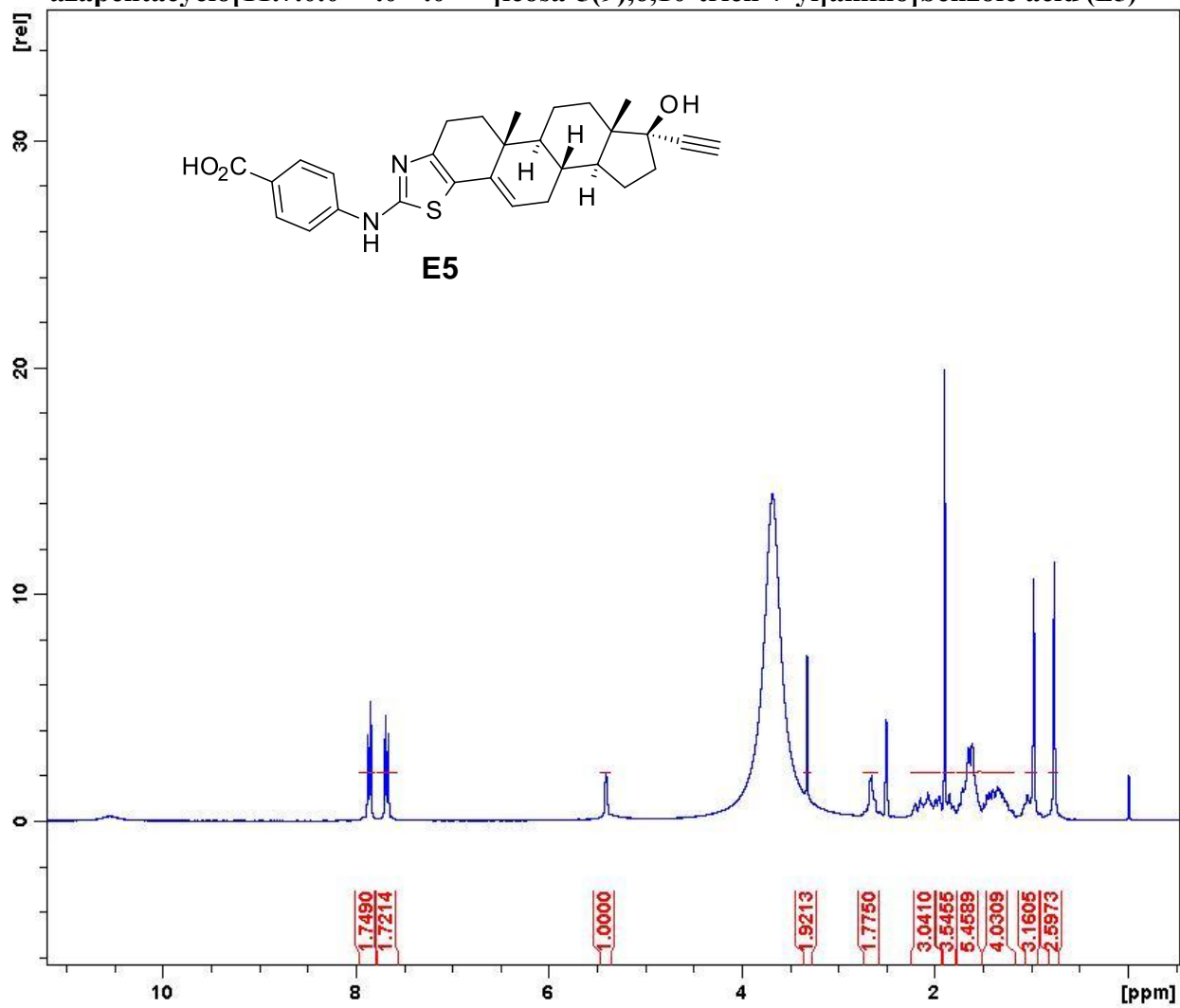


Figure S-10: ¹H NMR spectrum of compound **E5** in DMSO-*d*₆

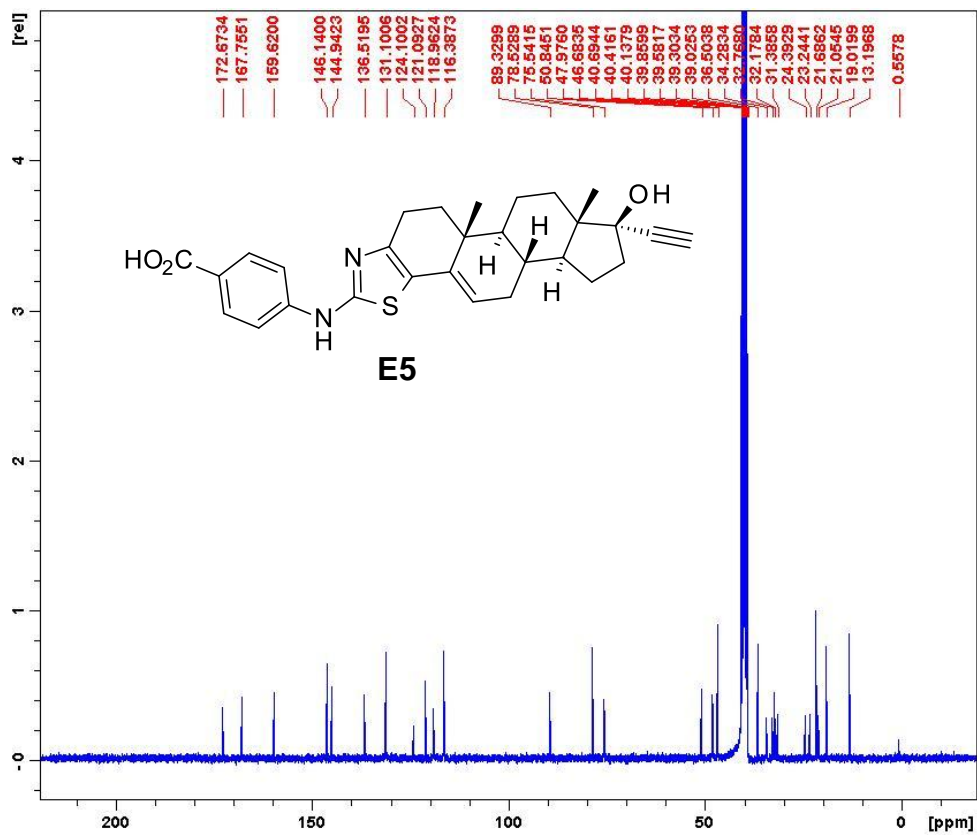


Figure S-11: ^{13}C NMR spectrum of compound **E5** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-4
 Sample id#: 5182
 Instrument: Shimadzu IT-TOF

9/20/2023

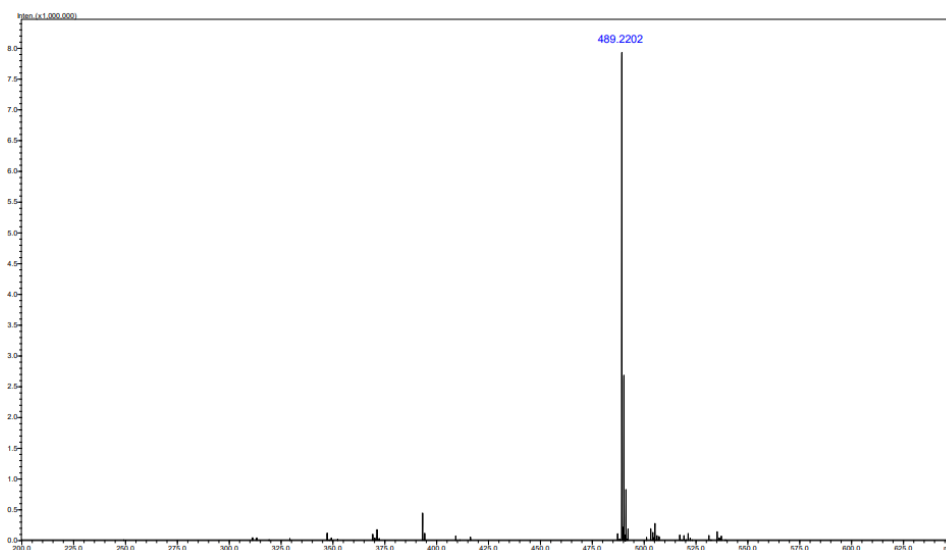


Figure S-12: High-resolution mass spectrum of compound **E5**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-(3,5-Dimethylanilino)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E7)

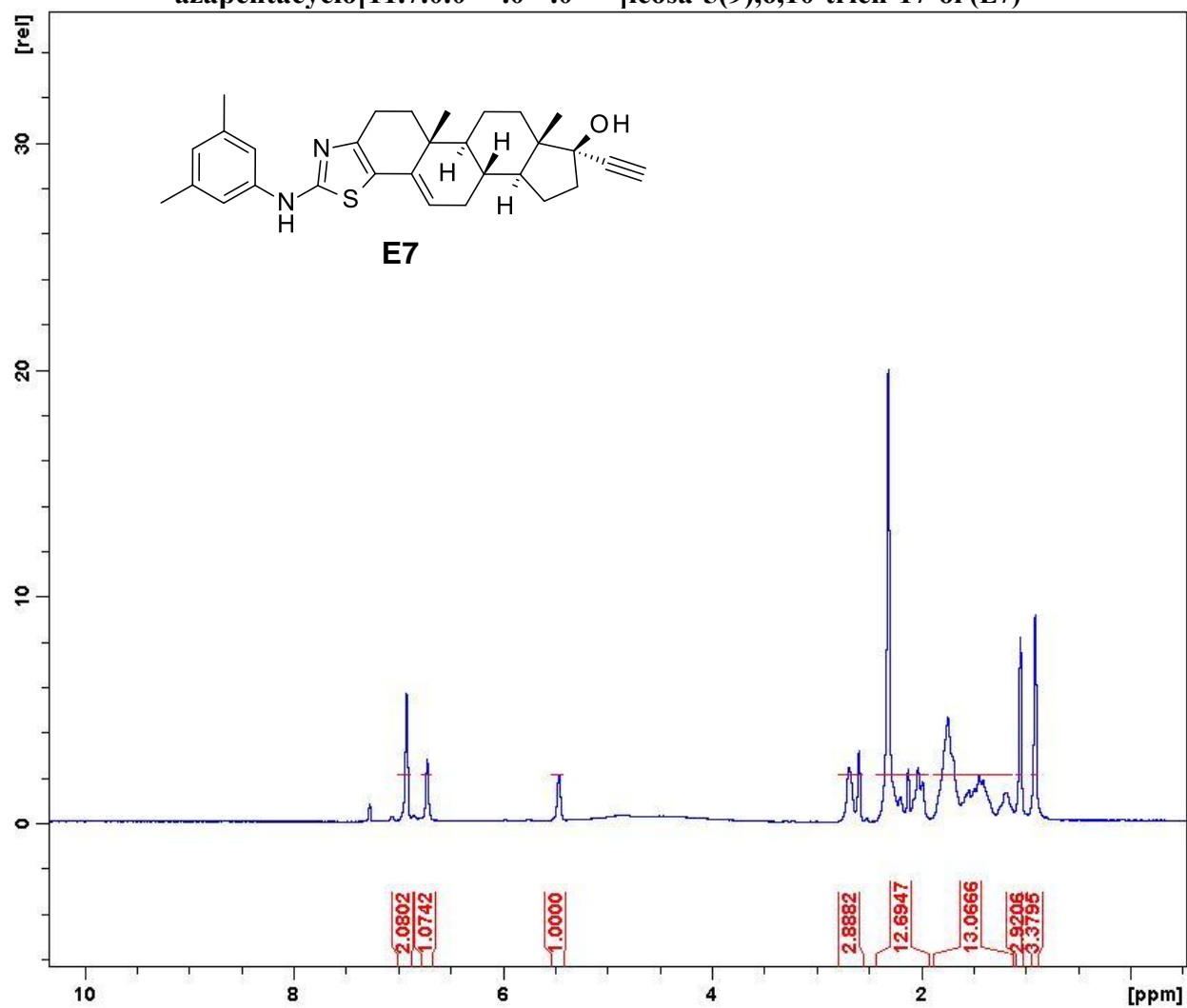


Figure S-13: ¹H NMR spectrum of compound E7 in CDCl₃

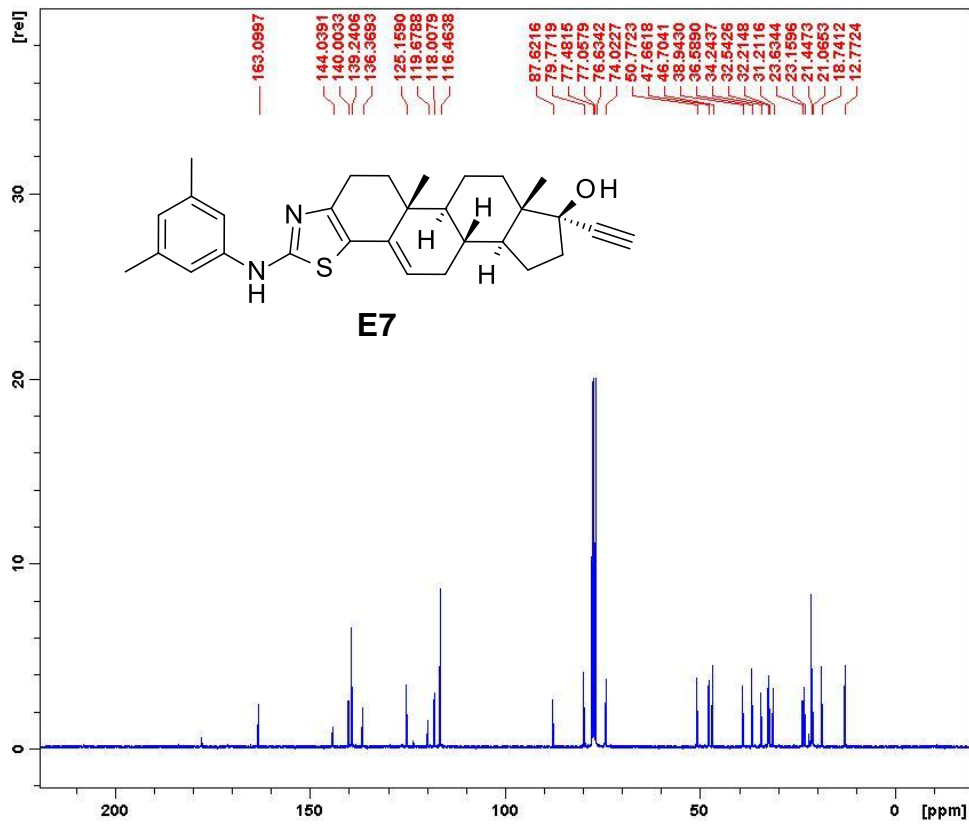


Figure S-14: ^{13}C NMR spectrum of compound E7 in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-5
 Sample id#: 5183
 Instrument: Shimadzu IT-TOF

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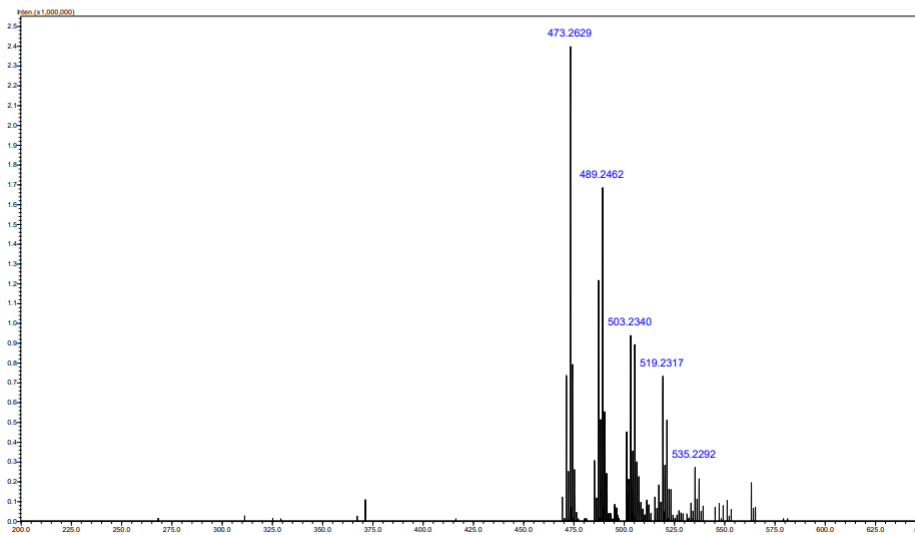


Figure S-15: High-resolution mass spectrum of compound E7

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-(3-Chloro-4-methyl-anilino)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E11)

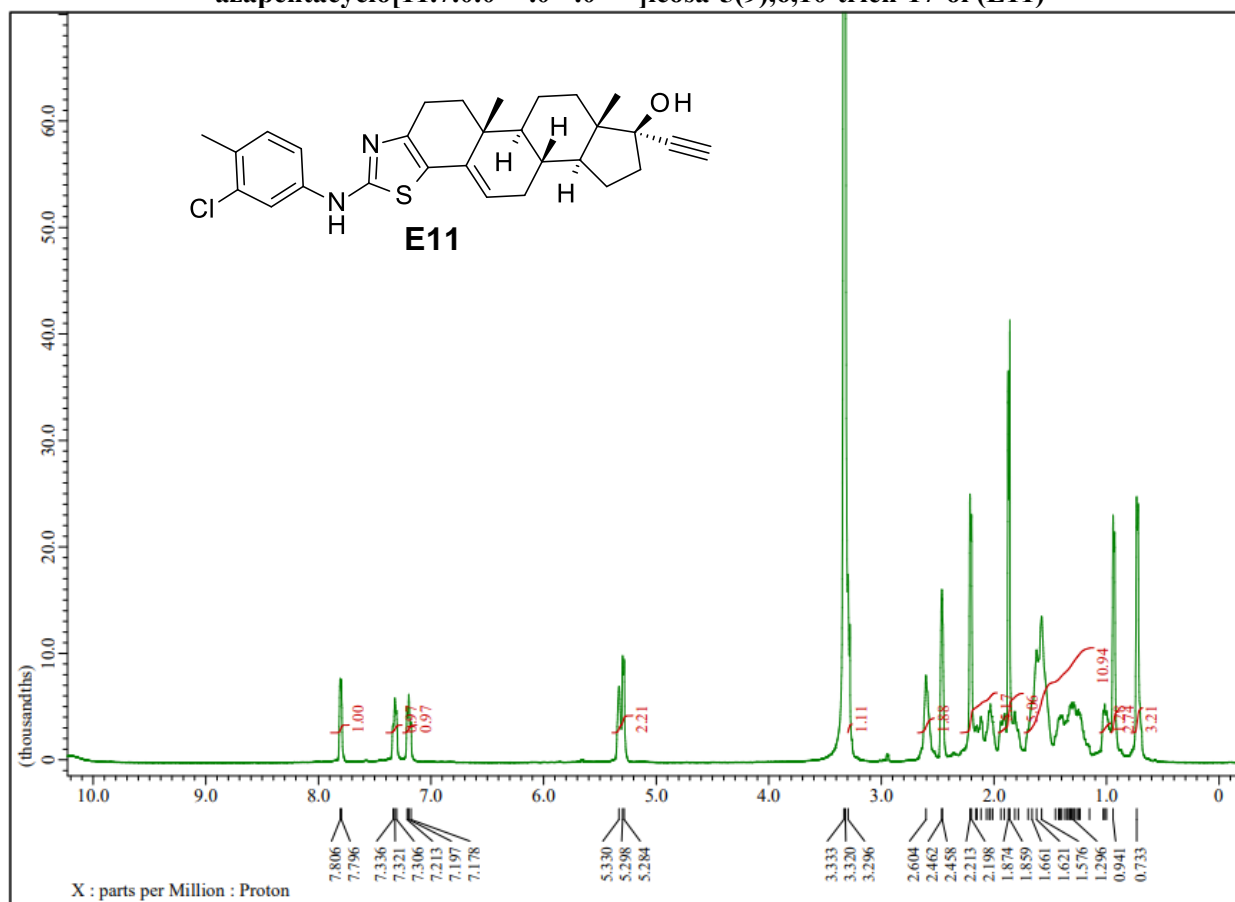


Figure S-16: ¹H NMR spectrum of compound E11 in DMSO-*d*₆

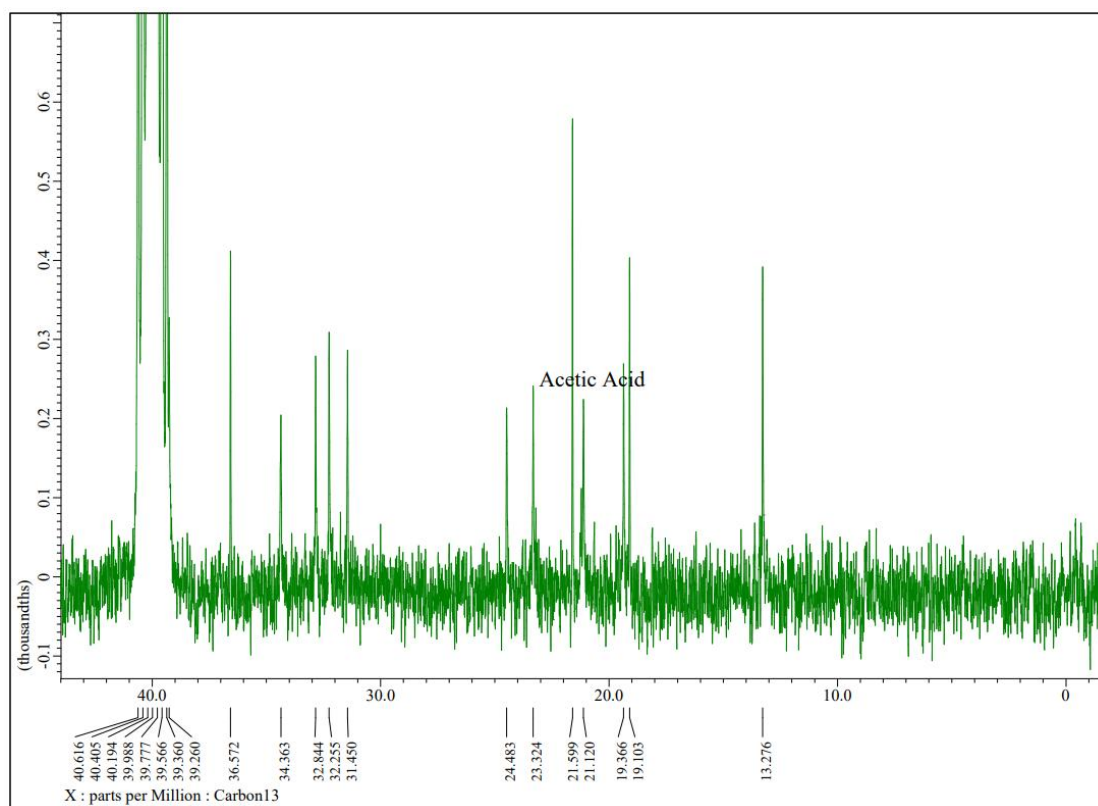
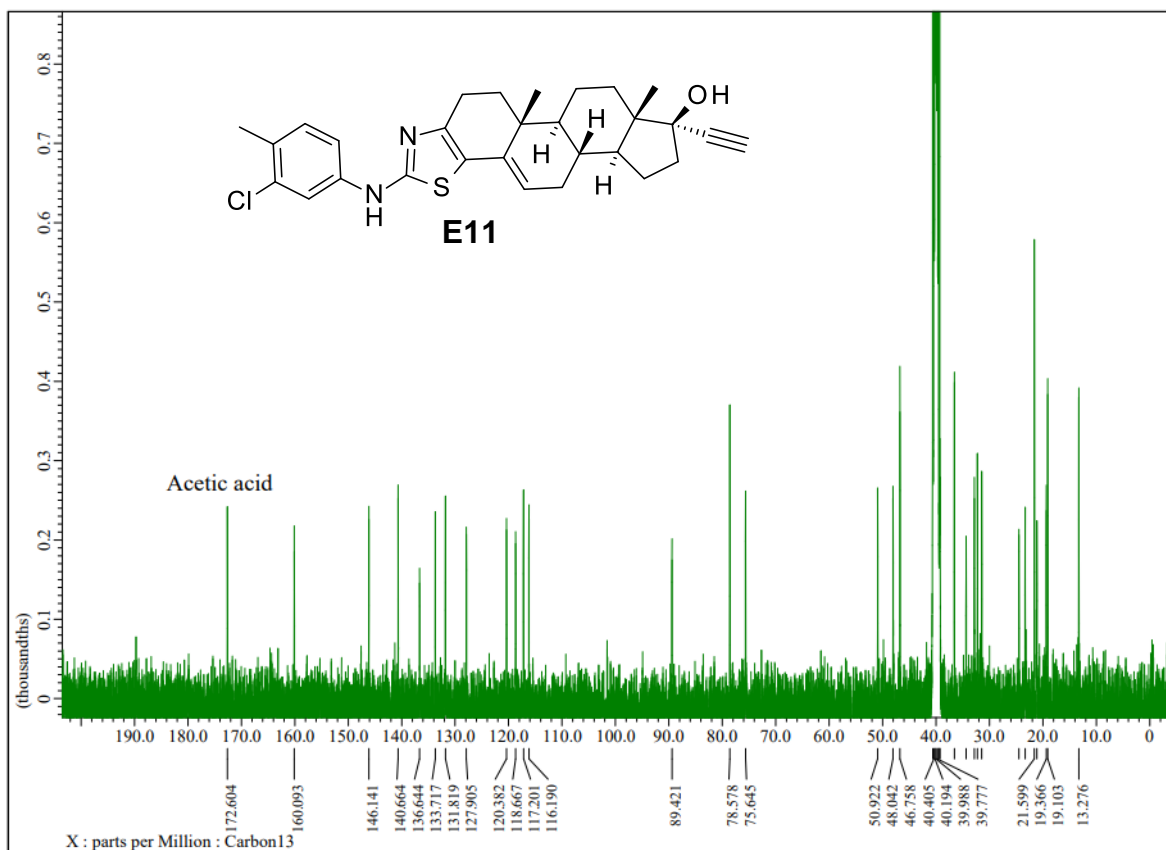


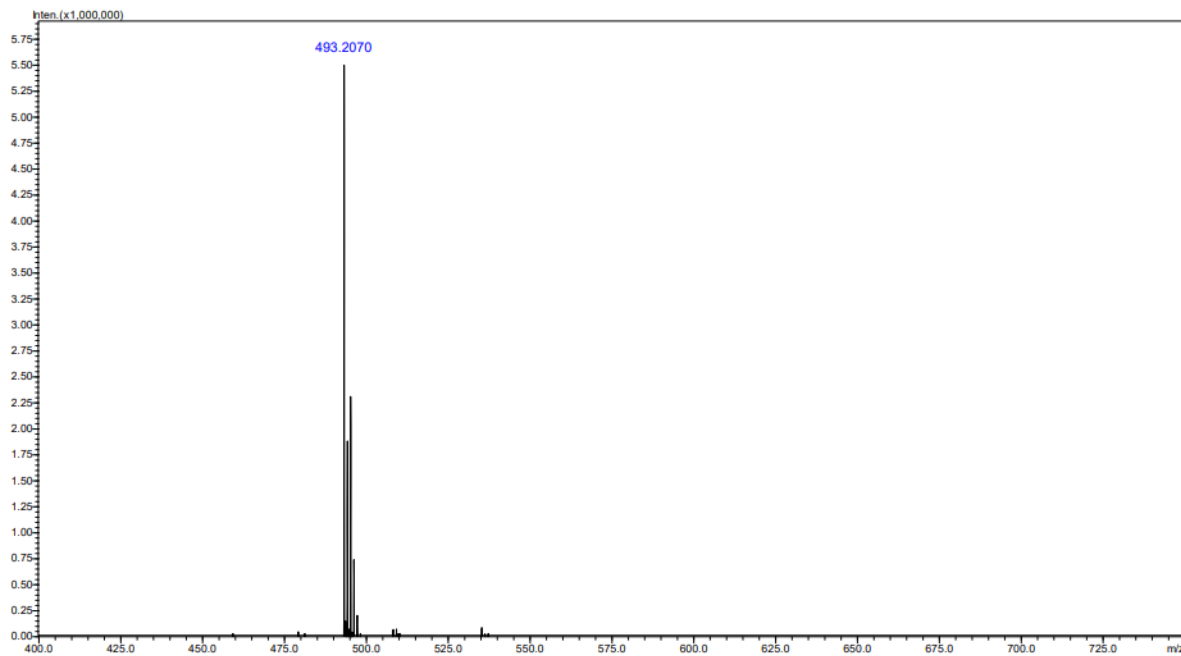
Figure S-17: ^{13}C NMR spectrum of compound **E11** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-3Cl-4Me
Sample id#: 4306
Instrument: Shimadzu IT-TOF

8/27/2021



Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-3Cl-4Me
Sample id#: 4306
Instrument: Shimadzu IT-TOF

8/27/2021

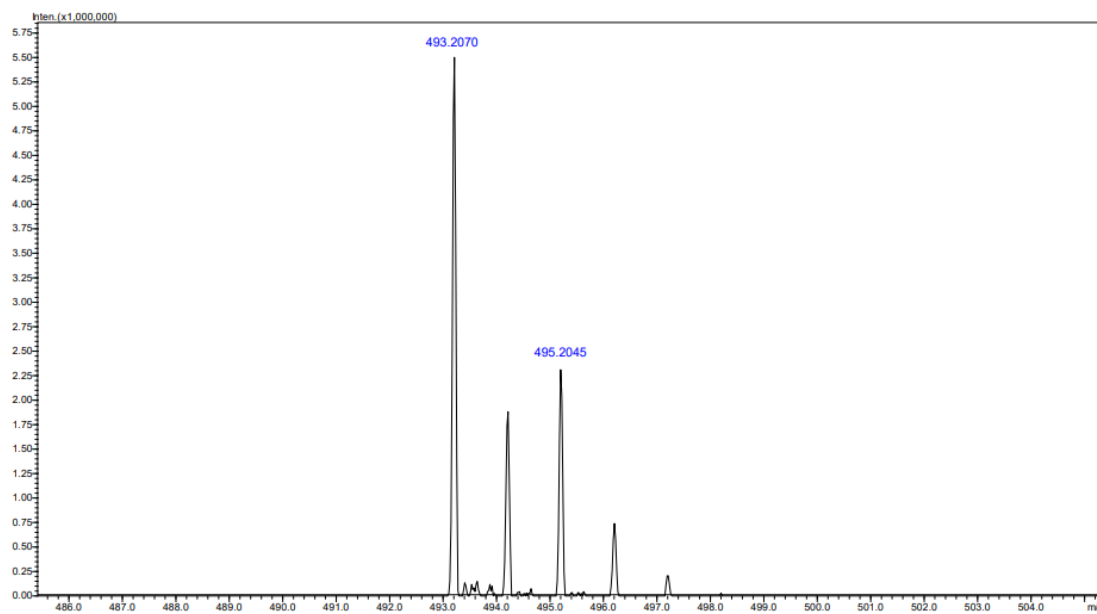


Figure S-18: High-resolution mass spectrum of compound E11

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-(*N*-methylanilino)-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]jicosa-5(9),6,10-trien-17-ol (E13)

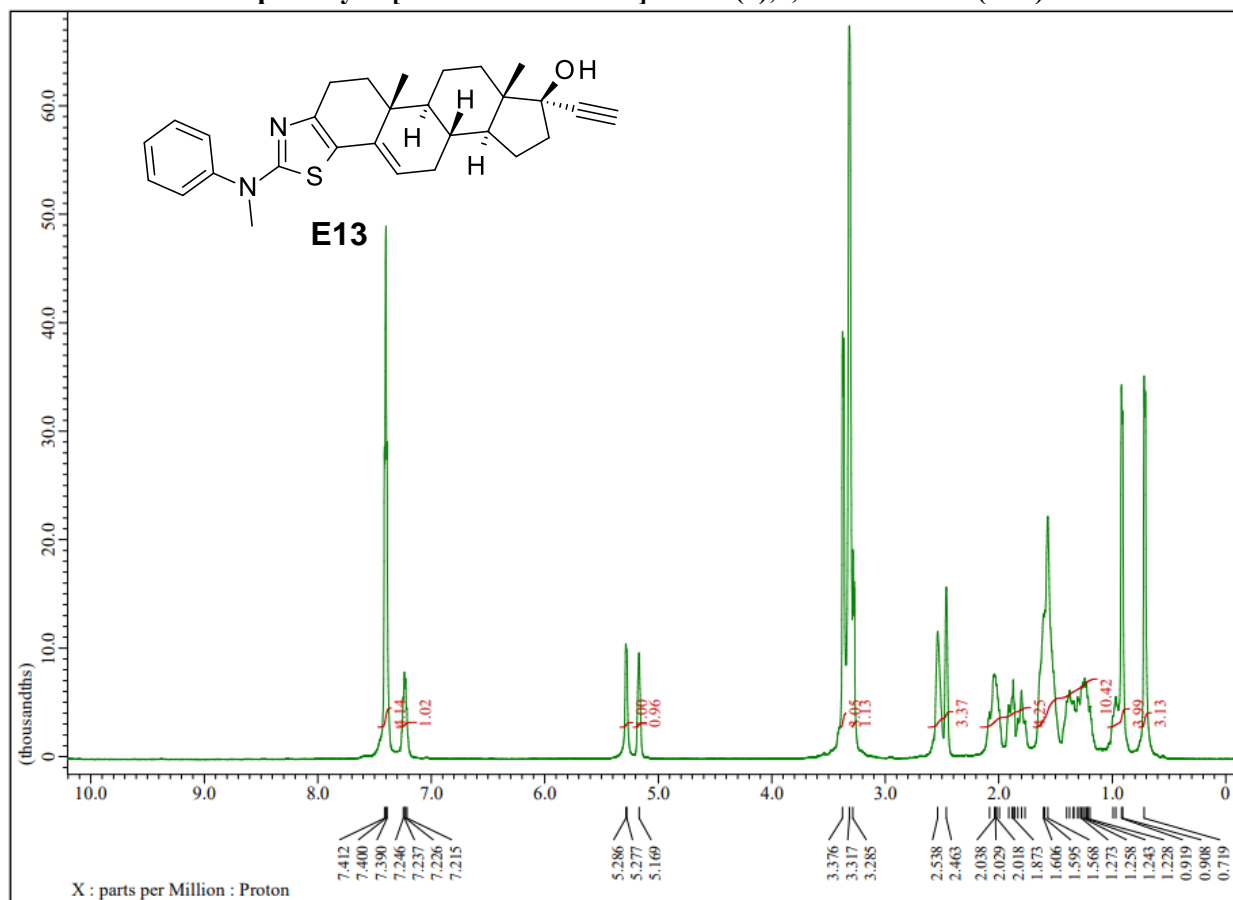


Figure S-19: ¹H NMR spectrum of compound E13 in DMSO-*d*₆

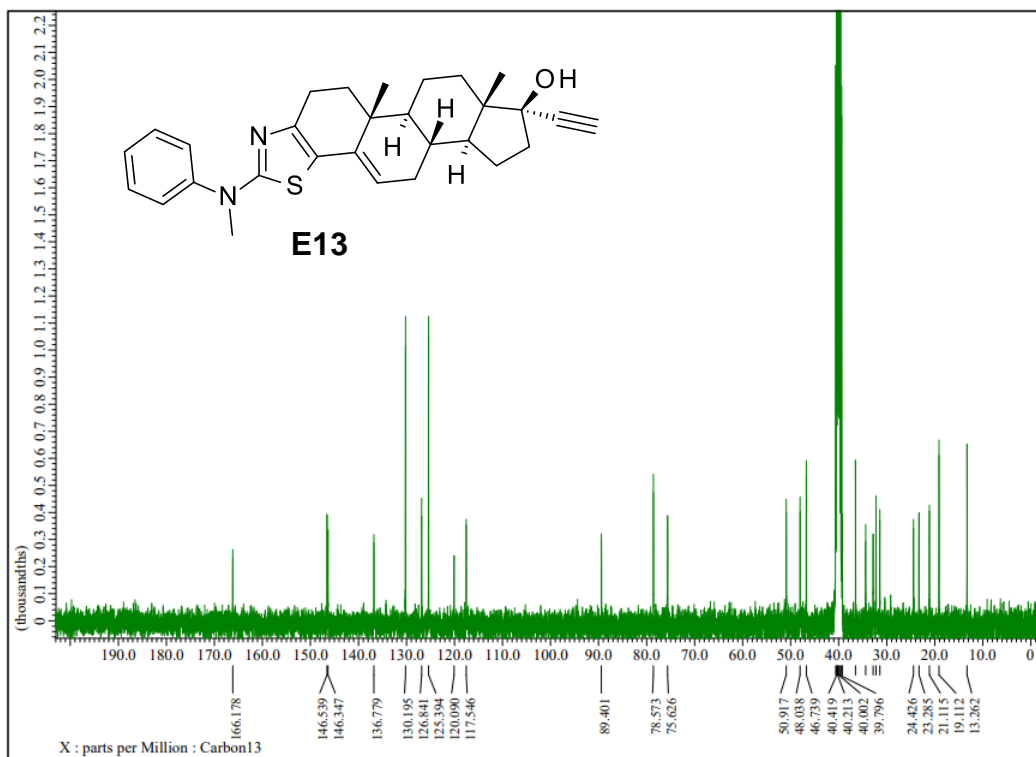


Figure S-20: ^{13}C NMR spectrum of compound **E13** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-7
 Sample id#: 5185
 Instrument: Shimadzu IT-TOF

9/20/2023

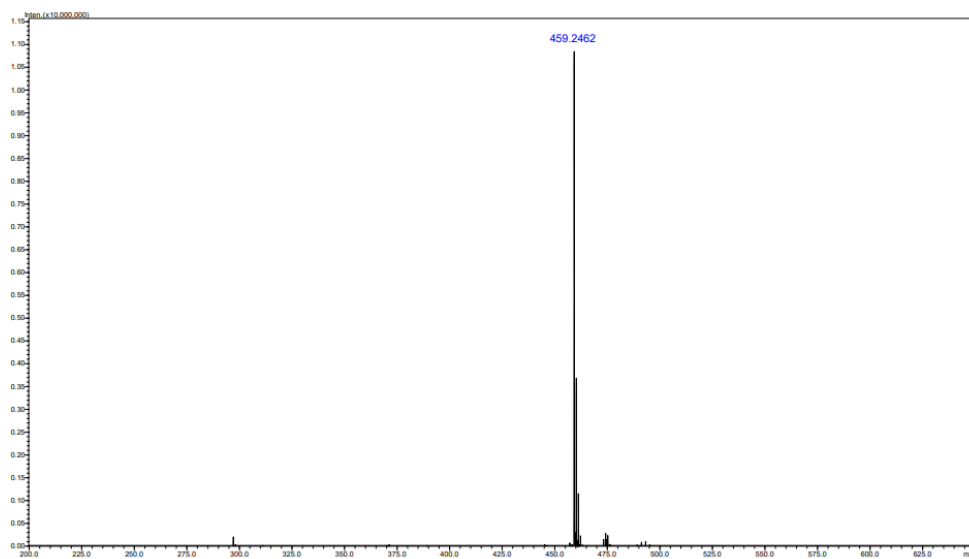


Figure S-21: High-resolution mass spectrum of compound **E13**

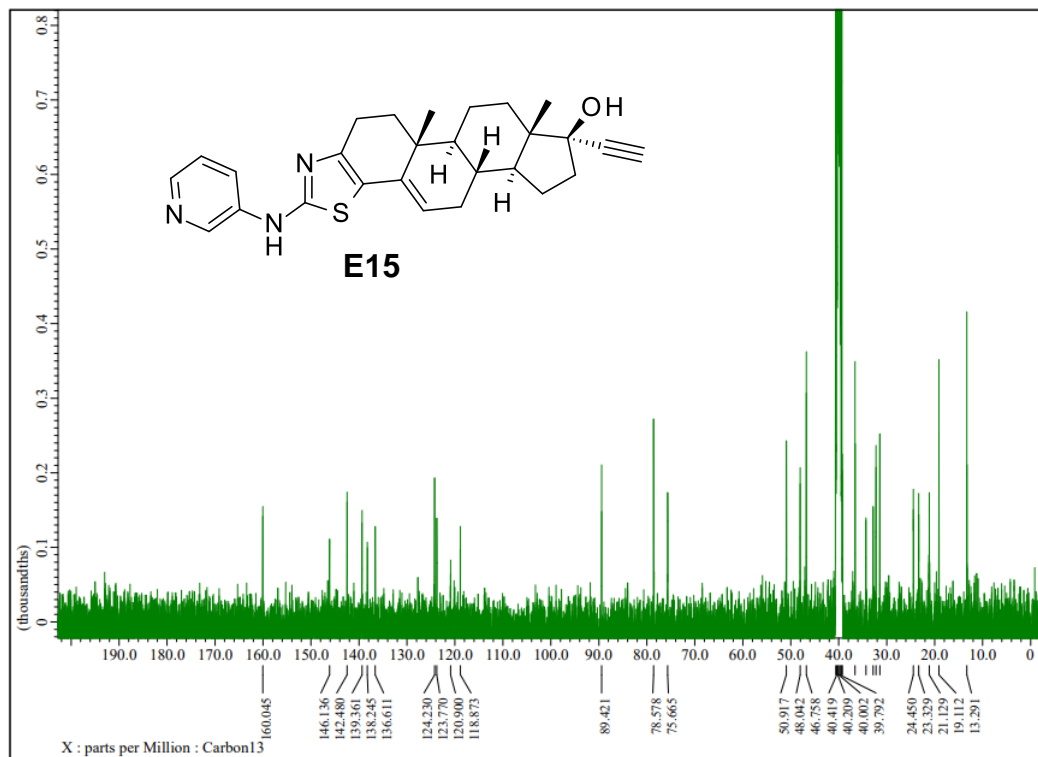


Figure S-23: ^{13}C NMR spectrum of compound **E15** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-8

Sample id#: 5186

Instrument: Shimadzu IT-TOF

9/20/2023

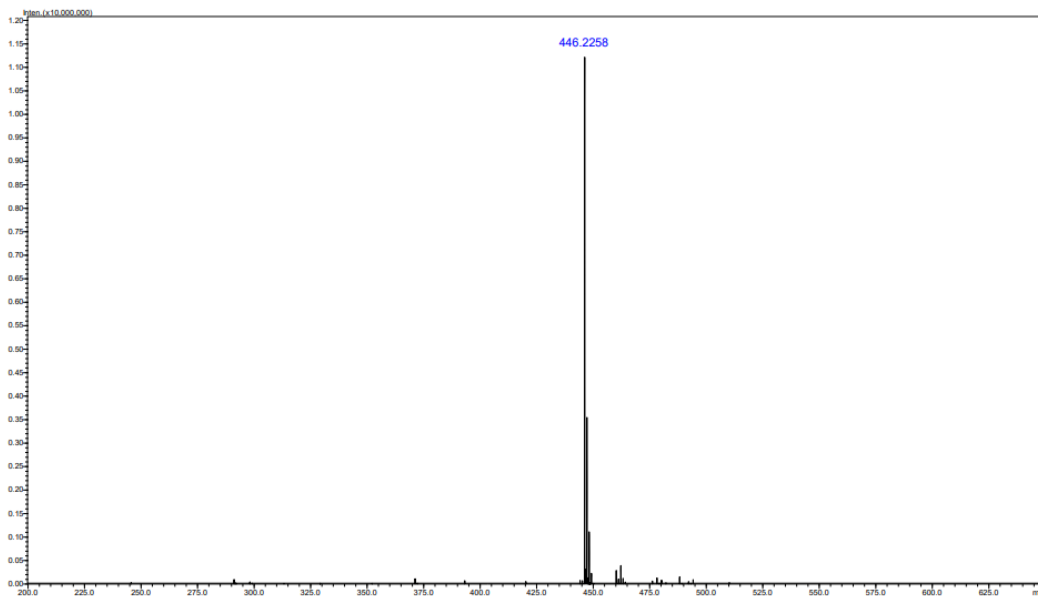


Figure S-24: High-resolution mass spectrum of compound **E15**

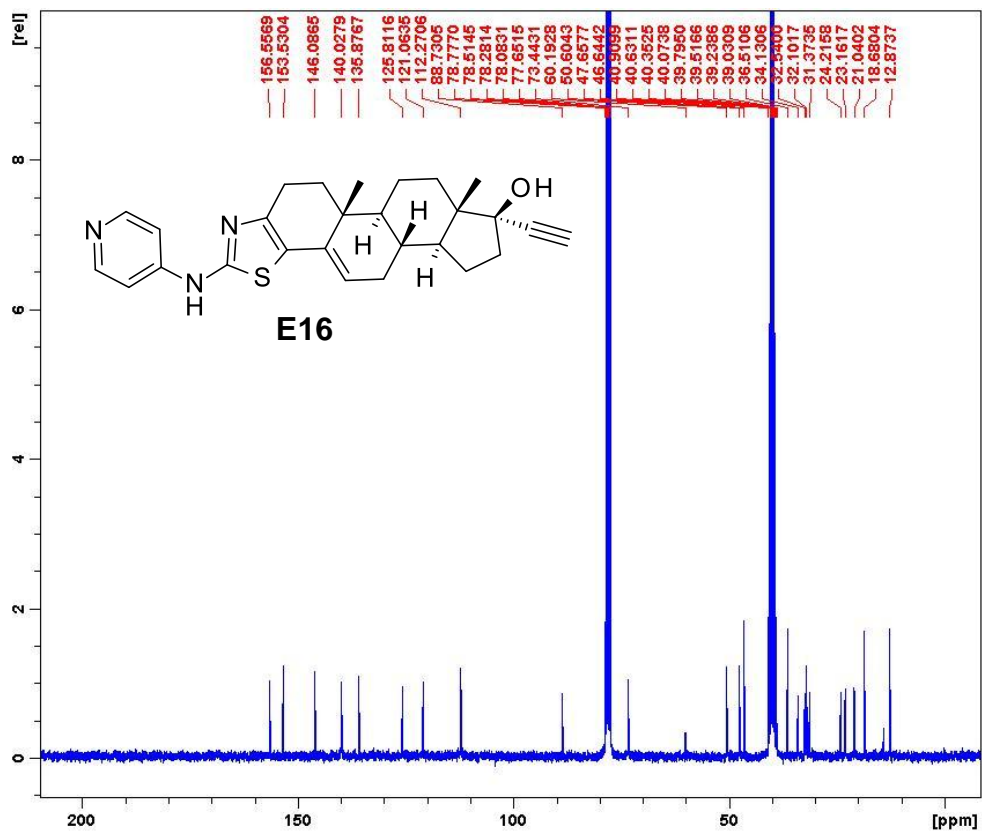


Figure S-26: ¹³C NMR spectrum of compound E16 in DMSO-*d*₆ and CDCl₃

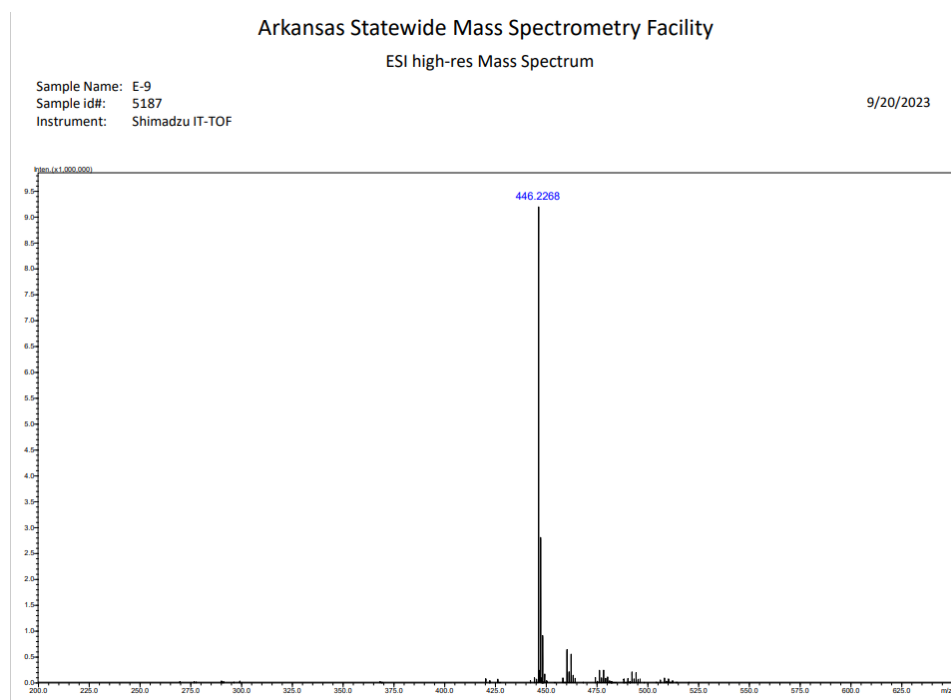


Figure S-27: High-resolution mass spectrum of compound E16

(1*S*,2*R*,13*R*,14*S*,17*R*,18*E*)-17-Ethynyl-2,18-dimethyl-7-[(3-methyl-2-pyridyl)amino]-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E17)

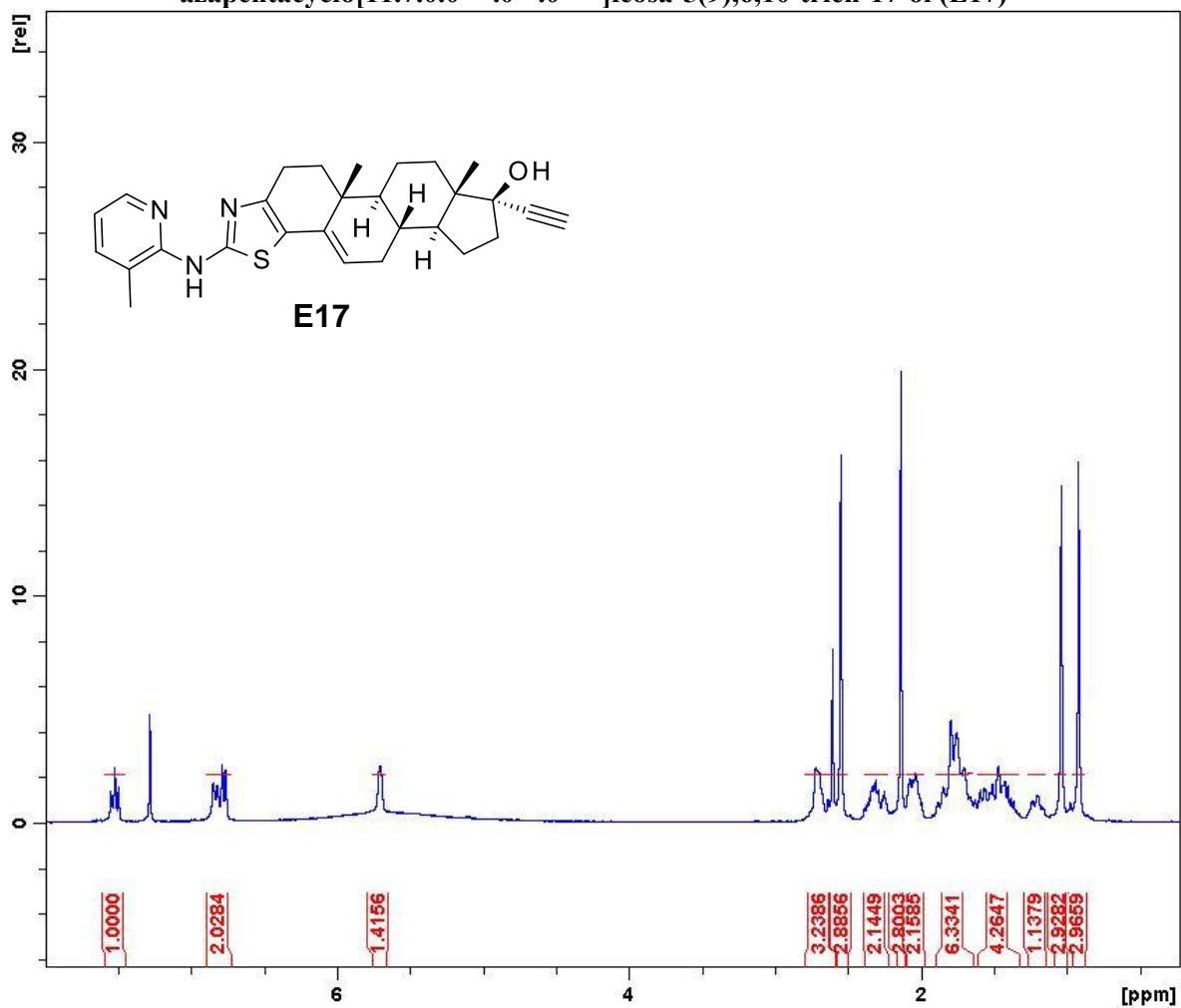


Figure S-28: ¹H NMR spectrum of compound E17 in CDCl₃

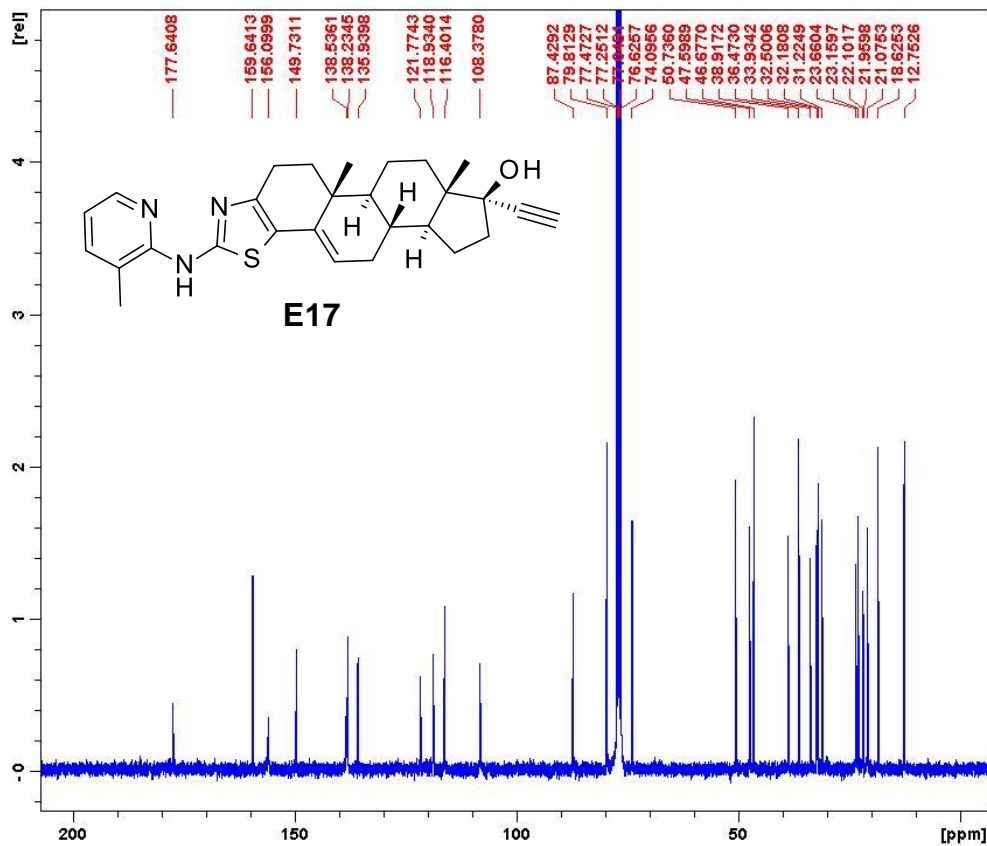


Figure S-29: ^{13}C NMR spectrum of compound **E17** in CDCl_3

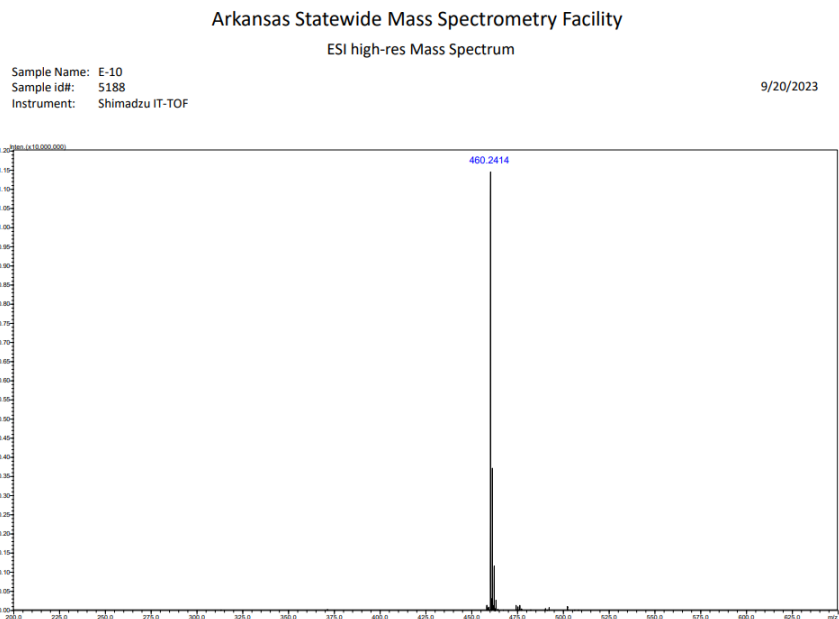


Figure S-30: High-resolution mass spectrum of compound **E17**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-[(5-methyl-2-pyridyl)amino]-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E18)

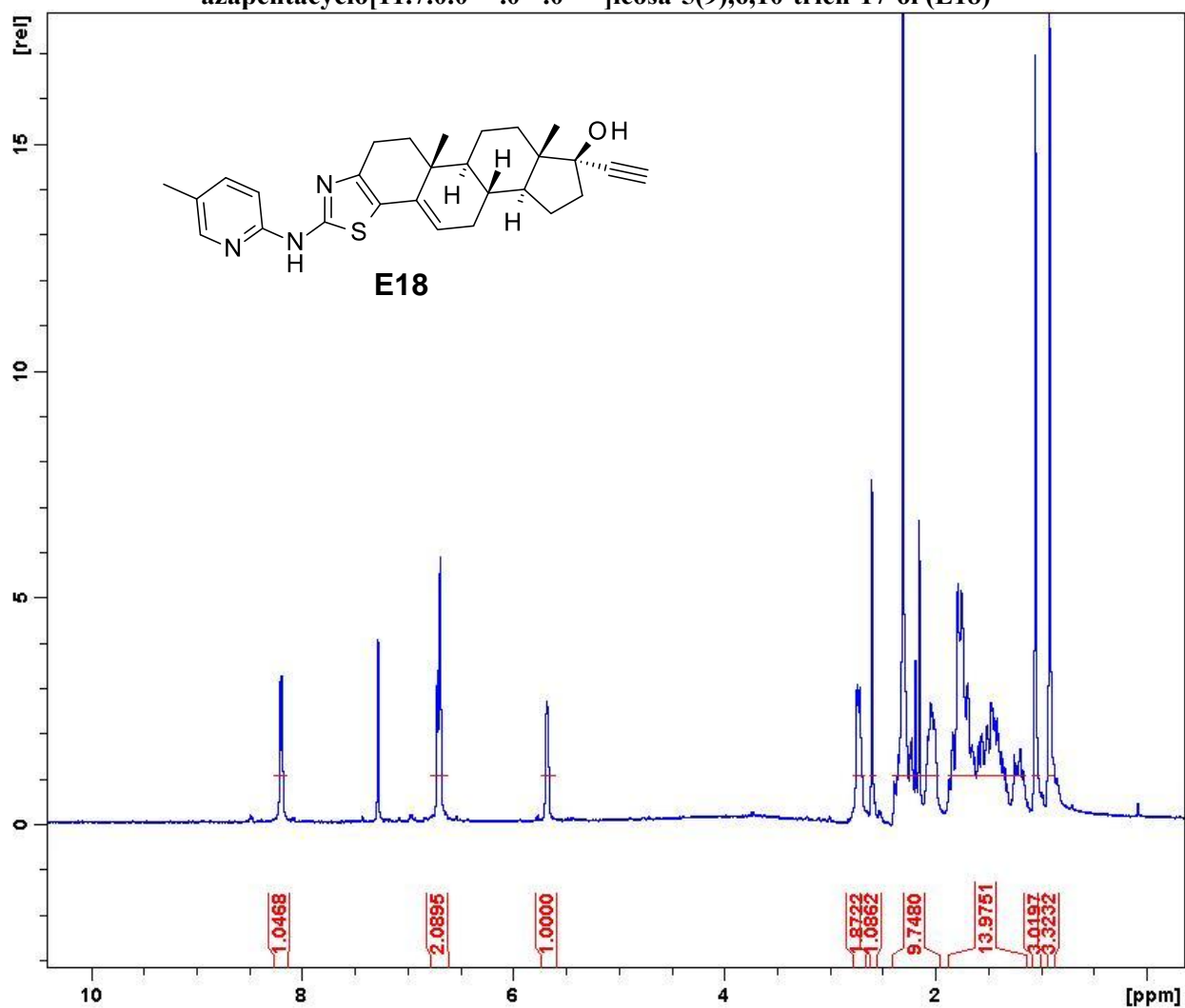


Figure S-31: ¹H NMR spectrum of compound E18 in CDCl₃

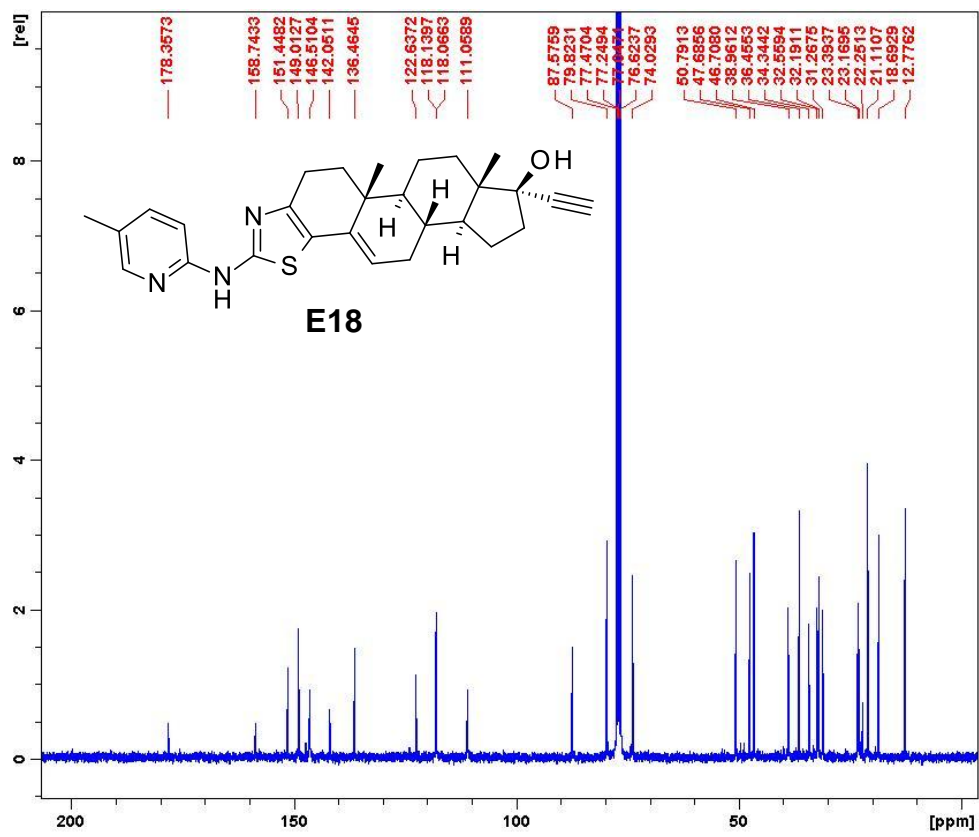


Figure S-32: ^{13}C NMR spectrum of compound **E18** in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-11
 Sample id#: 5189
 Instrument: Shimadzu IT-TOF

9/20/2023

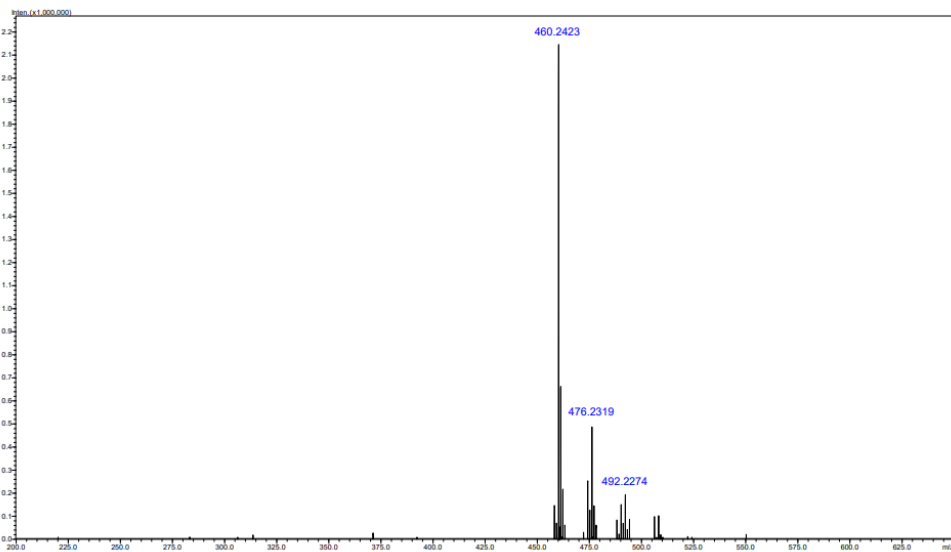


Figure S-33: High-resolution mass spectrum of compound **E18**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-[(6-methyl-2-pyridyl)amino]-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E19)

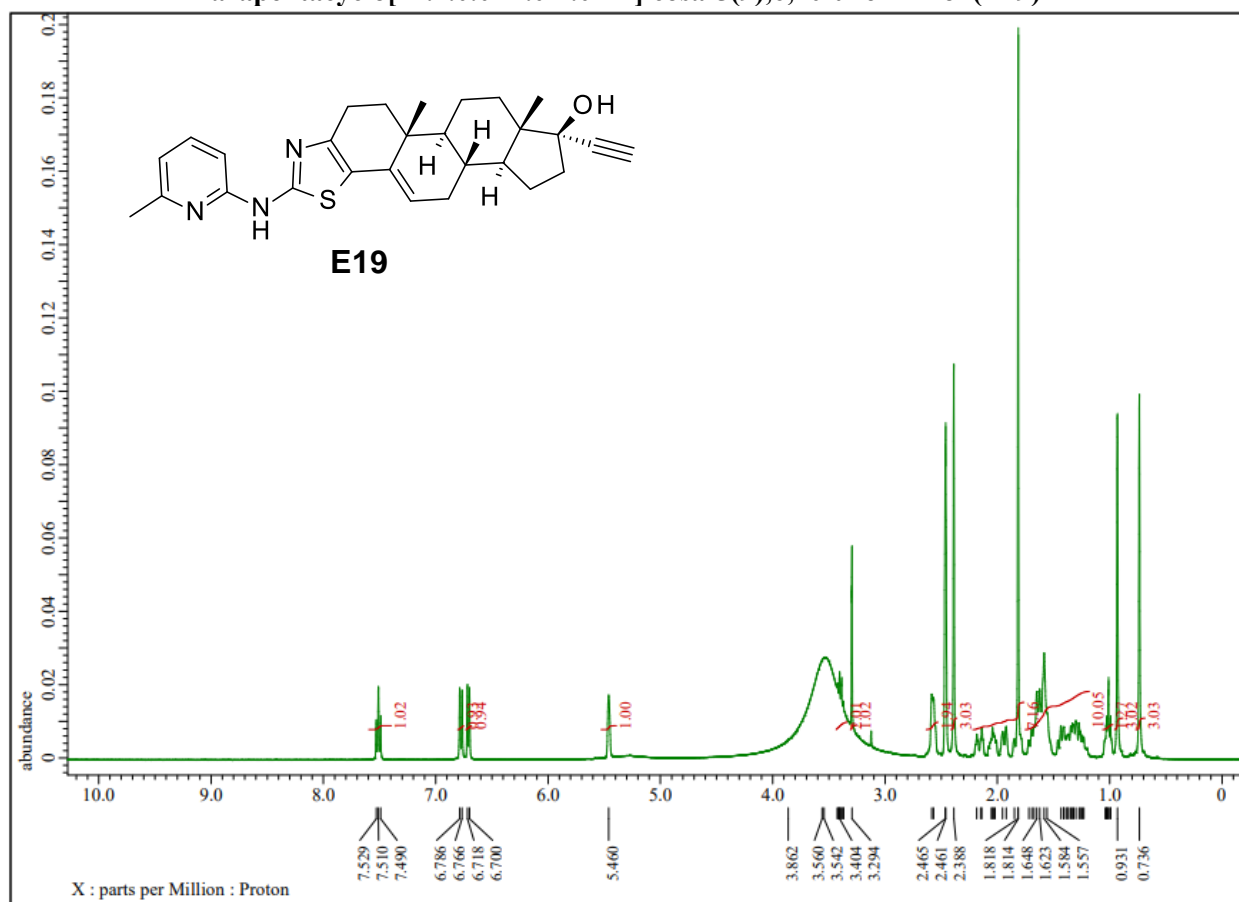


Figure S-34: ¹H NMR spectrum of compound **E19** in DMSO-*d*₆

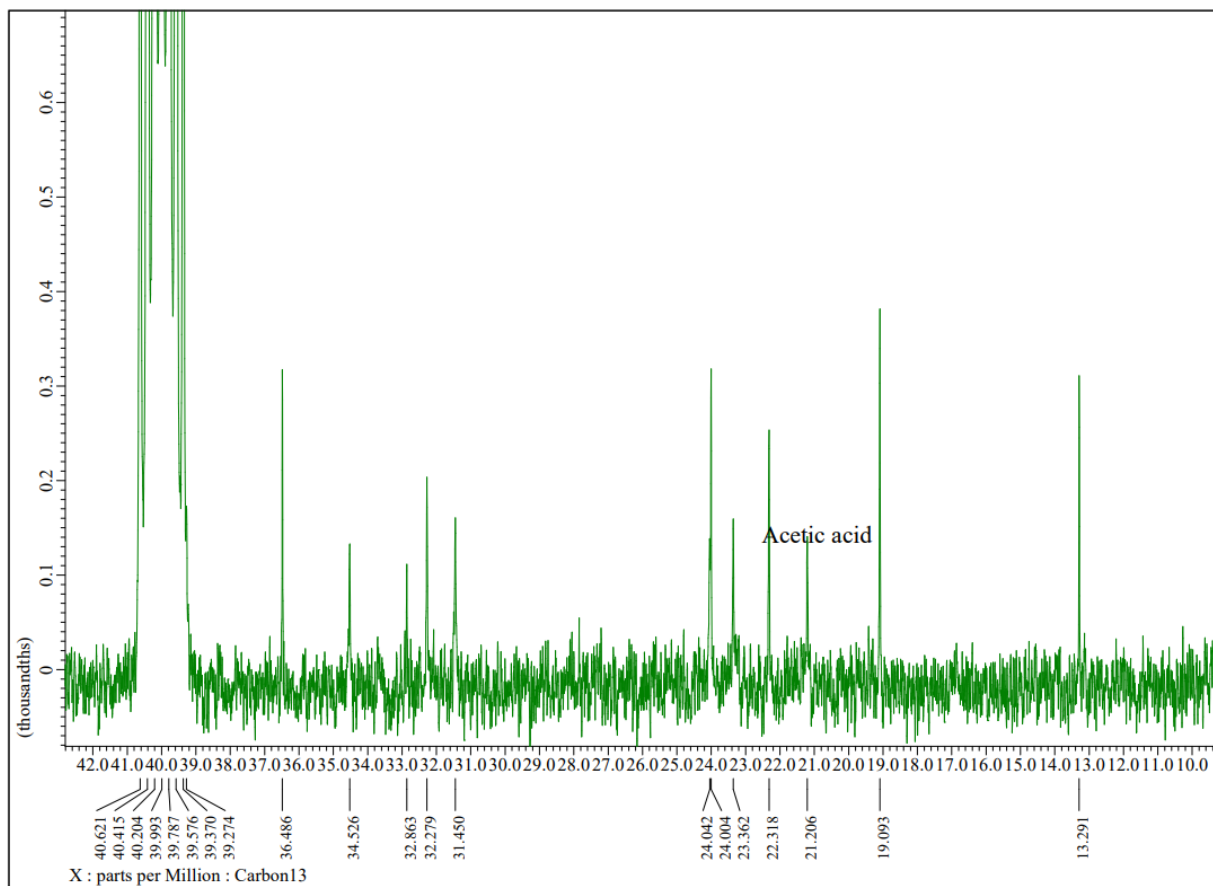
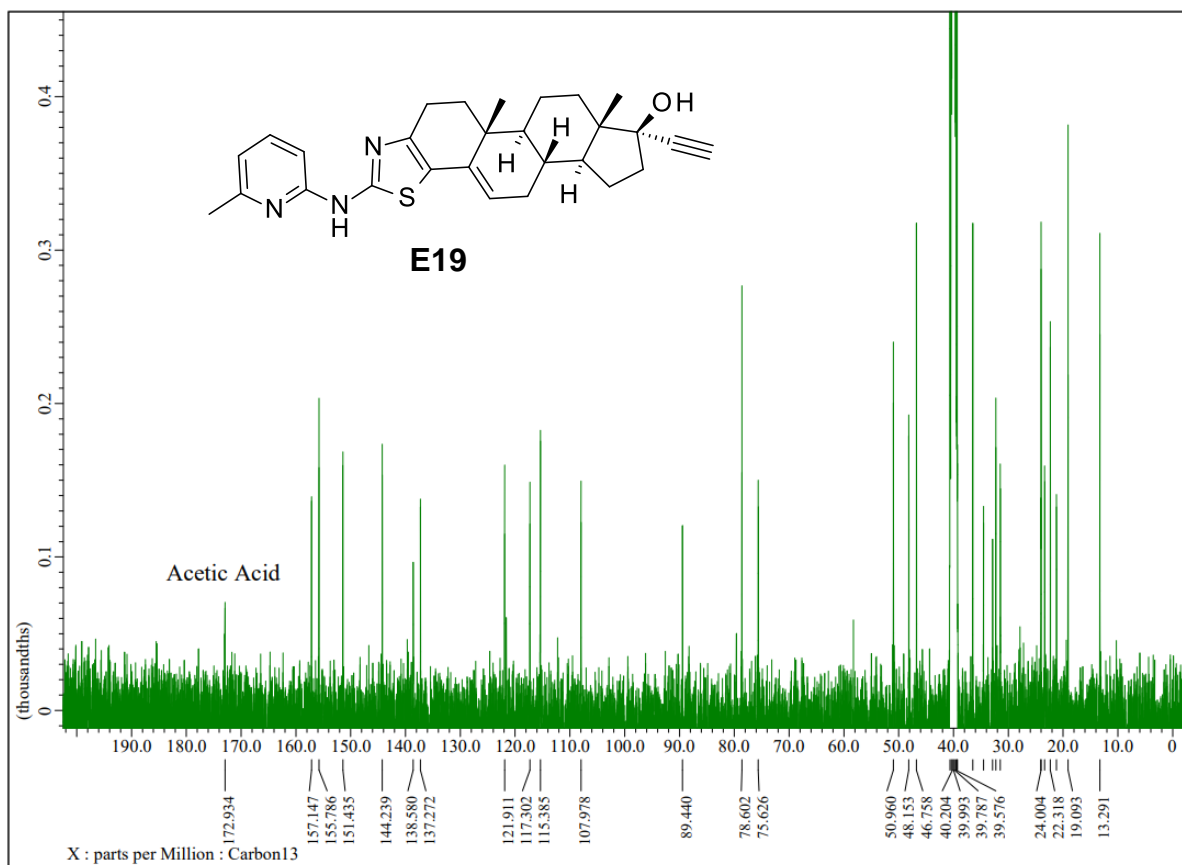


Figure S-35: ^{13}C NMR spectrum of compound **E19** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-12
Sample id#: 5190
Instrument: Shimadzu IT-TOF

9/20/2023

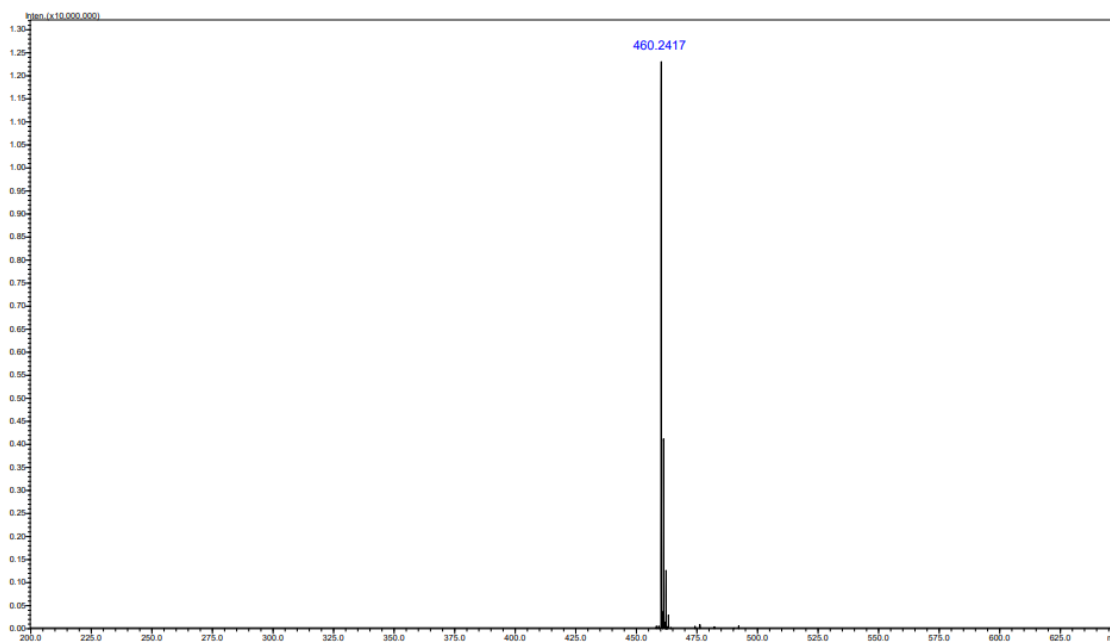


Figure S-36: High-resolution mass spectrum of compound E19

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-7-[(5-fluoro-2-pyridyl)amino]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E20)

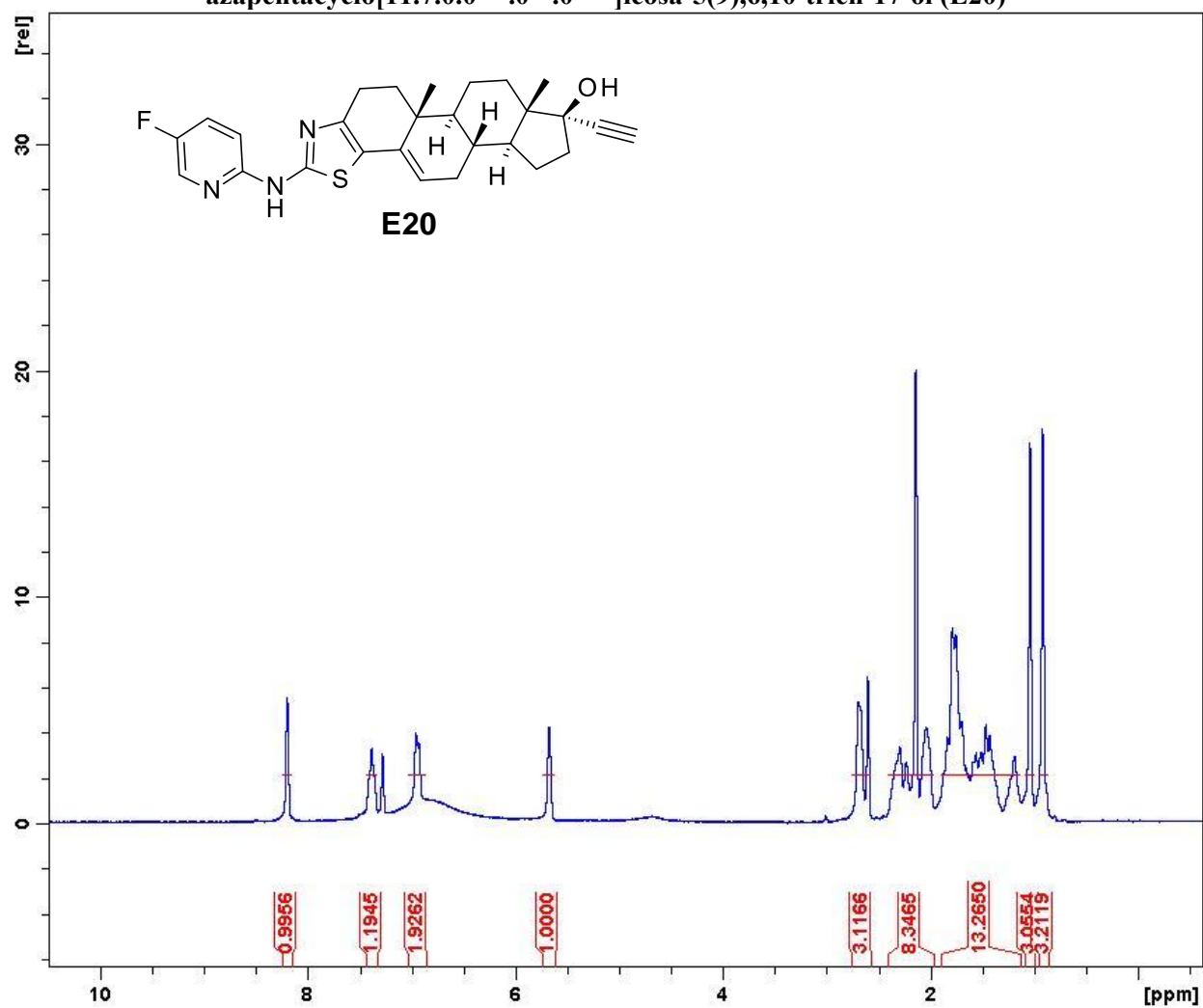


Figure S-37: ¹H NMR spectrum of compound E20 in CDCl₃

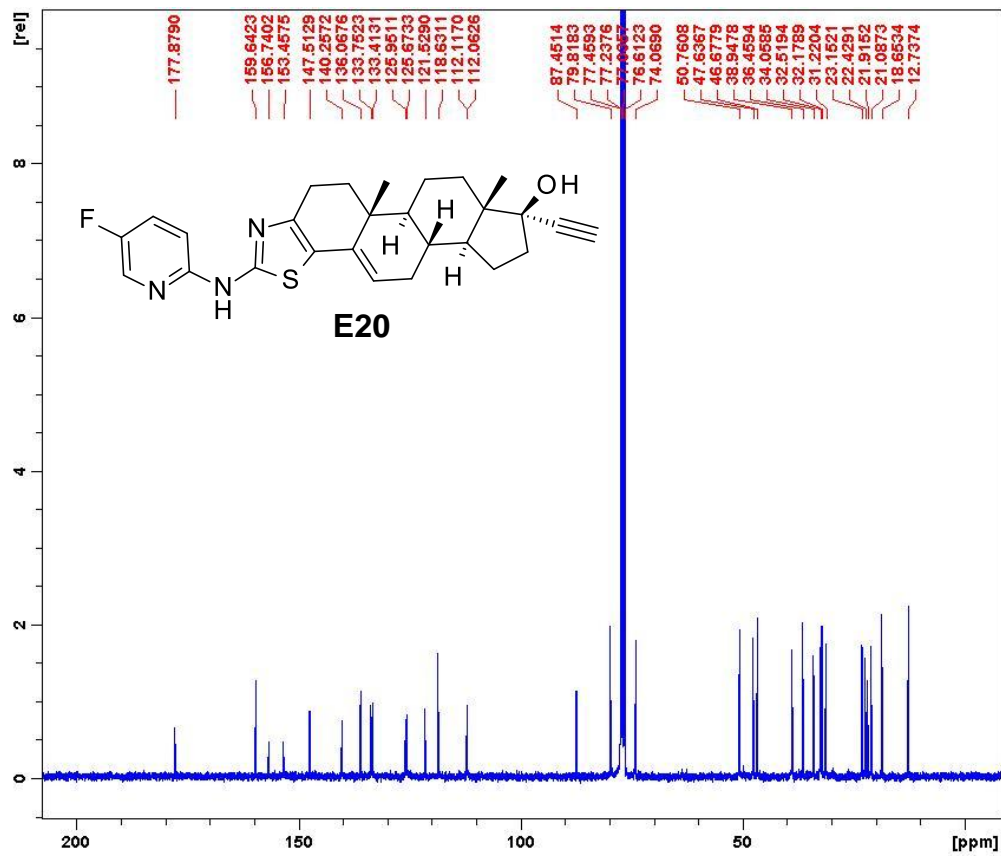


Figure S-38: ^{13}C NMR spectrum of compound E20 in CDCl_3

Arkansas Statewide Mass Spectrometry Facility
ESI high-res Mass Spectrum

Sample Name: E-13
Sample id#: 5191
Instrument: Shimadzu IT-TOF

9/20/2023

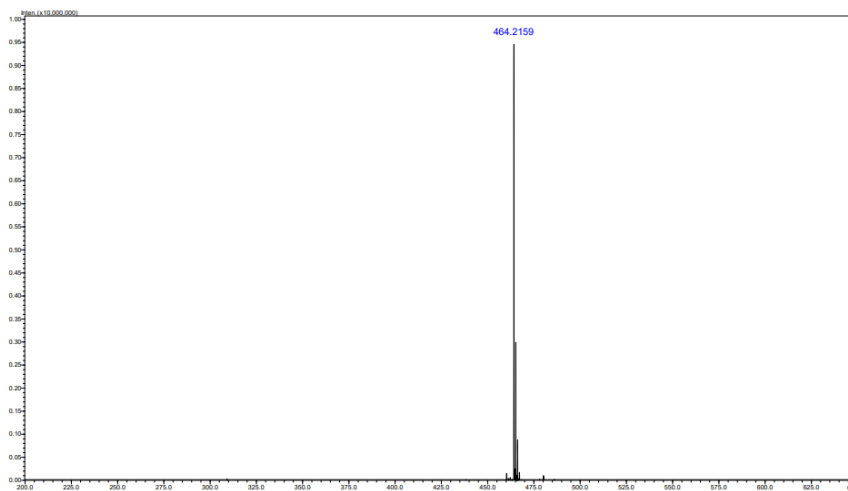


Figure S-39: High-resolution mass spectrum of compound E20

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-[(4-Chloro-2-pyridyl)amino]-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E21)

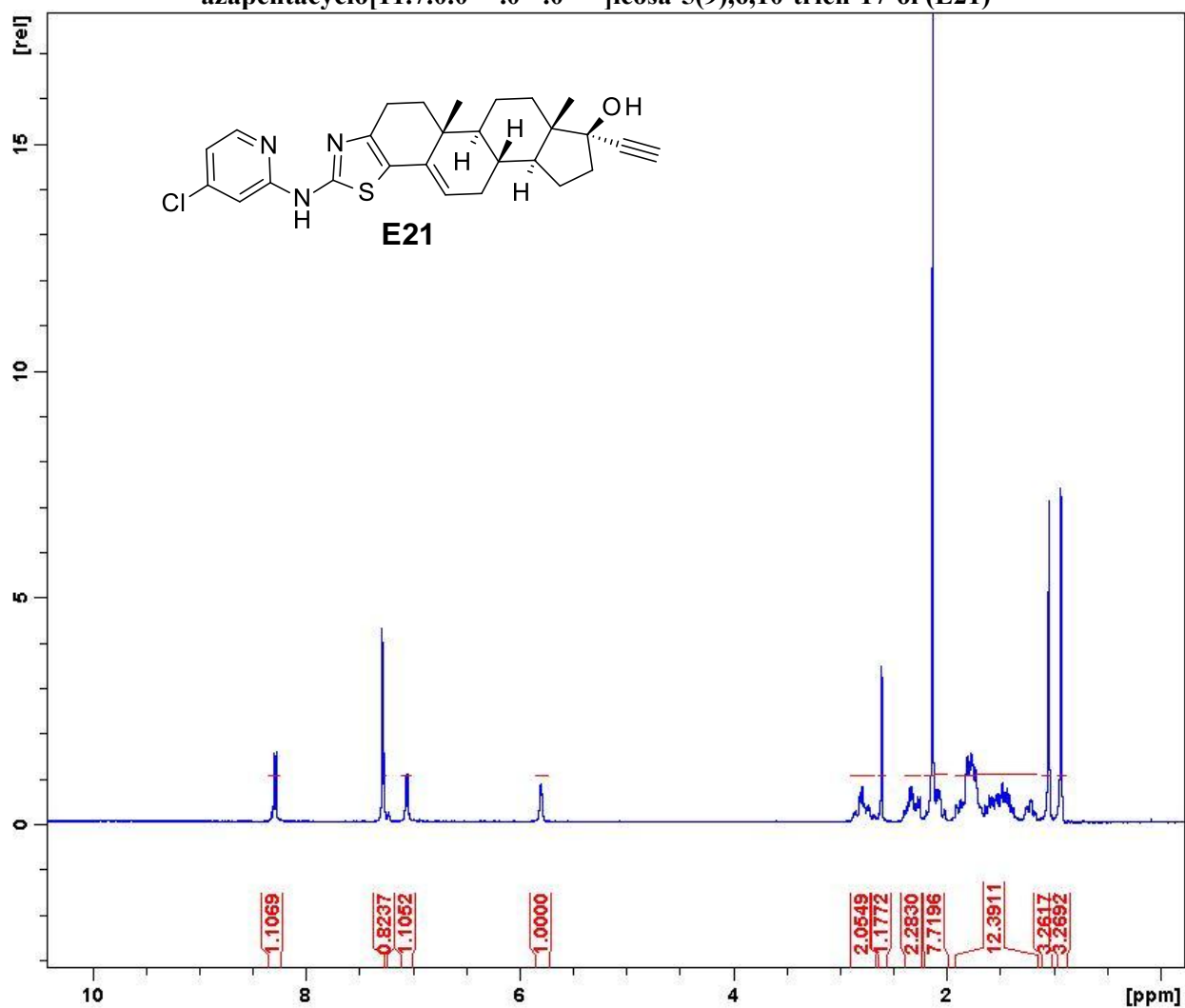


Figure S-40: ¹H NMR spectrum of compound E21 in CDCl₃

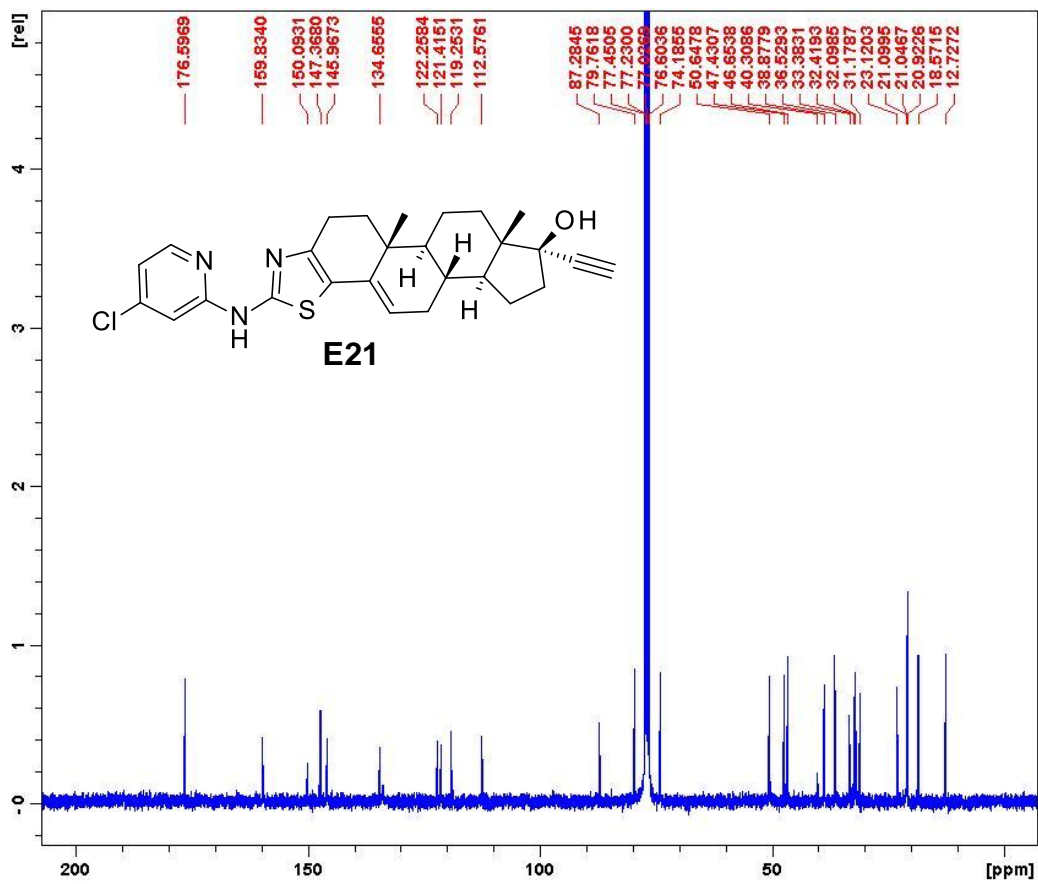


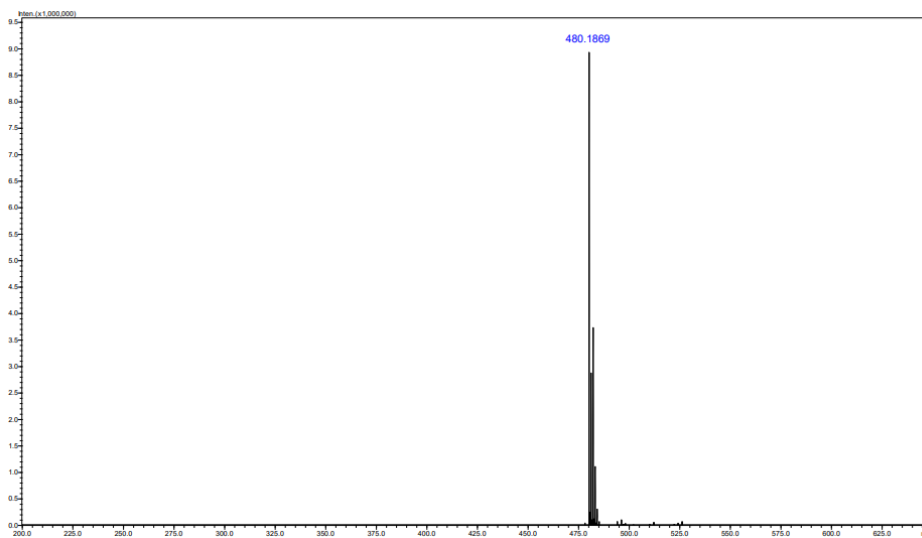
Figure S-41: ¹³C NMR spectrum of compound E21 in CDCl₃

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-14
 Sample id#: 5192
 Instrument: Shimadzu IT-TOF

9/20/2023



Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-14
Sample id#: 5192
Instrument: Shimadzu IT-TOF

9/20/2023

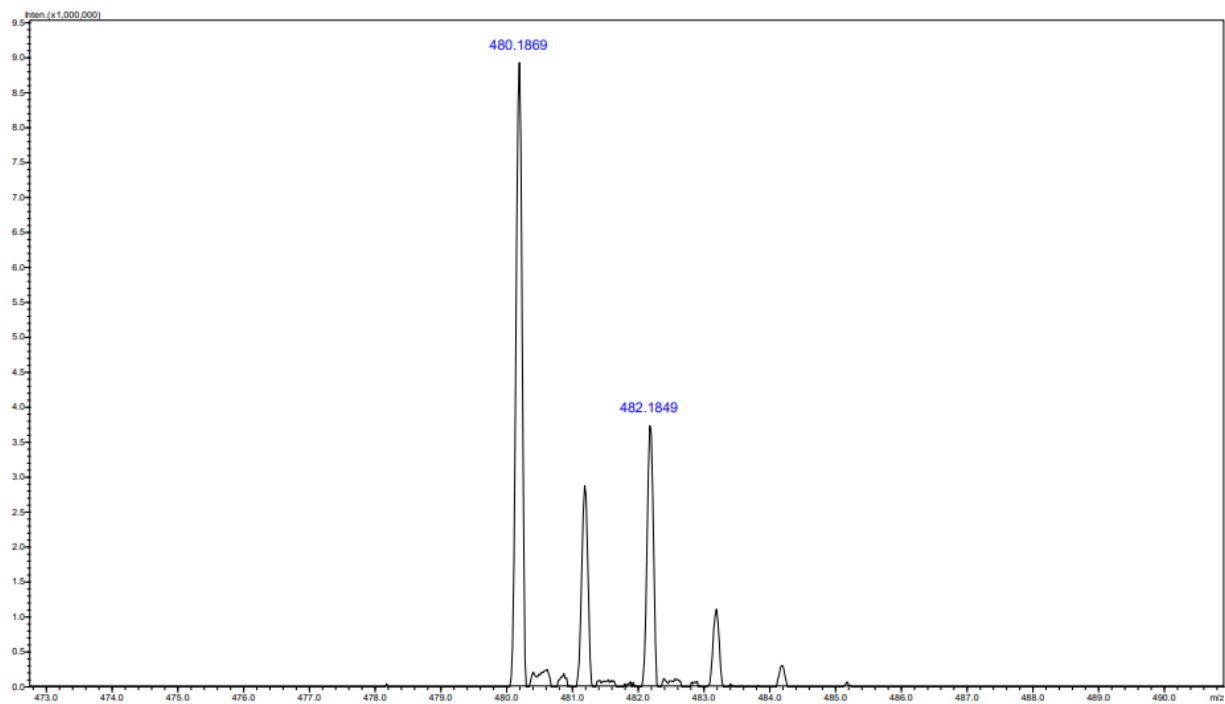


Figure S-42: High-resolution mass spectrum of compound **E21**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-[(5-Chloro-2-pyridyl)amino]-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E22)

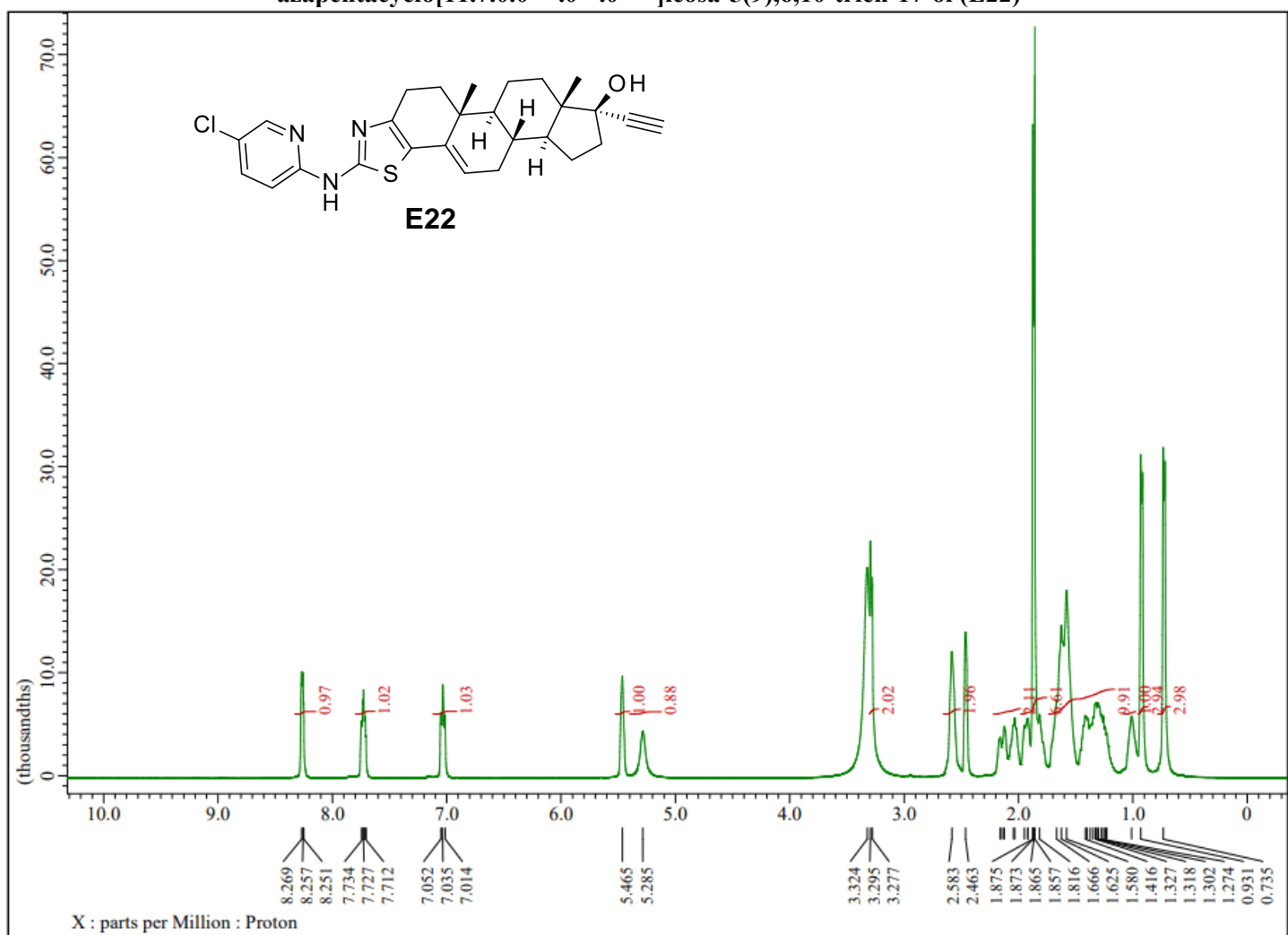


Figure S-43: ¹H NMR spectrum of compound E22 in DMSO-*d*₆

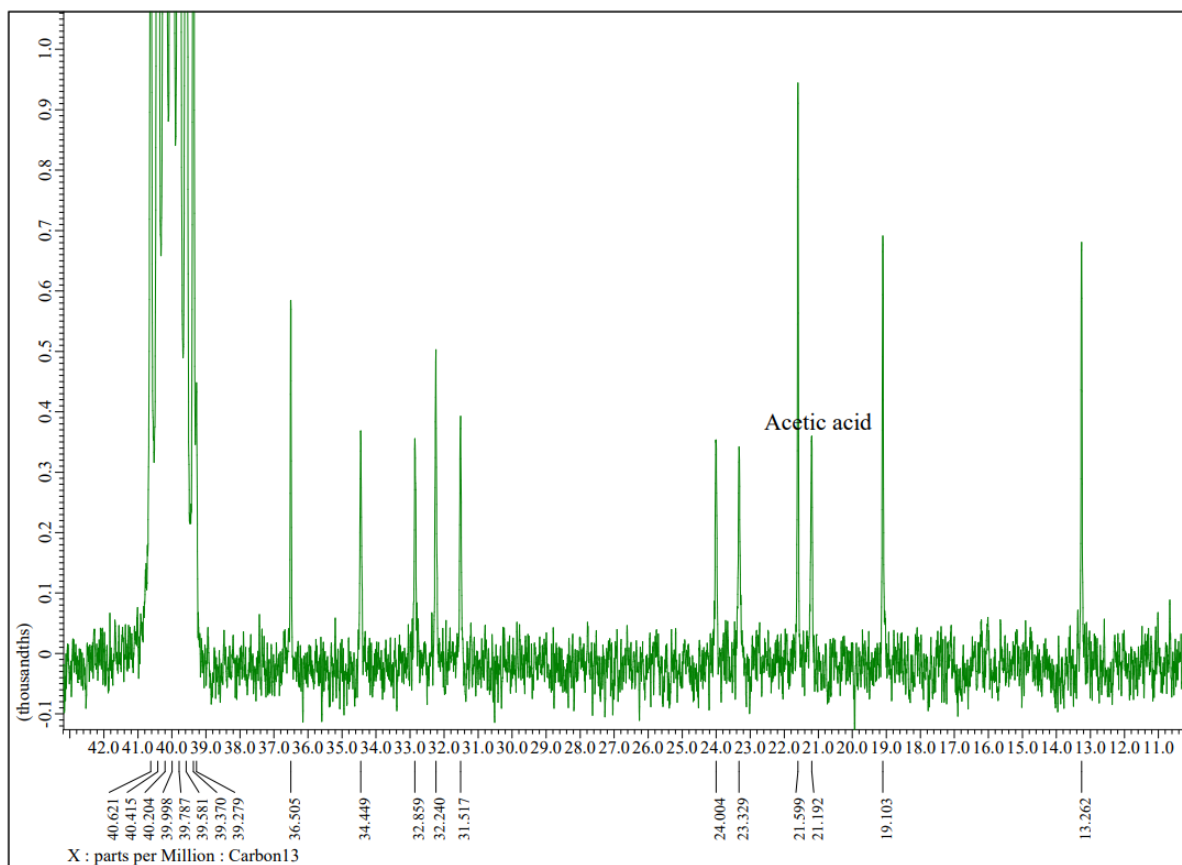
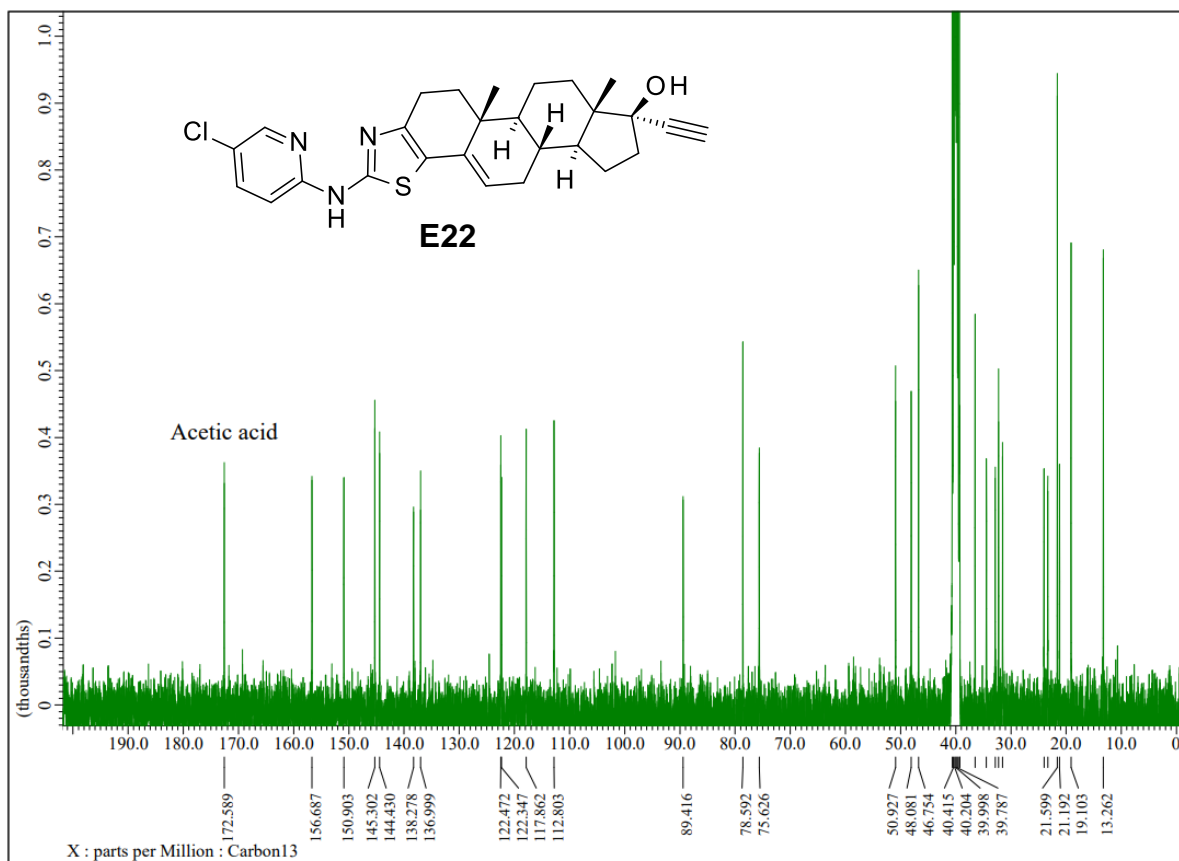


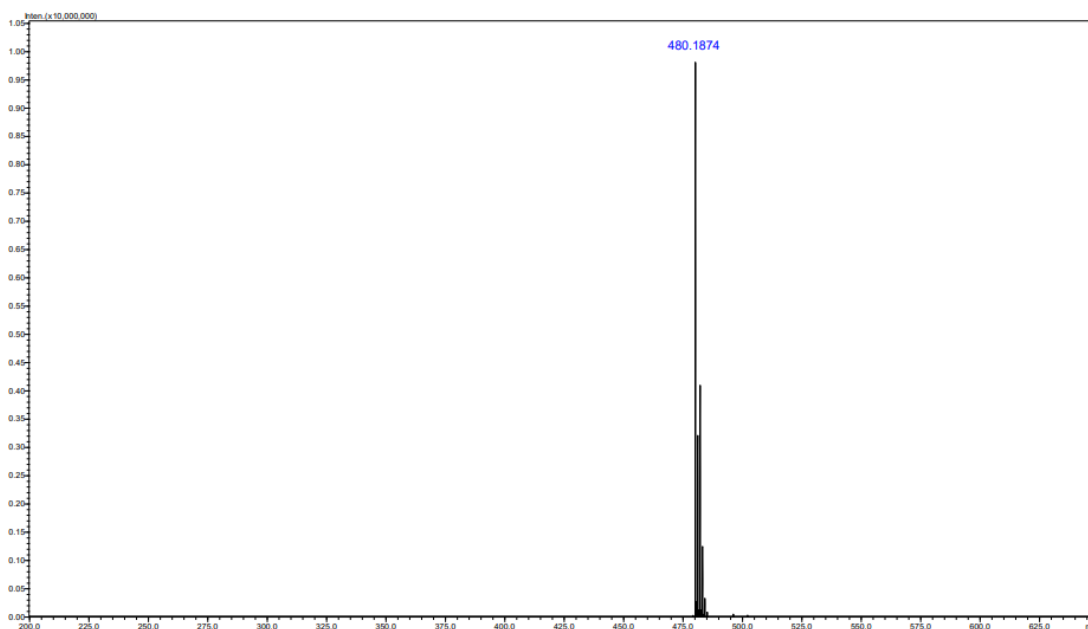
Figure S-44: ^{13}C NMR spectrum of compound **E22** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-15
Sample id#: 5193
Instrument: Shimadzu IT-TOF

9/20/2023



Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-15
Sample id#: 5193
Instrument: Shimadzu IT-TOF

9/20/2023

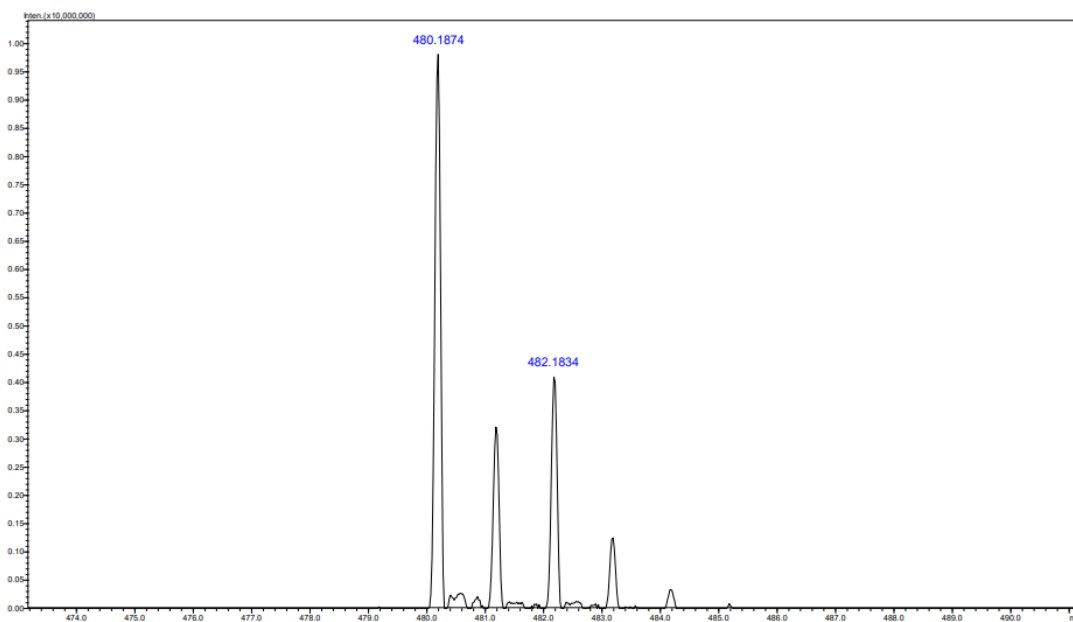


Figure S-45: High-resolution mass spectrum of compound E22

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-[(6-Chloro-2-pyridyl)amino]-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E23)

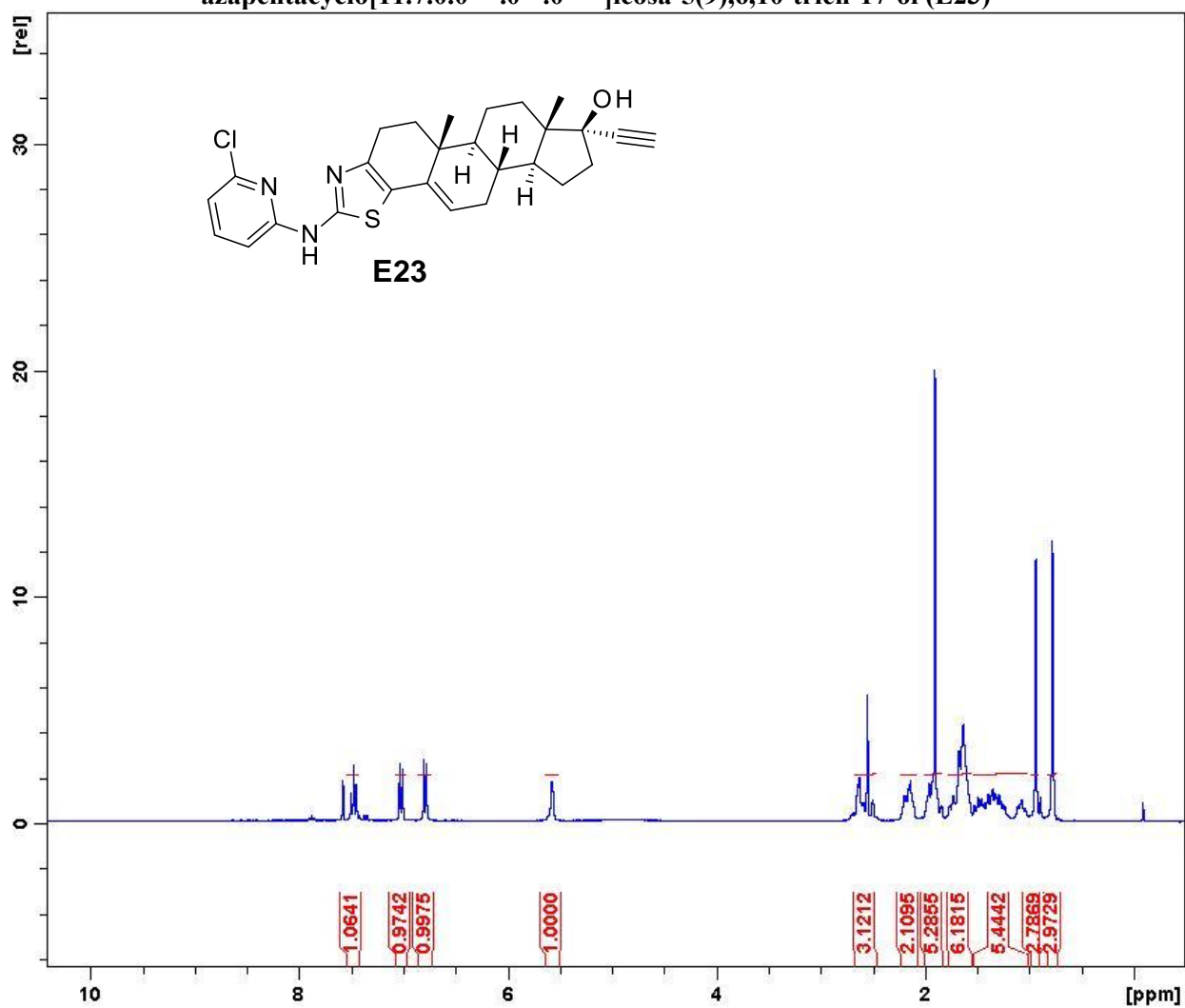


Figure S-46: ¹H NMR spectrum of compound E23 in CDCl₃

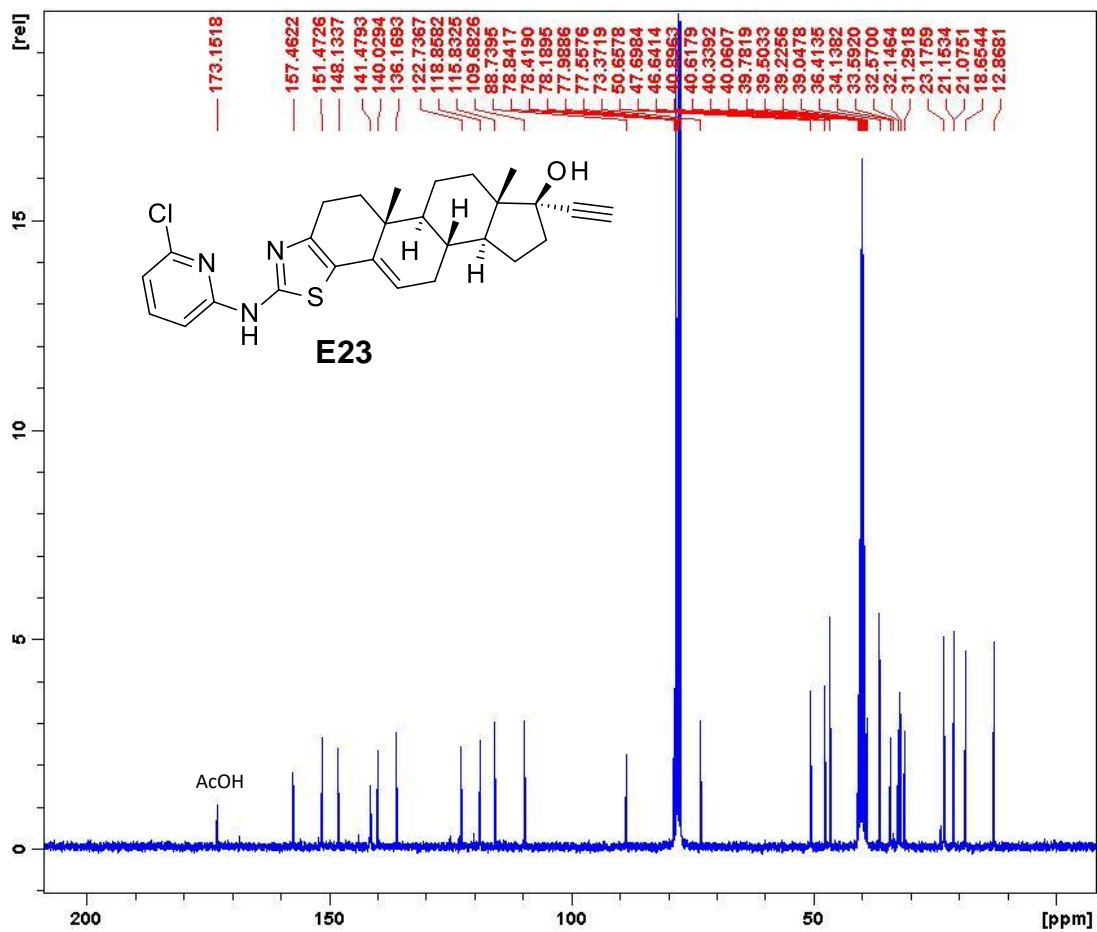
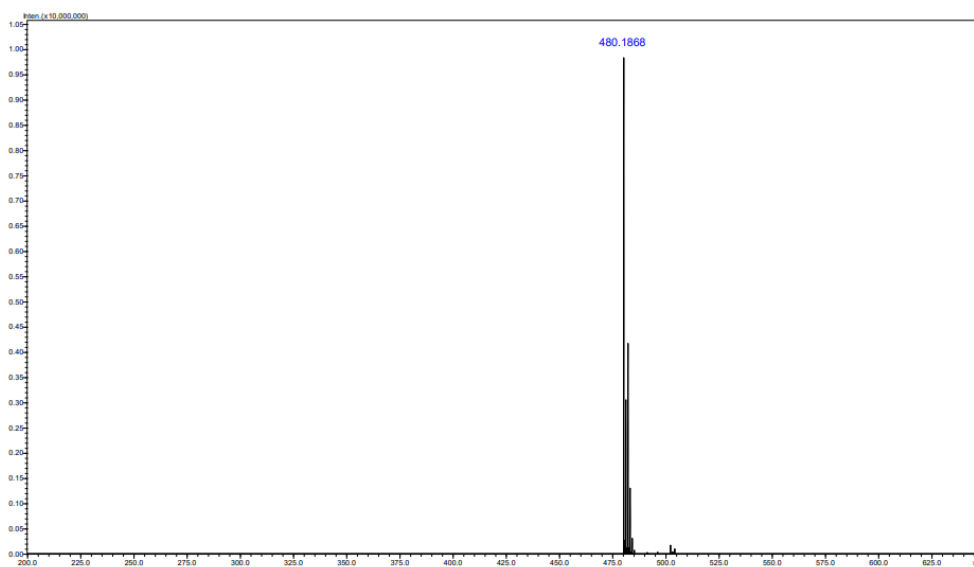


Figure S-47: ^{13}C NMR spectrum of compound E23 in CDCl_3 and $\text{DMSO}-d_6$

Arkansas Statewide Mass Spectrometry Facility
ESI high-res Mass Spectrum

Sample Name: E-16
Sample id#: 5194
Instrument: Shimadzu IT-TOF

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Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-16
Sample id#: 5194
Instrument: Shimadzu IT-TOF

9/20/2023

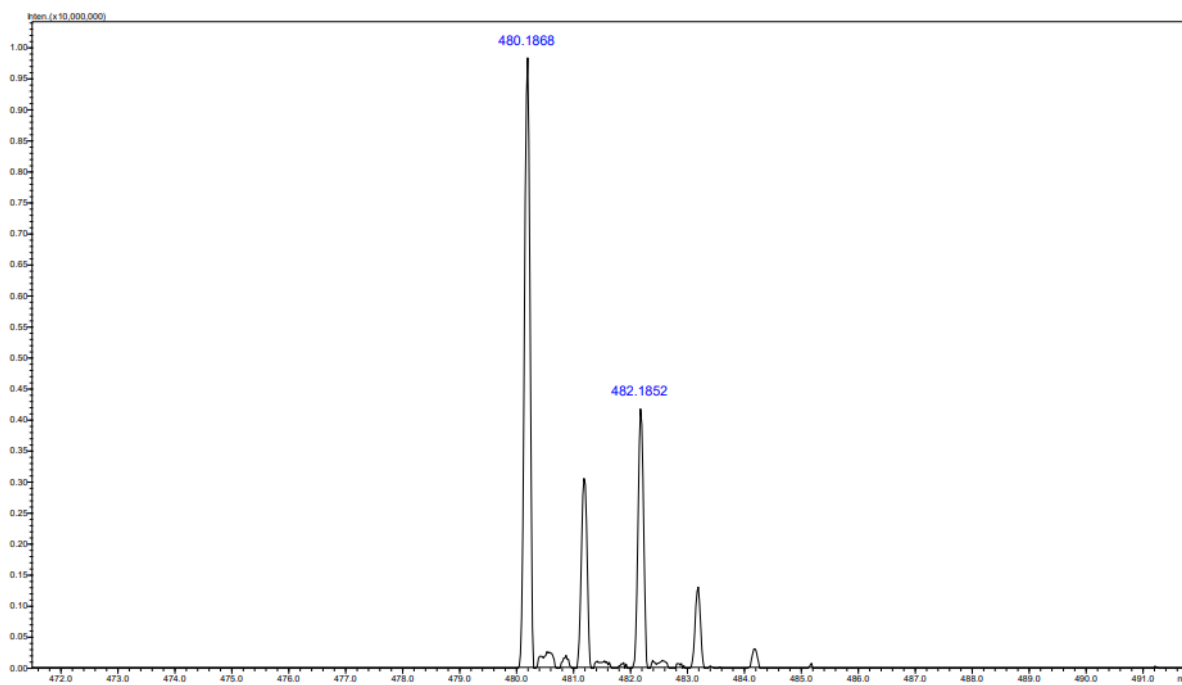


Figure S-48: High-resolution mass spectrum of compound E23

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-[(4,6-Dimethyl-2-pyridyl)amino]-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E24)

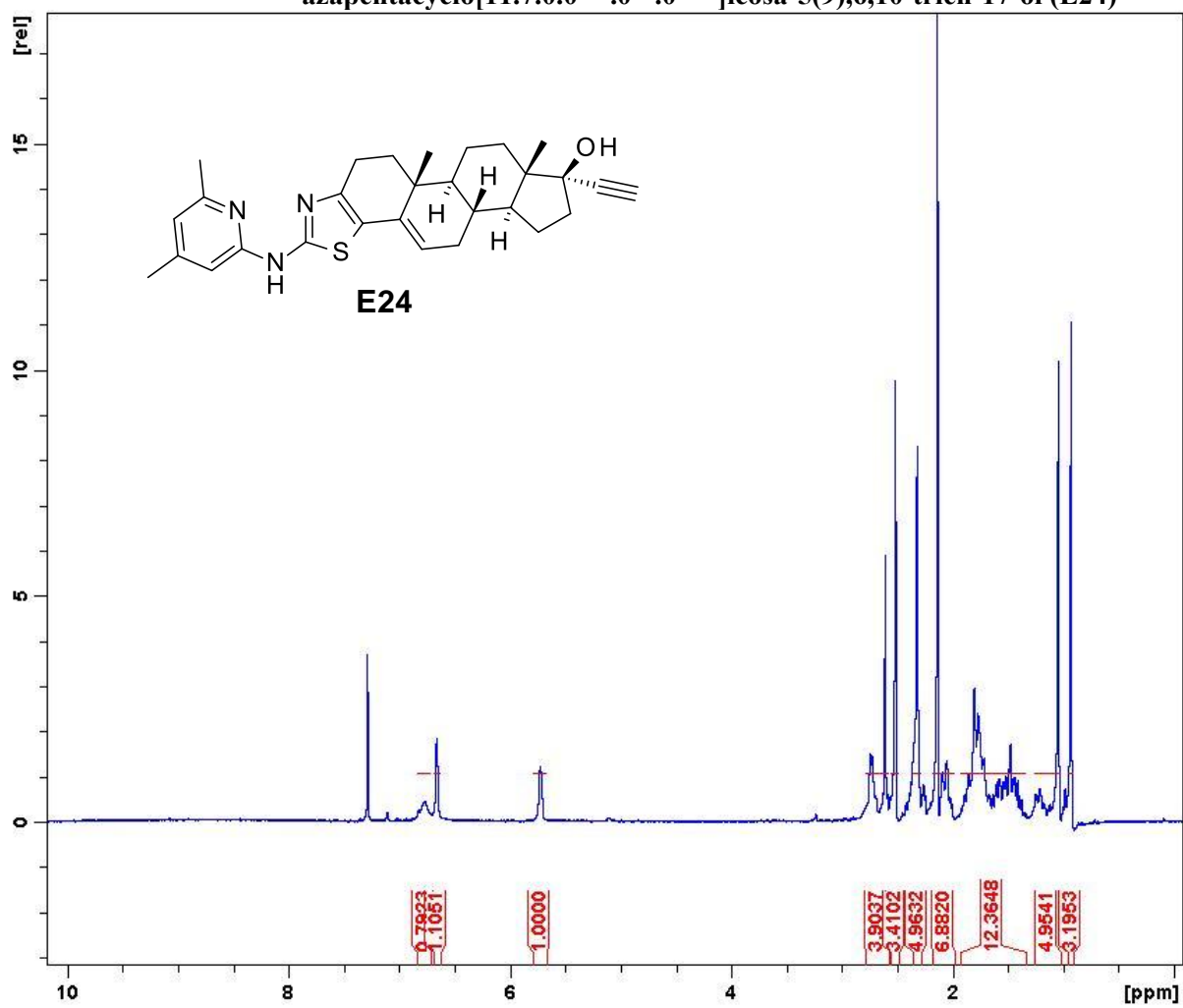


Figure S-49: ¹H NMR spectrum of compound E24 in CDCl₃

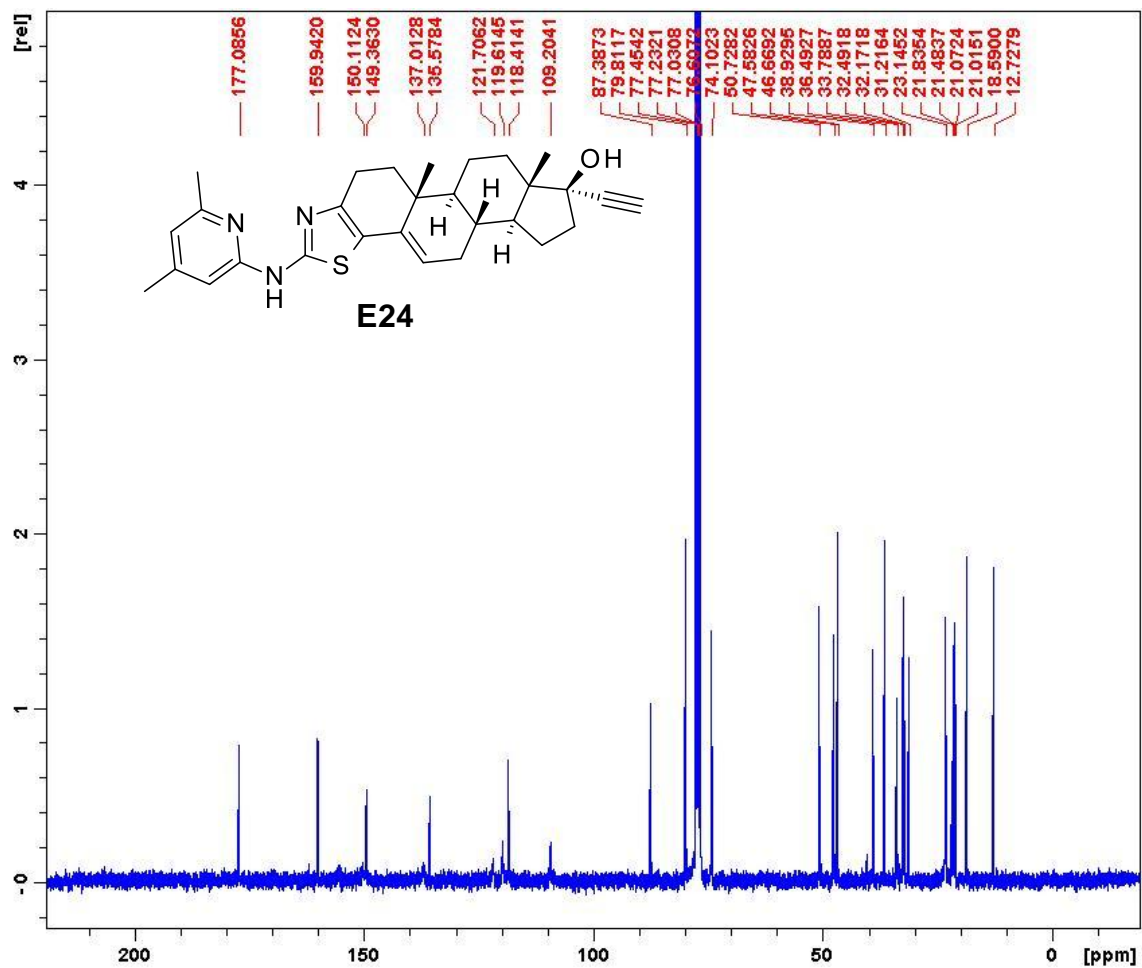


Figure S-50: ^{13}C NMR spectrum of compound **E24** in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-17
 Sample id#: 5195
 Instrument: Shimadzu IT-TOF

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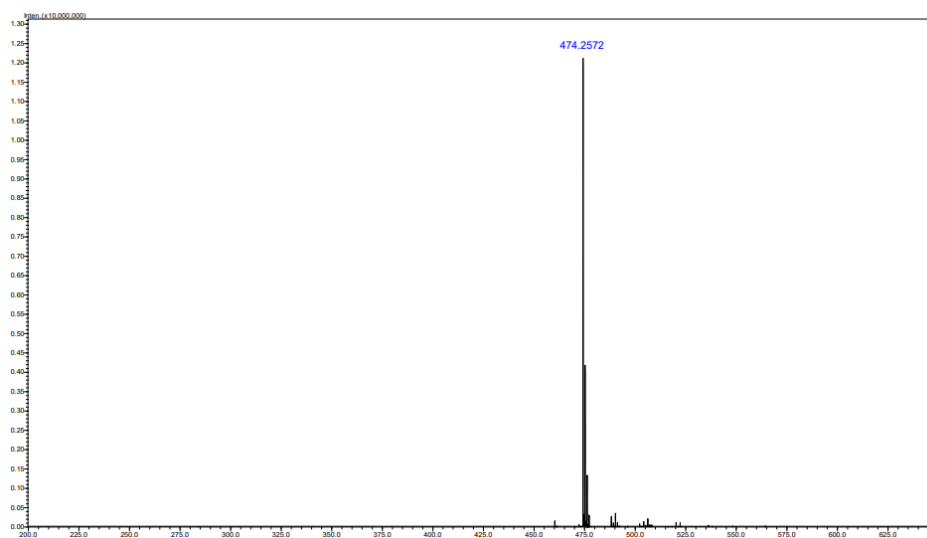


Figure S-51: High-resolution mass spectrum of compound **E24**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-7-[(4-methoxy-6-methyl-pyrimidin-2-yl)amino]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E26)

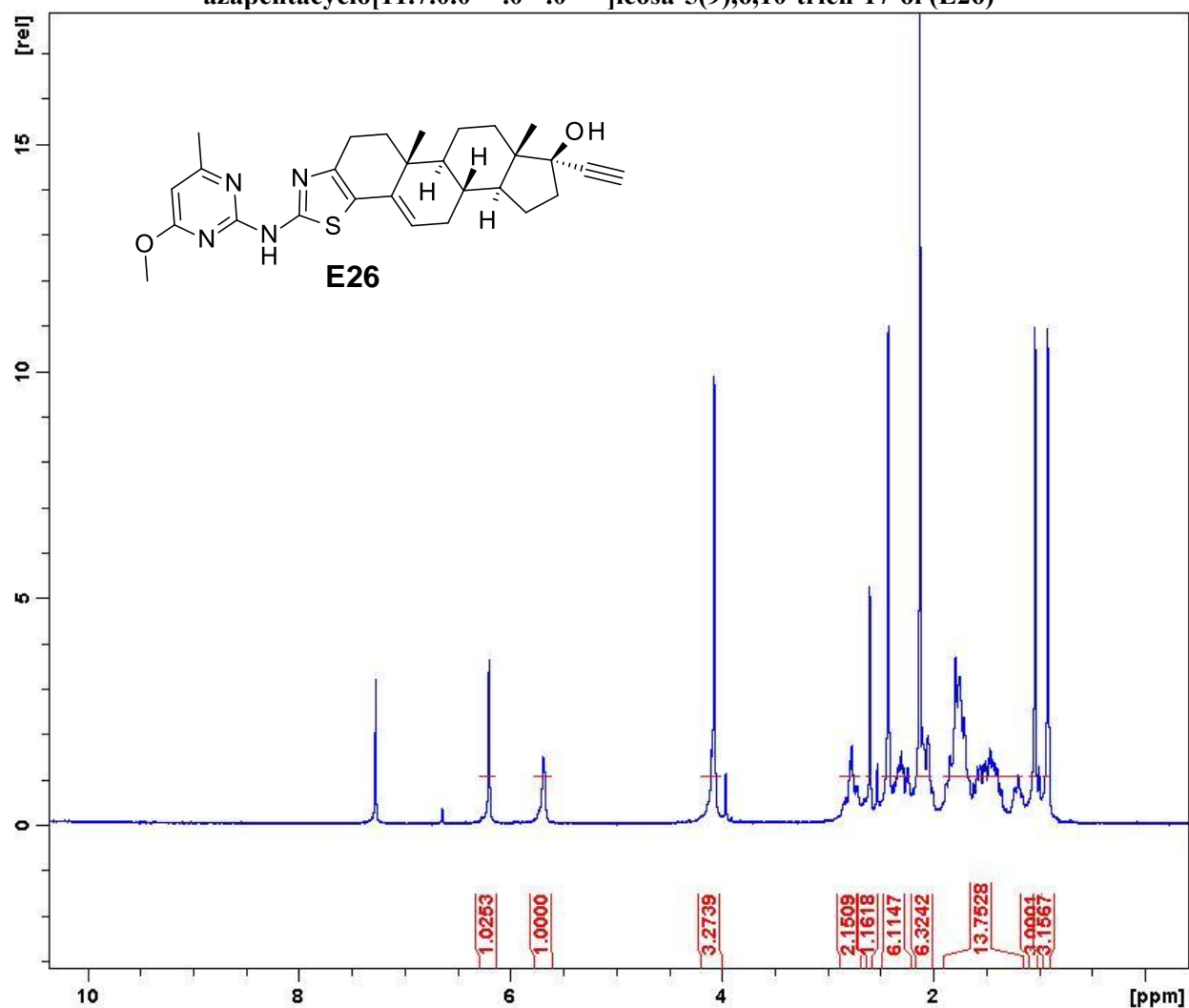


Figure S-52: ¹H NMR spectrum of compound E26 in CDCl₃

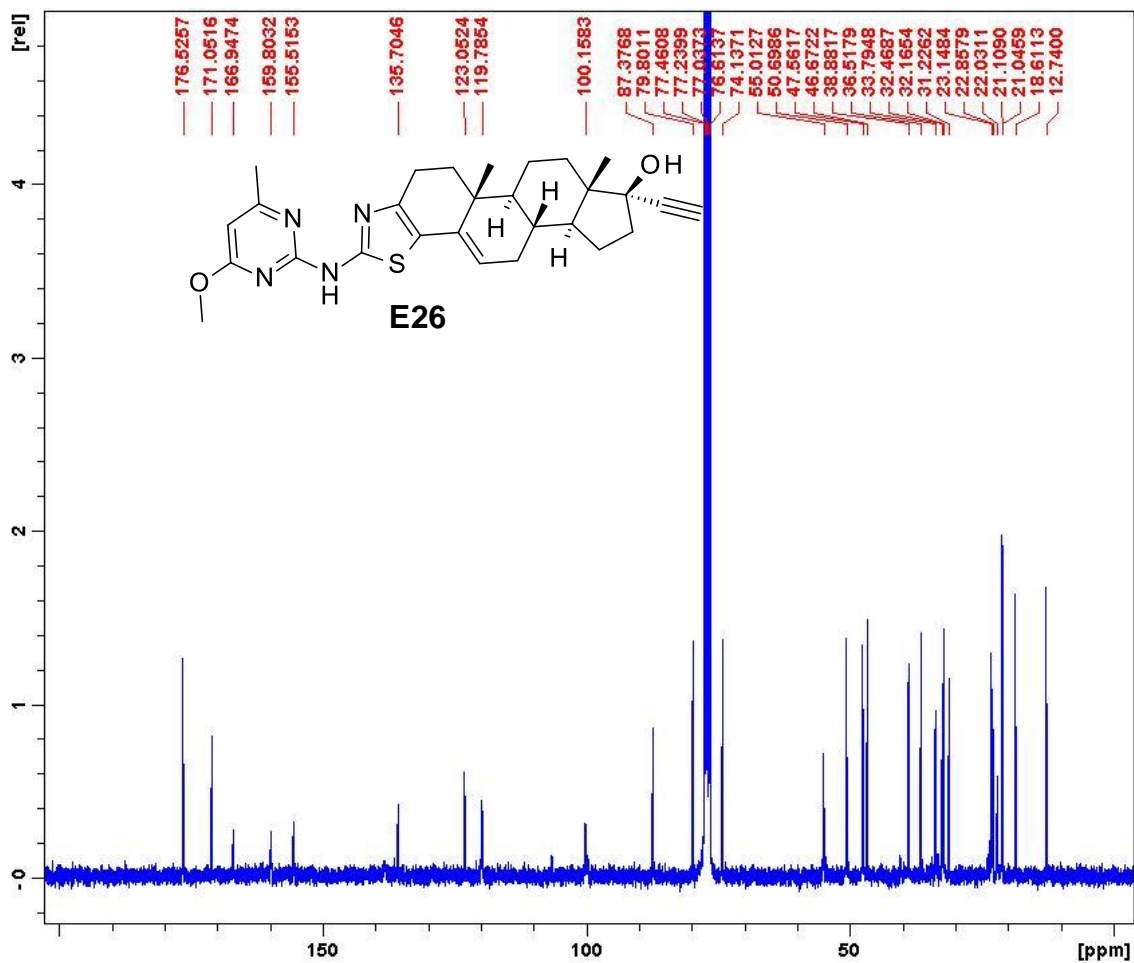


Figure S-53: ^{13}C NMR spectrum of compound **E26** in CDCl_3

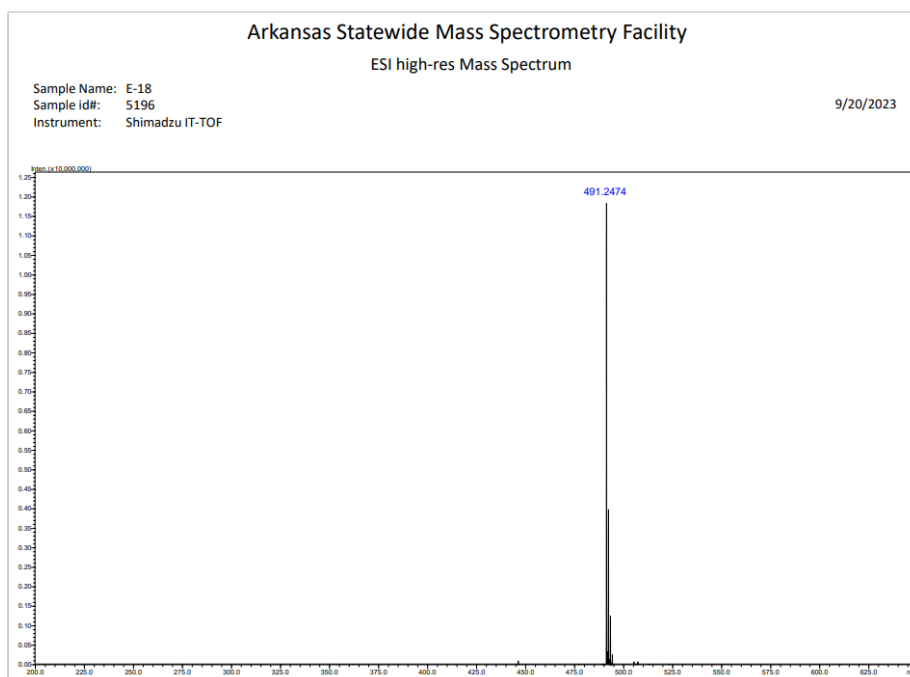


Figure S-54: High-resolution mass spectrum of compound **E26**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-(1-piperidyl)-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E27)

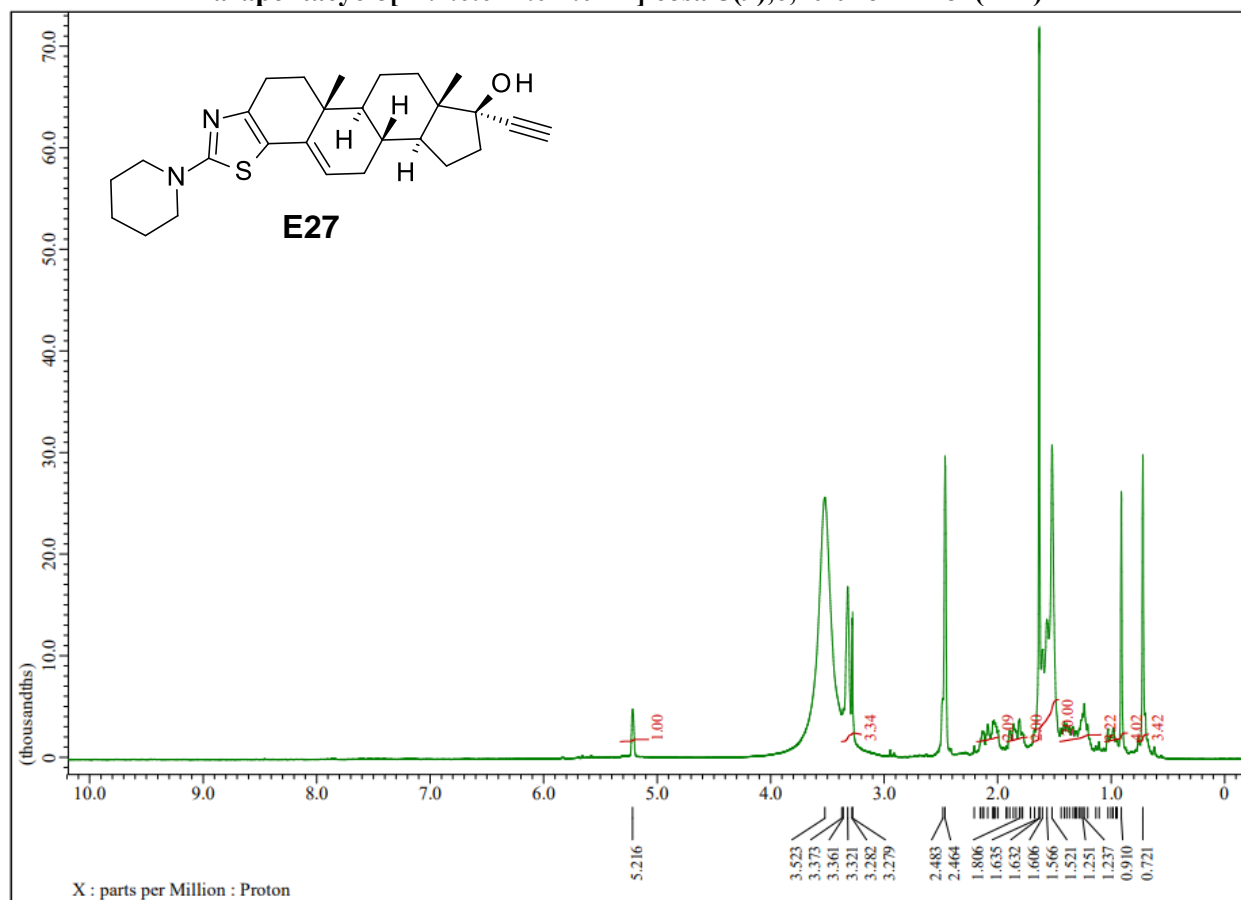


Figure S-55: ¹H NMR spectrum of compound E27 in DMSO-*d*₆

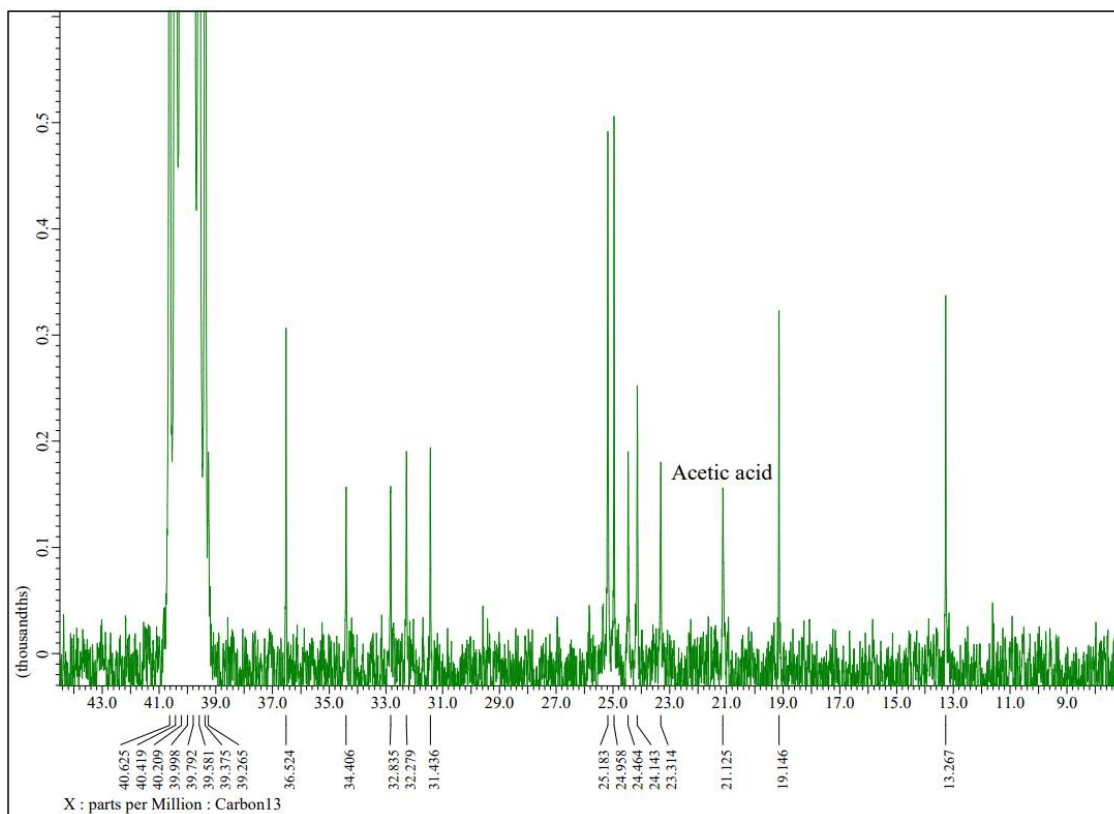
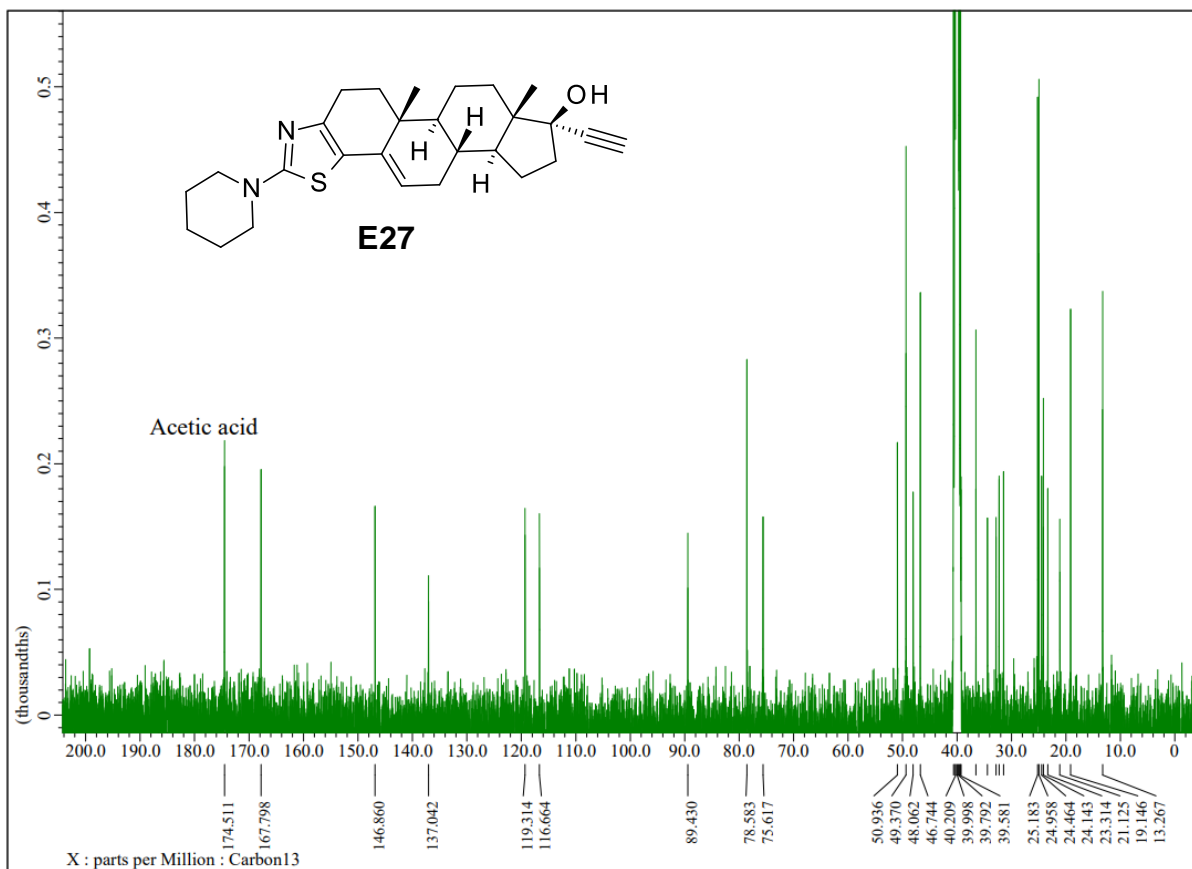


Figure S-56: ^{13}C NMR spectrum of compound **E27** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-19
Sample id#: 5197
Instrument: Shimadzu IT-TOF

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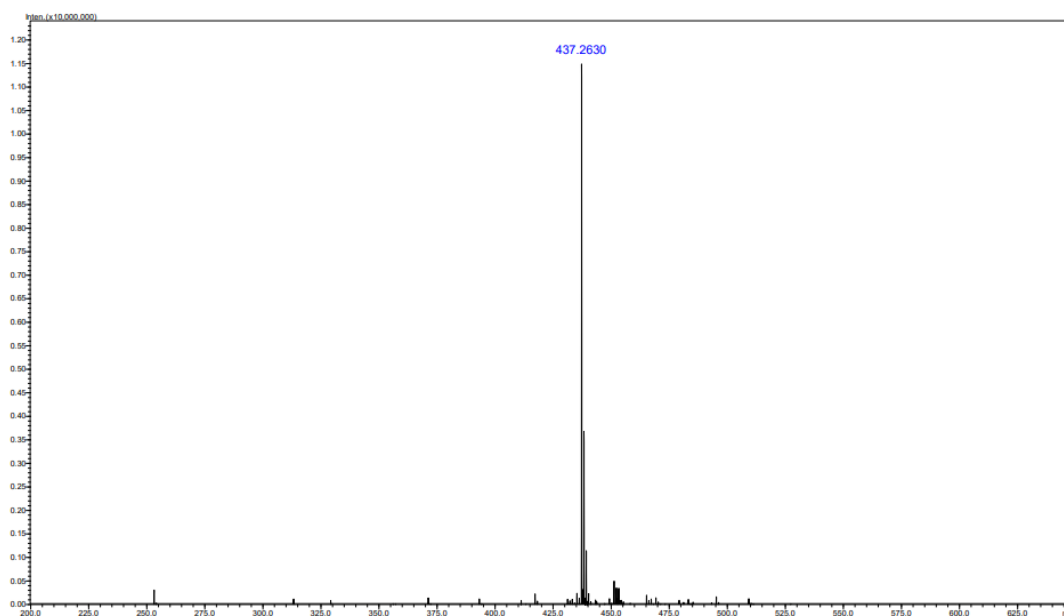


Figure S-57: High-resolution mass spectrum of compound E27

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-(4-methylpiperazin-1-yl)-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E28)

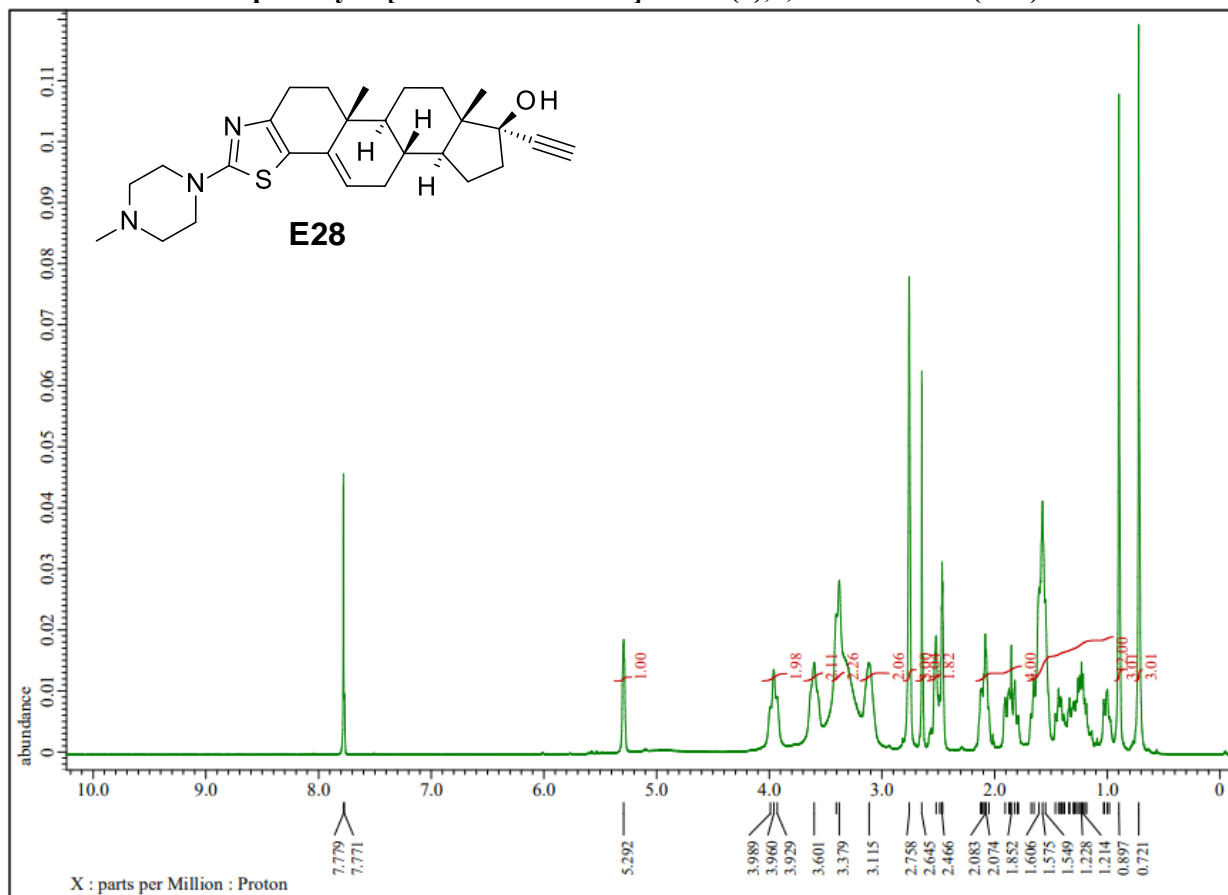


Figure S-58: ¹H NMR spectrum of compound E28 in DMSO-d₆

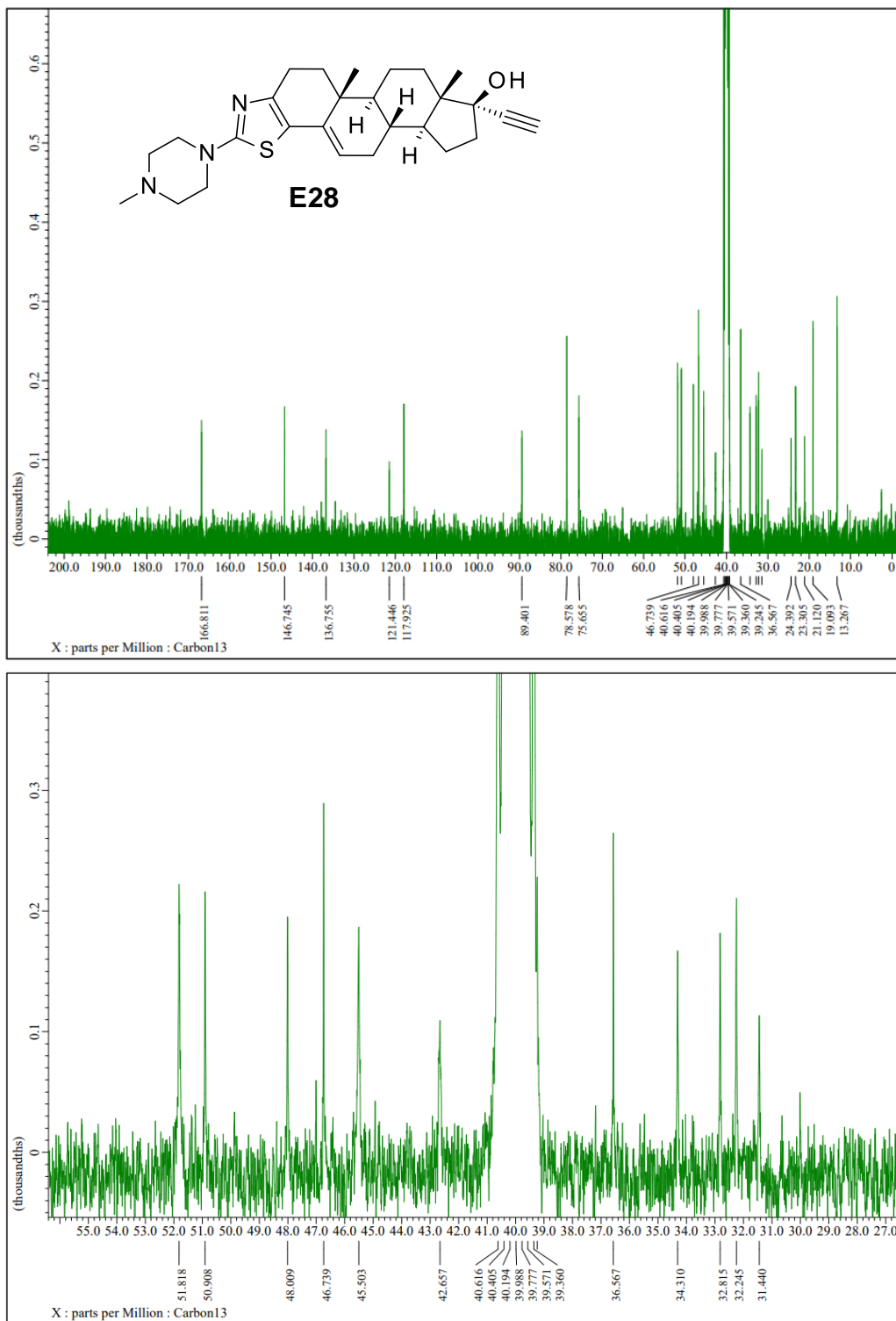


Figure S-59: ^{13}C NMR spectrum of compound **E28** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-20
Sample id#: 5198
Instrument: Shimadzu IT-TOF

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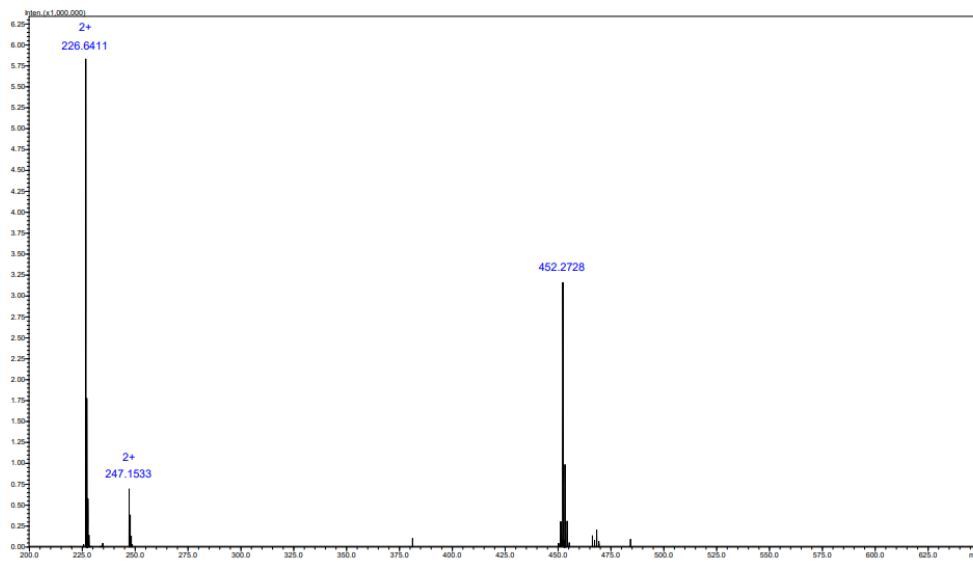


Figure S-60: High-resolution mass spectrum of compound **E28**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,7,18-trimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E29)

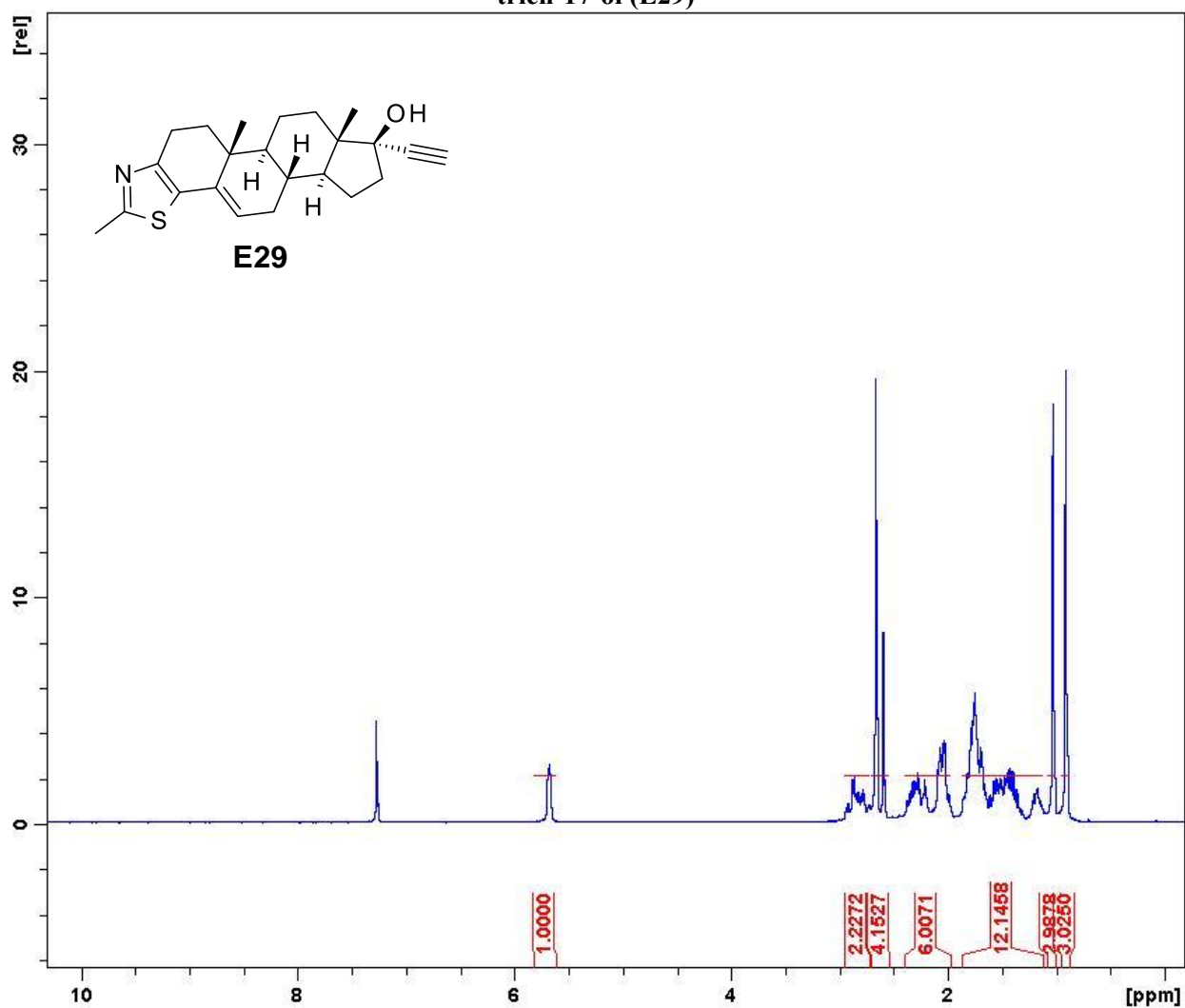


Figure S-61: ¹H NMR spectrum of compound E29 in CDCl₃

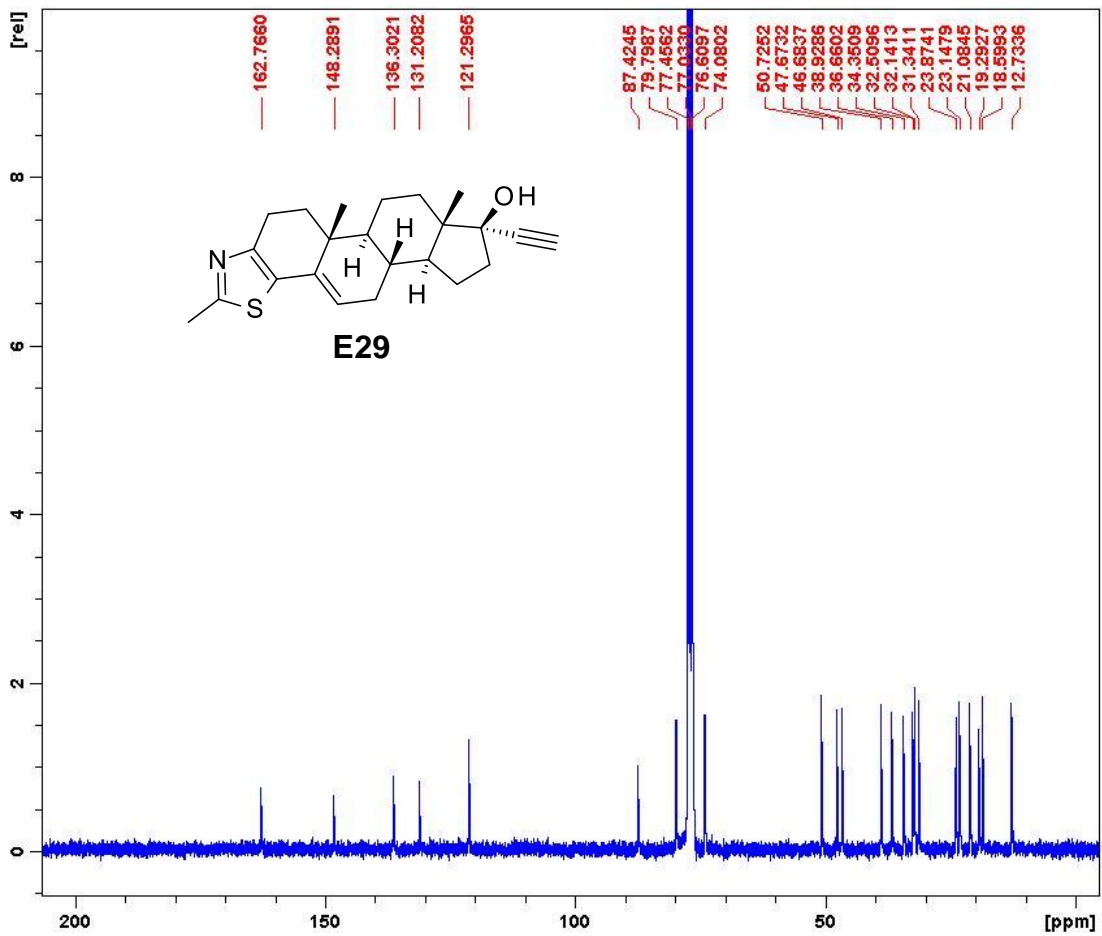


Figure S-62: ¹³C NMR spectrum of compound E29 in CDCl₃

Arkansas Statewide Mass Spectrometry Facility
ESI high-res Mass Spectrum

Sample Name: E-21
Sample id#: 5199
Instrument: Shimadzu IT-TOF

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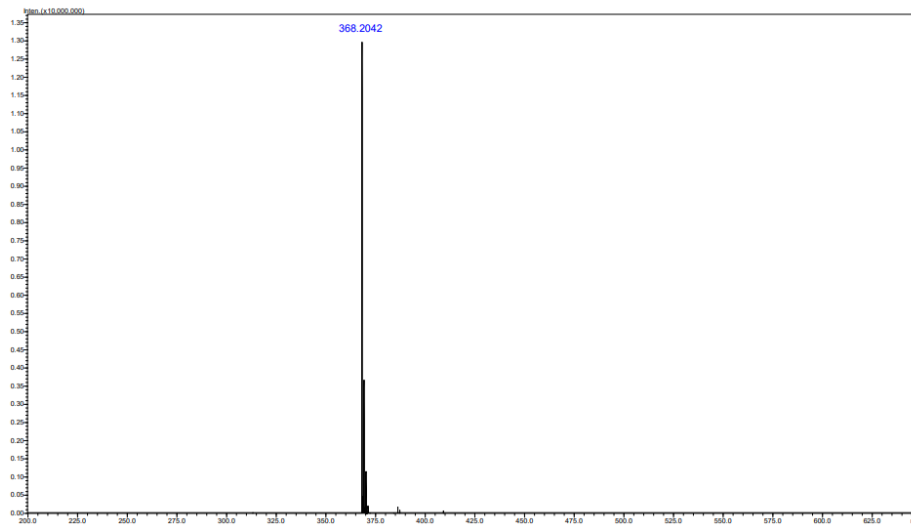


Figure S-63: High-resolution mass spectrum of compound E29

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-(*m*-tolyl)-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E34)

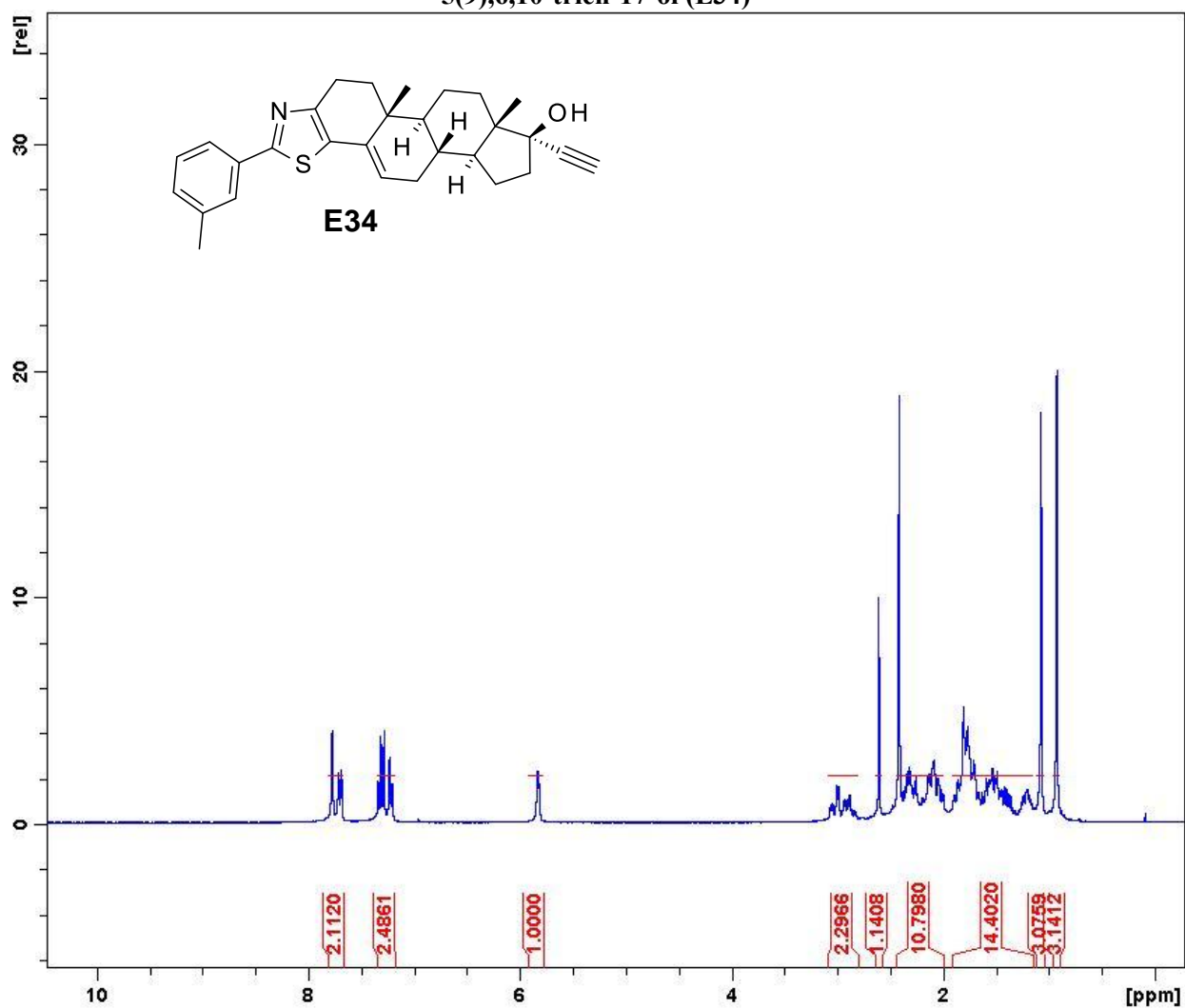


Figure S-64: ¹H NMR spectrum of compound E34 in CDCl₃

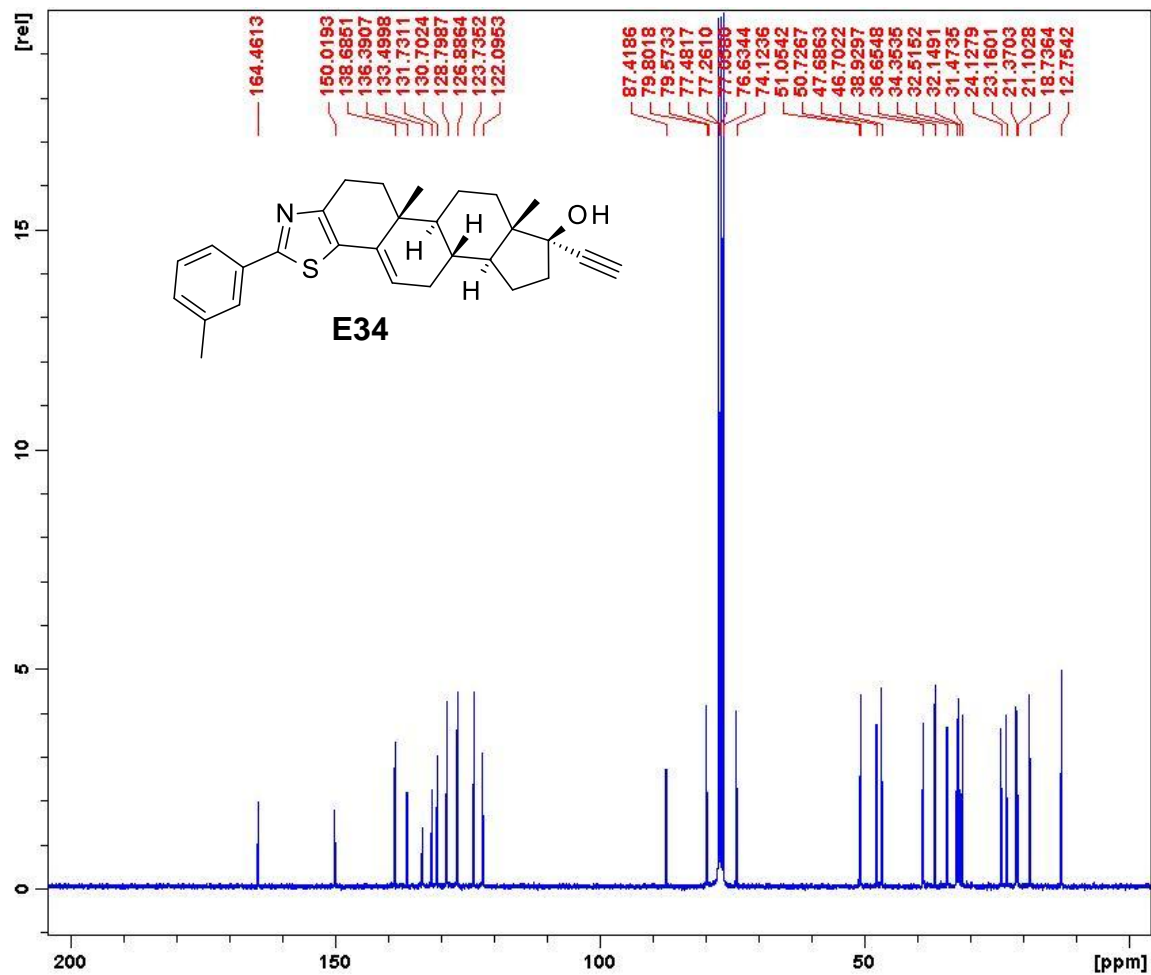


Figure S-65: ^{13}C NMR spectrum of compound **E34** in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-22
 Sample id#: 5200
 Instrument: Shimadzu IT-TOF

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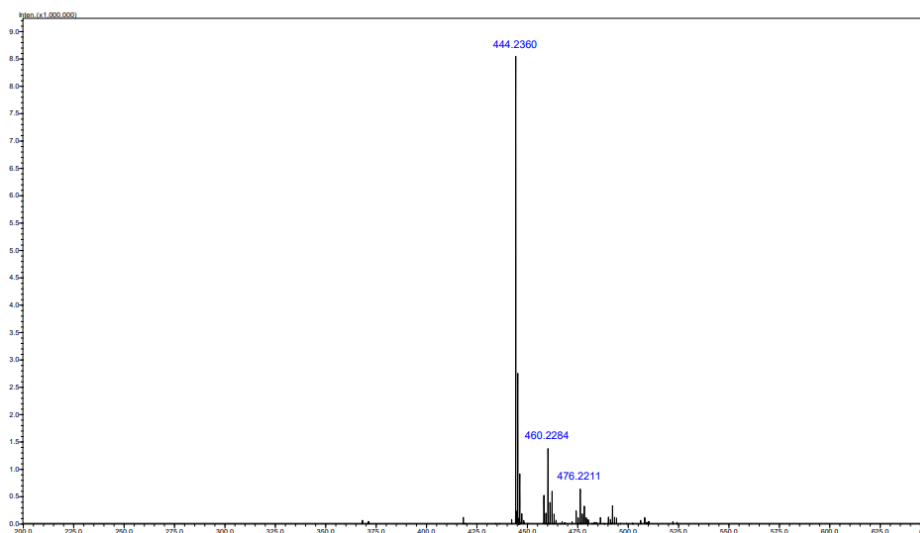


Figure S-66: High-resolution mass spectrum of compound **E34**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-7-(3-methoxyphenyl)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E36)

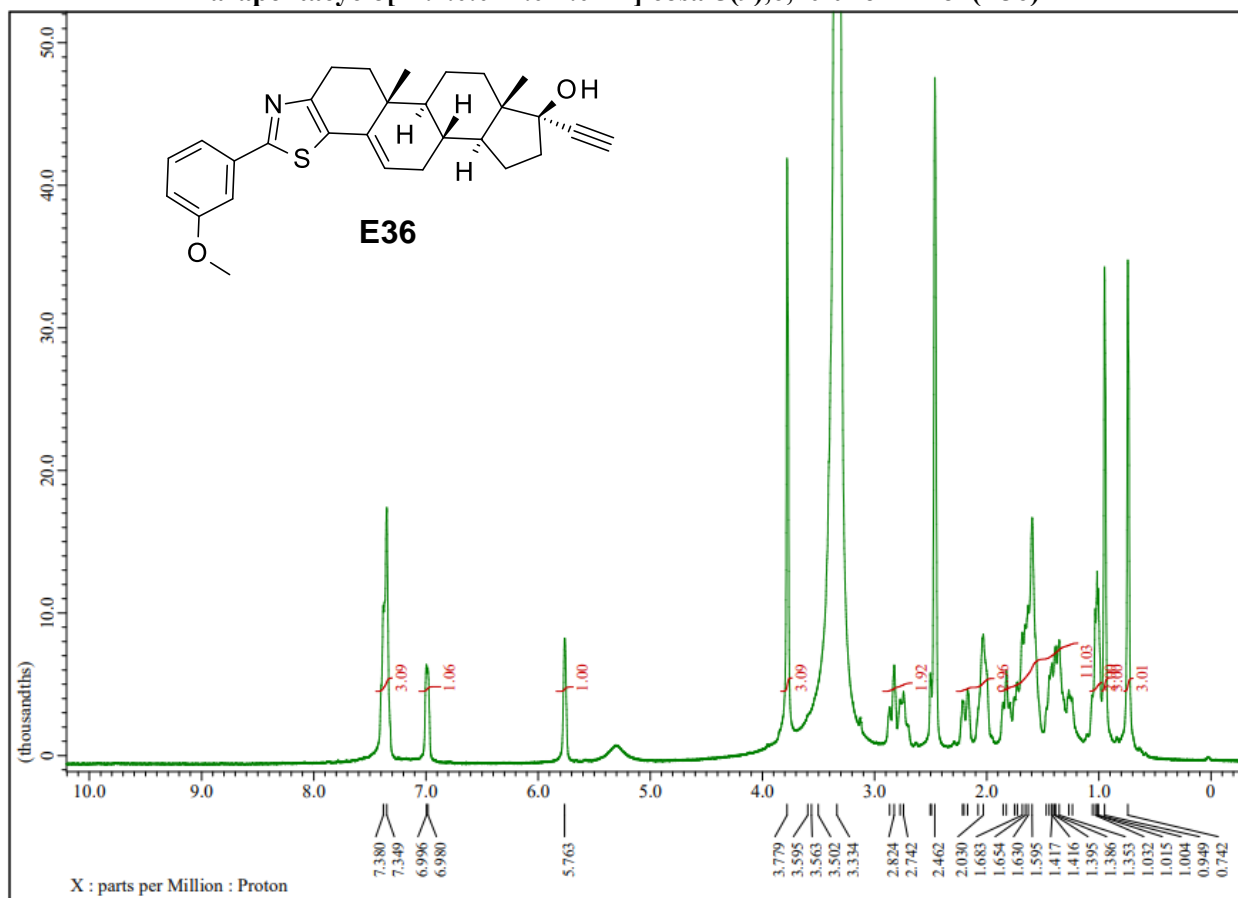


Figure S-67: ¹H NMR spectrum of compound **E36** in DMSO-*d*₆

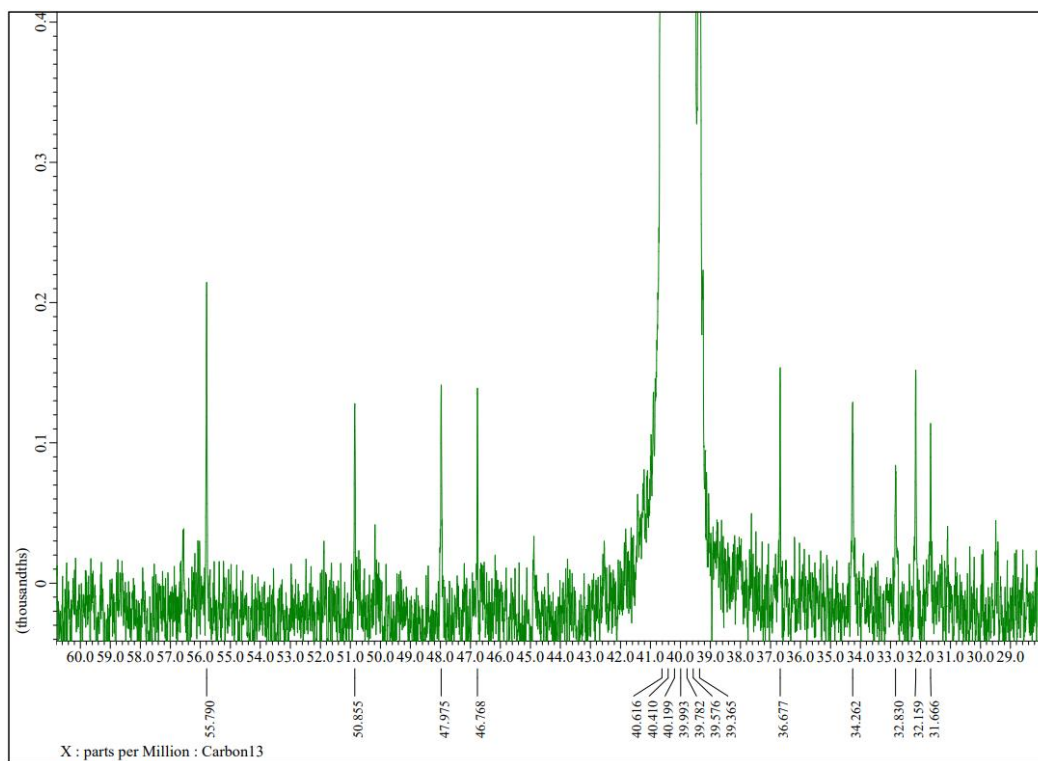
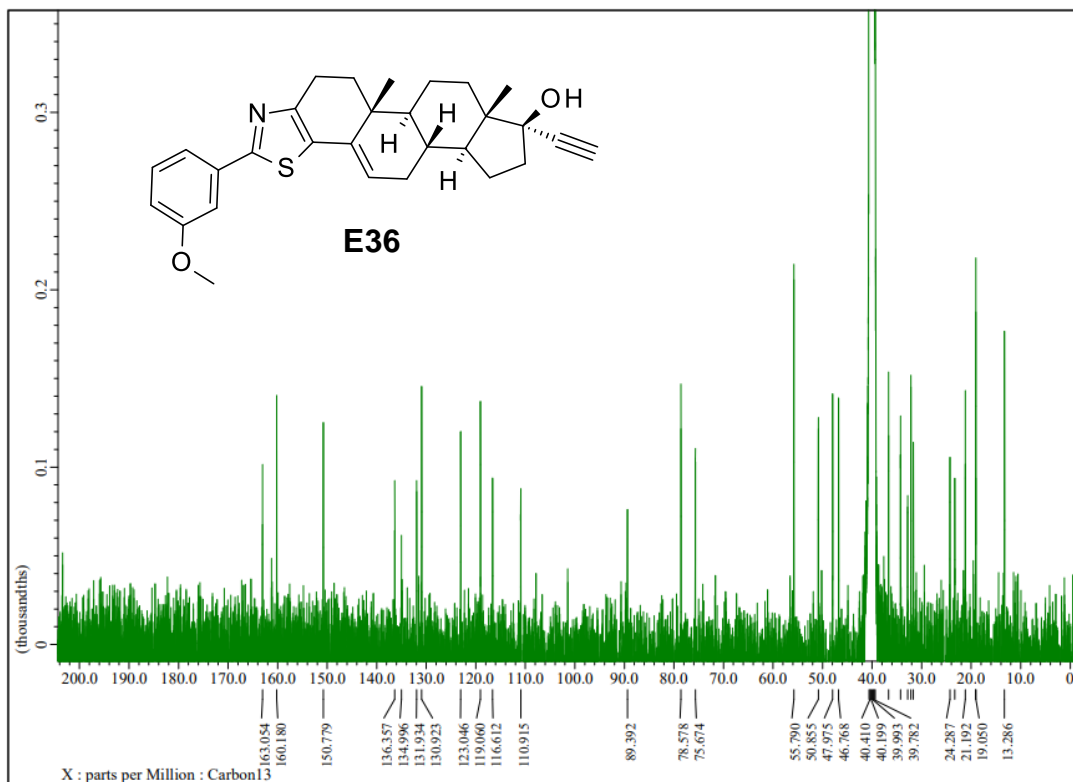


Figure S-68: ^{13}C NMR spectrum of compound **E36** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-23
Sample id#: 5201
Instrument: Shimadzu IT-TOF

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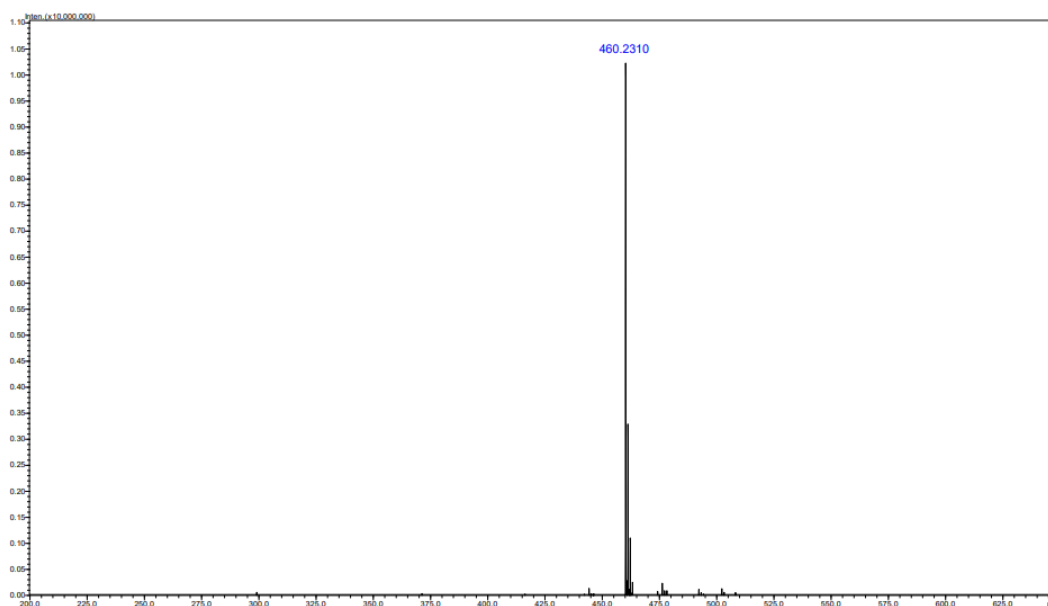


Figure S-69: High-resolution mass spectrum of compound **E36**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-7-(4-fluorophenyl)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E41)

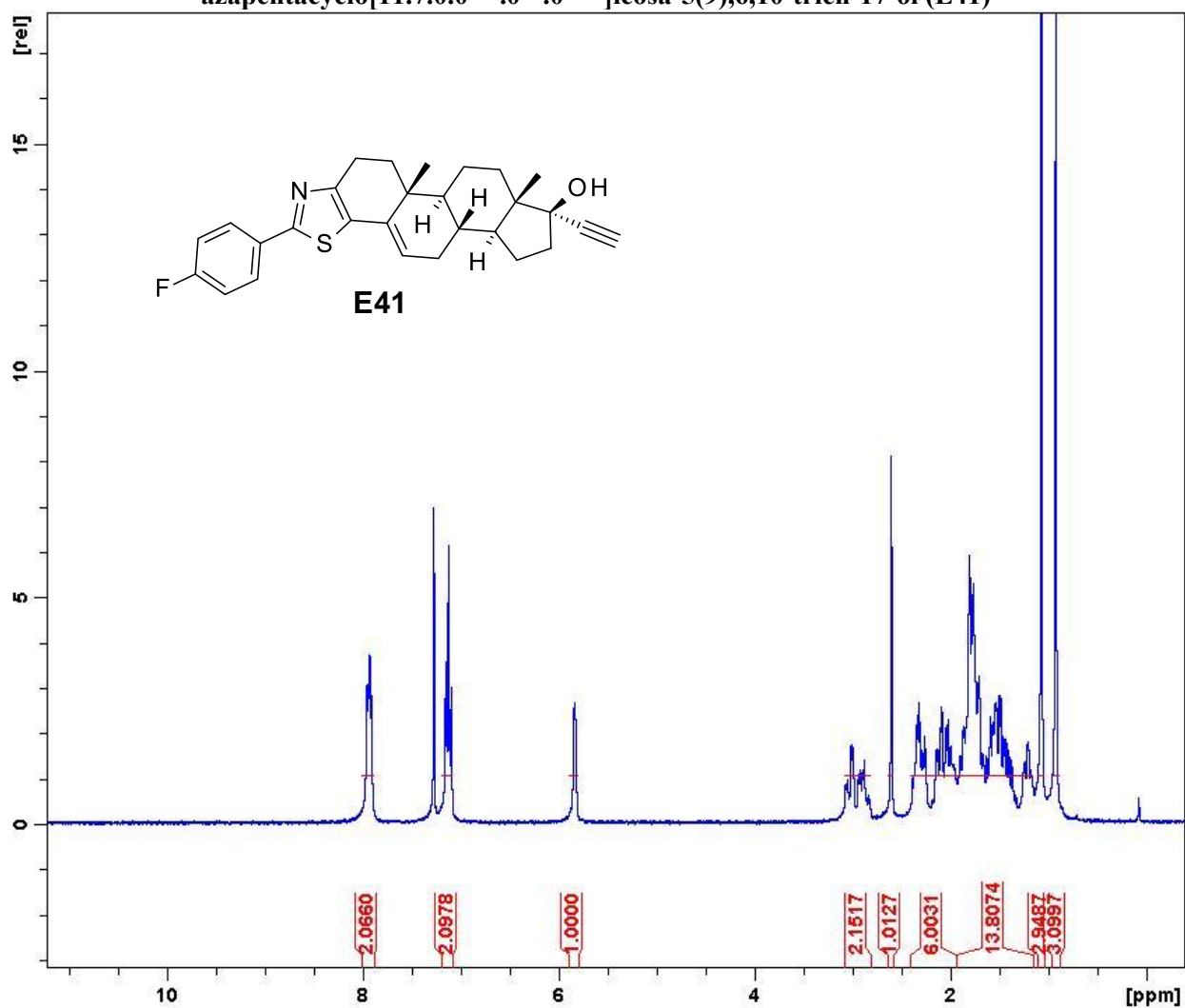


Figure S-70: ¹H NMR spectrum of compound E41 in CDCl₃

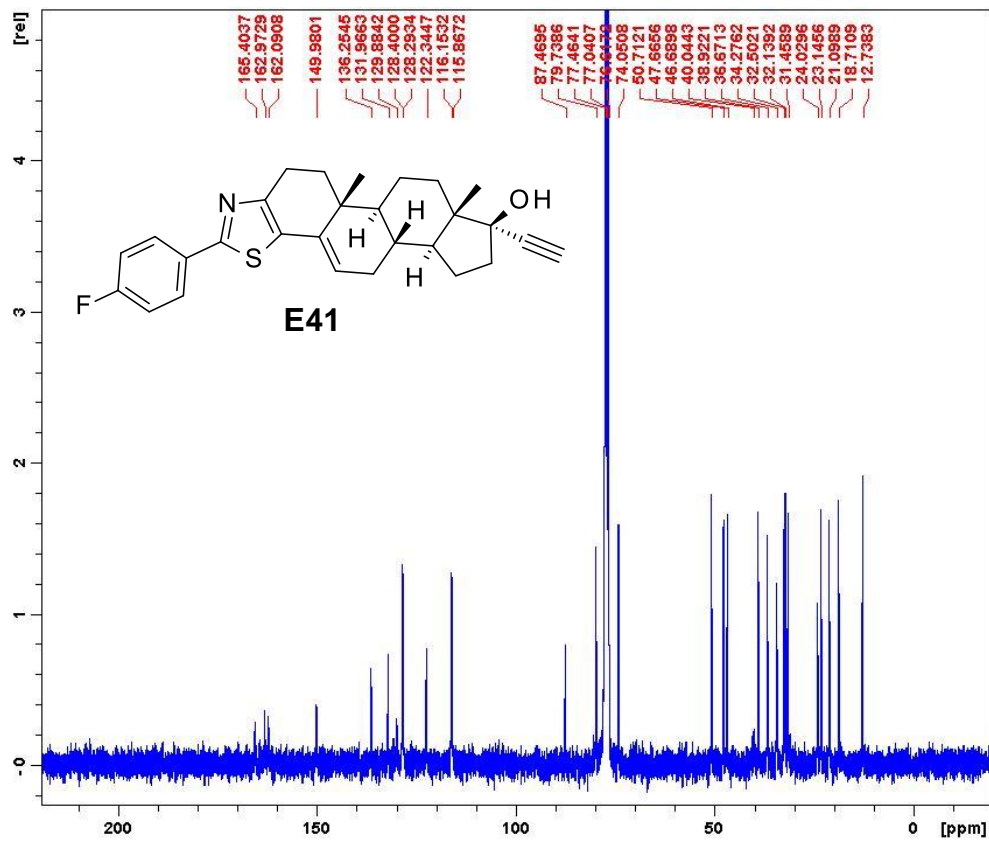


Figure S-71: ¹³C NMR spectrum of compound **E41** in CDCl₃

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-24
 Sample id#: 5202
 Instrument: Shimadzu IT-TOF

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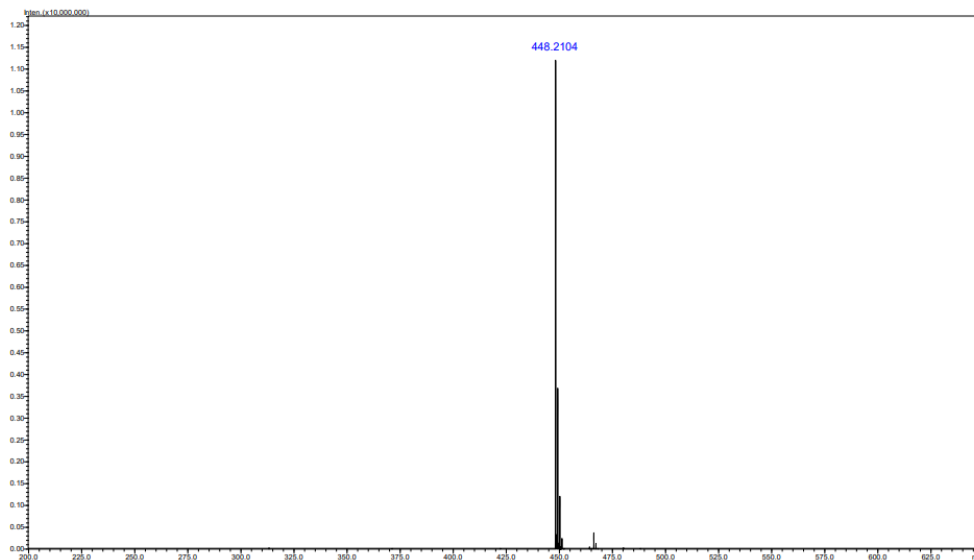


Figure S-72: High-resolution mass spectrum of compound **E41**

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-(3-Chlorophenyl)-17-ethynyl-2,18-dimethyl-8-thia-
azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E43)

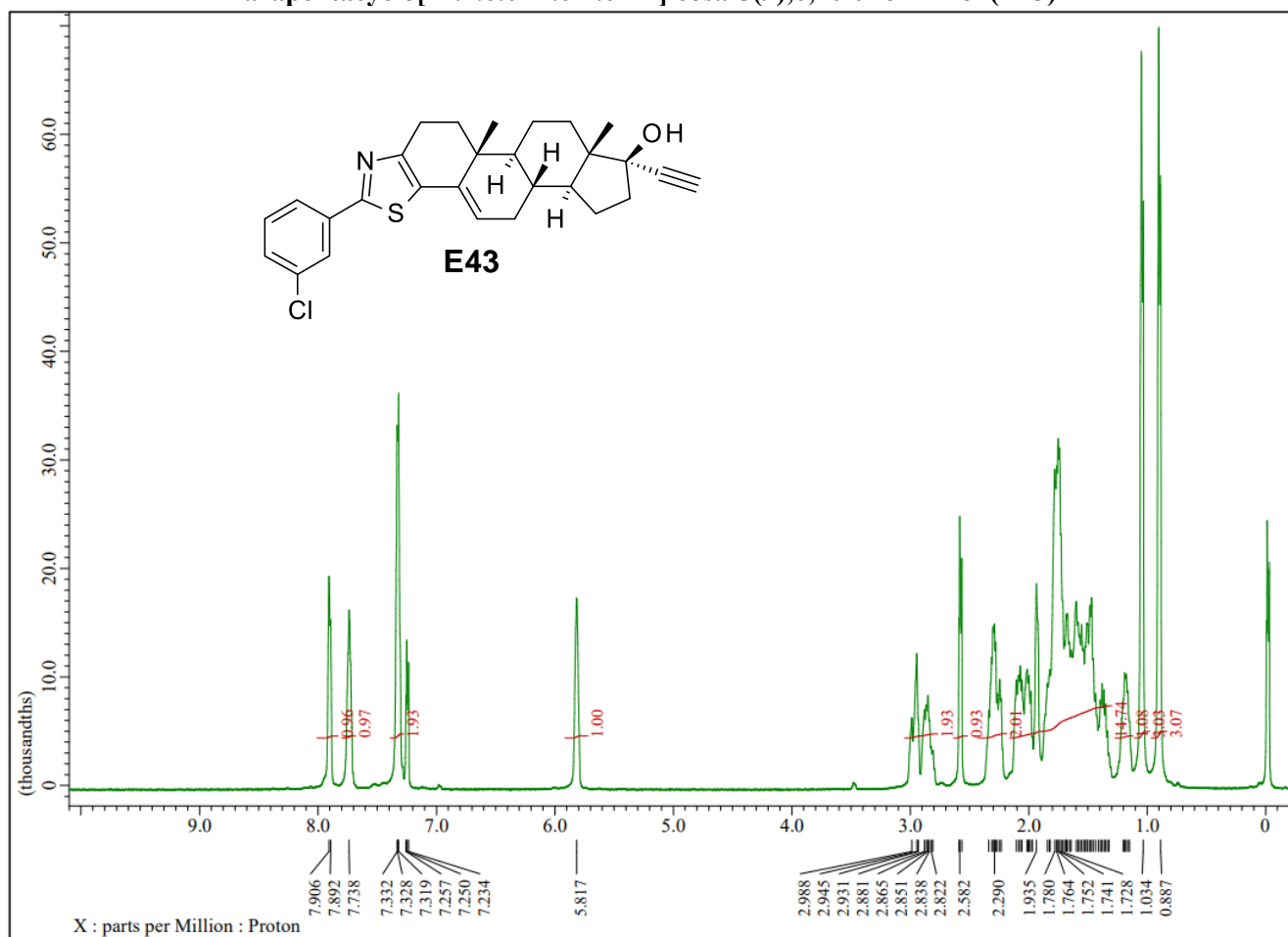


Figure S-73: ¹H NMR spectrum of compound E43 in CDCl₃

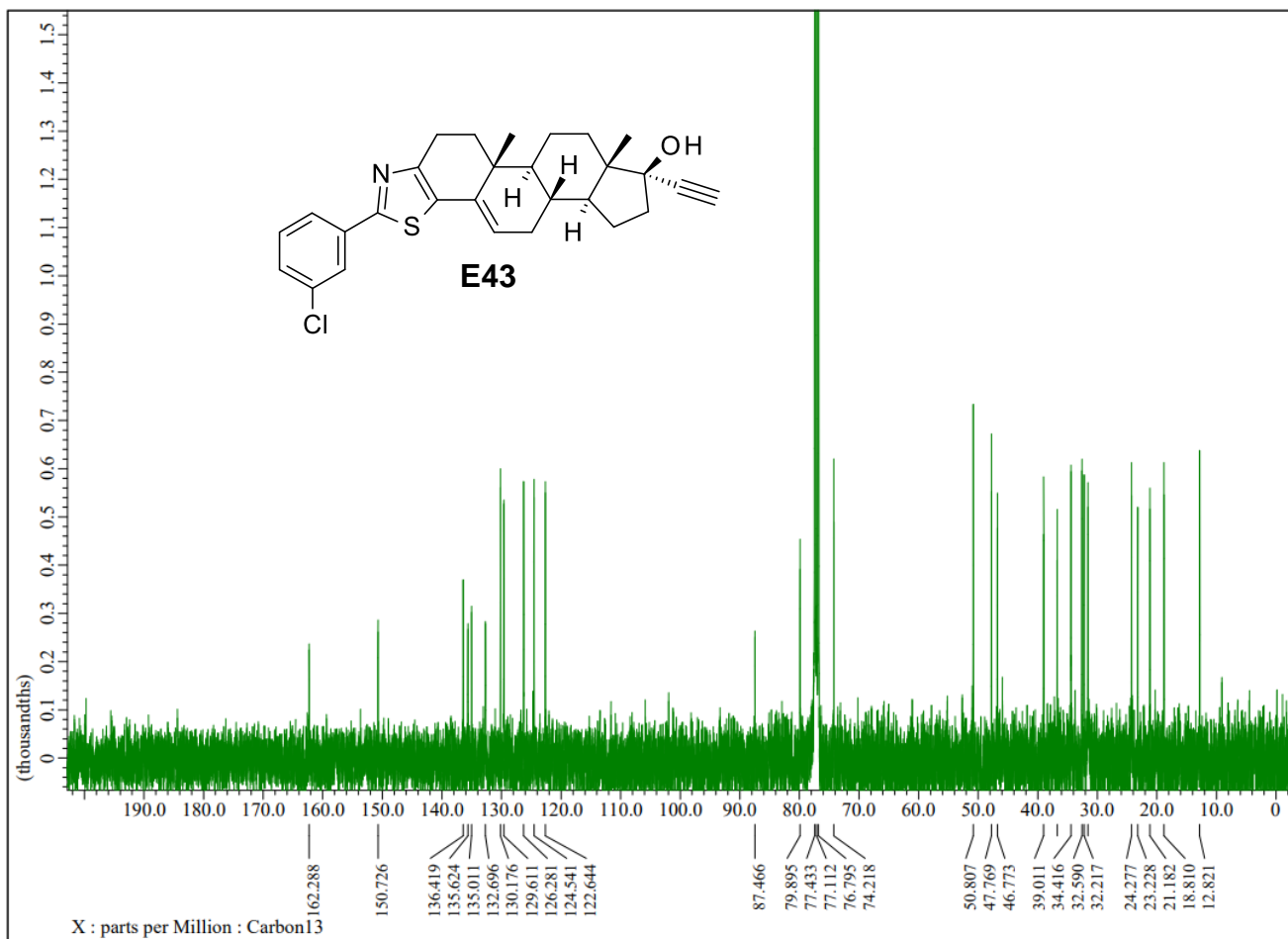


Figure S-74: ¹³C NMR spectrum of compound **E43** in CDCl₃

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-(4-Bromophenyl)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E44)

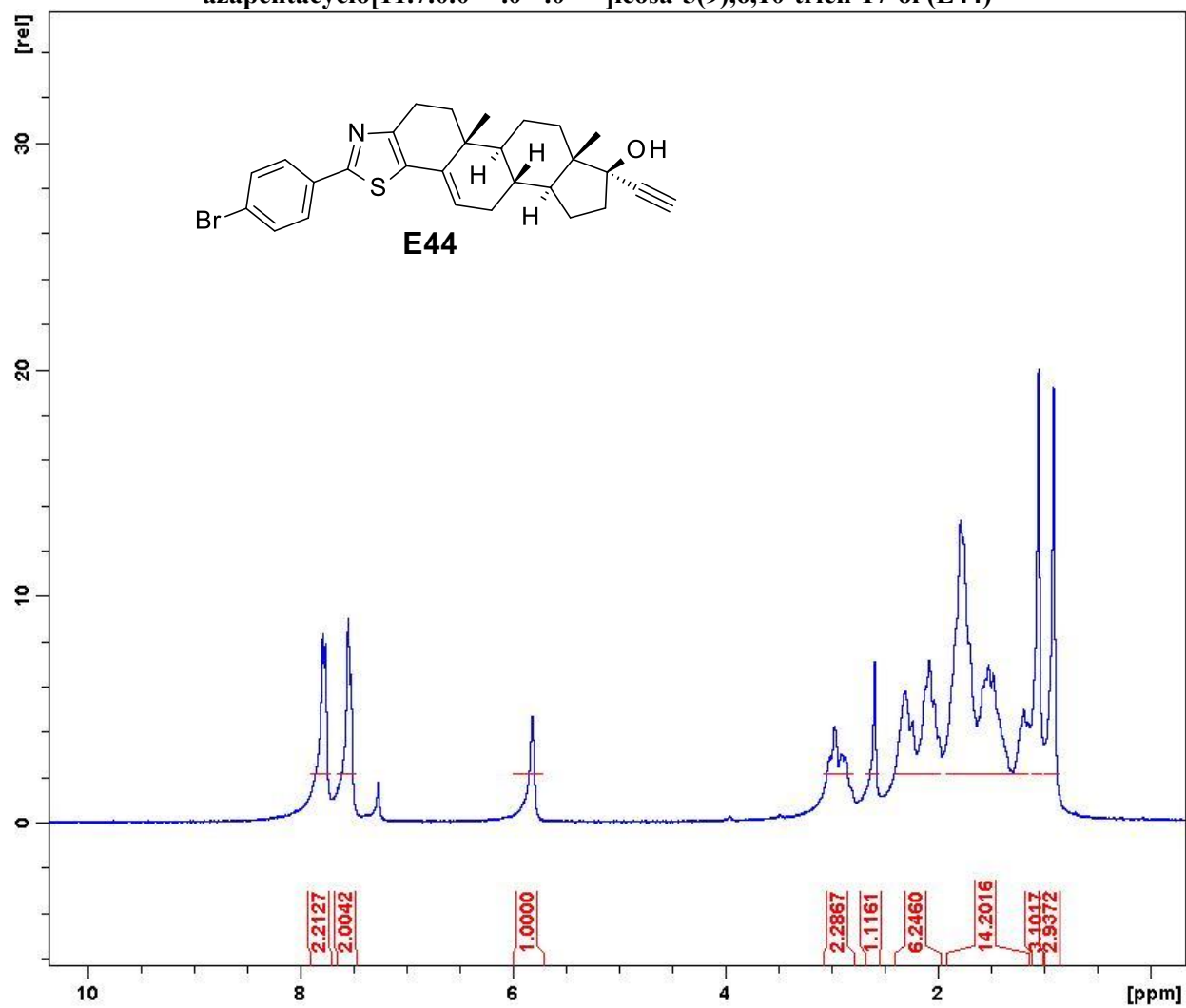


Figure S-75: ¹H NMR spectrum of compound E44 in CDCl₃

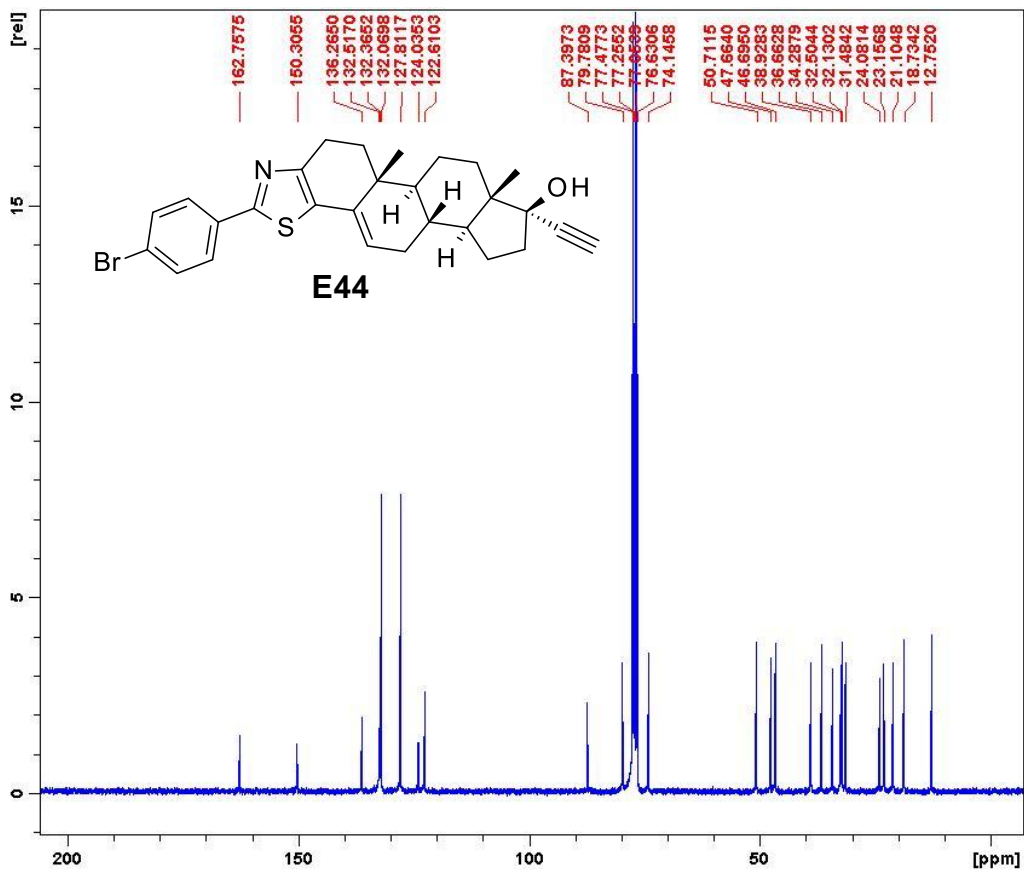
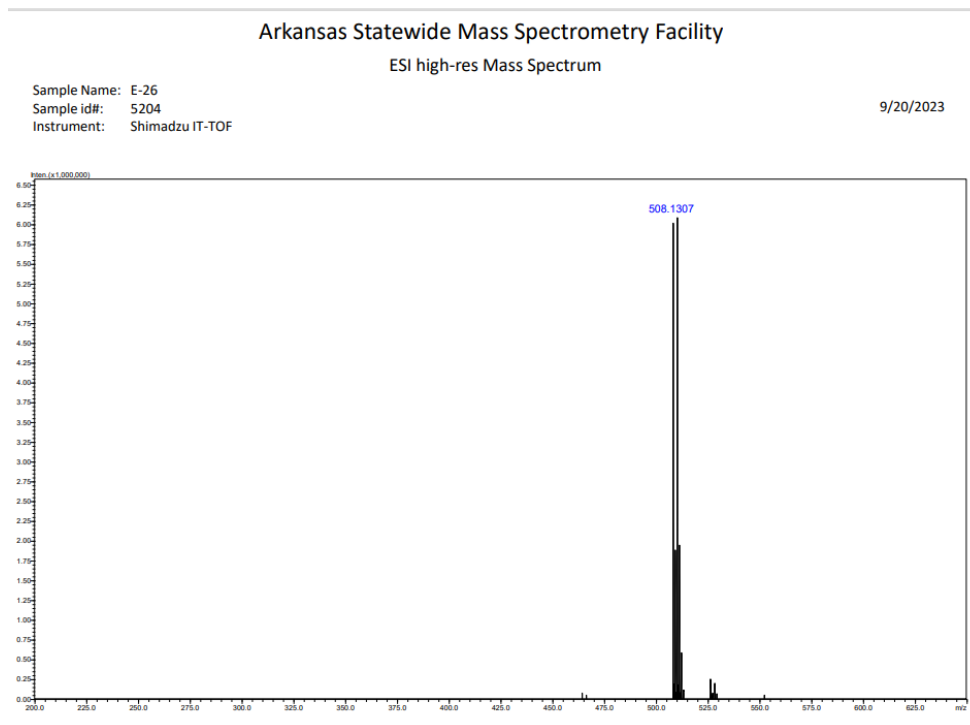


Figure S-76: ¹³C NMR spectrum of compound E44 in CDCl₃



Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-26

Sample id#: 5204

Instrument: Shimadzu IT-TOF

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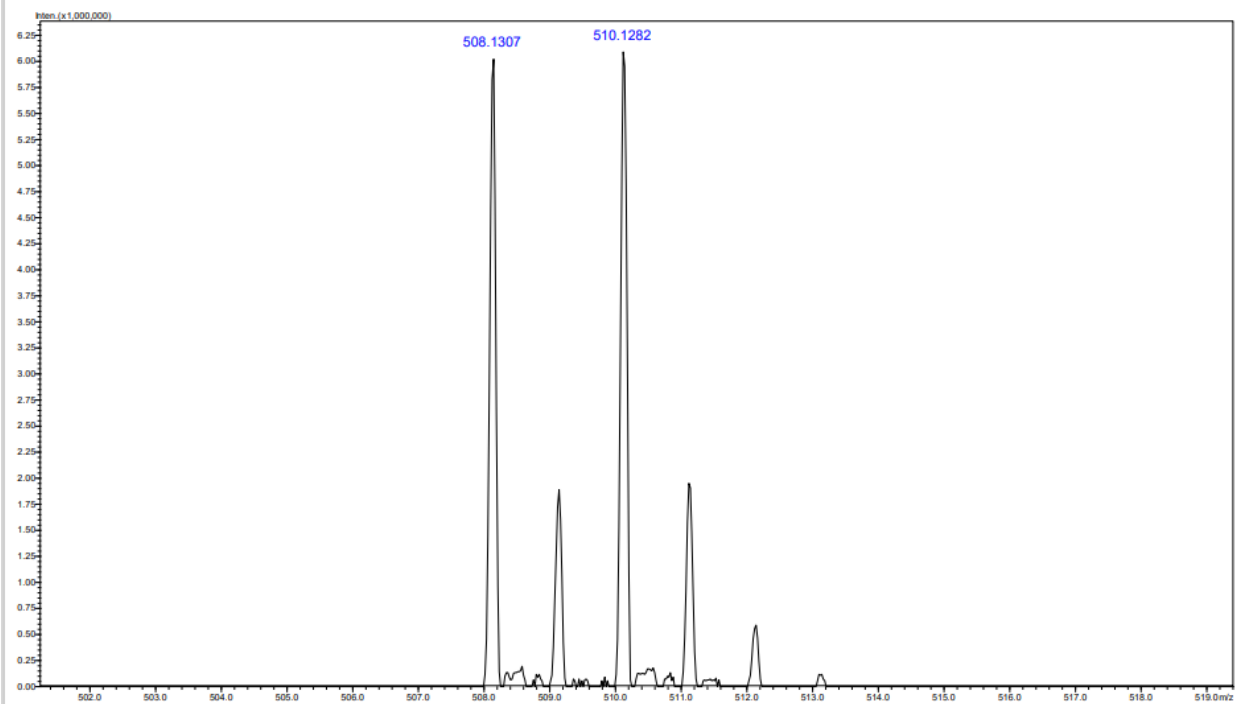


Figure S-77: High-resolution mass spectrum of compound E44

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-(1,3-Benzodioxol-5-yl)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E46)

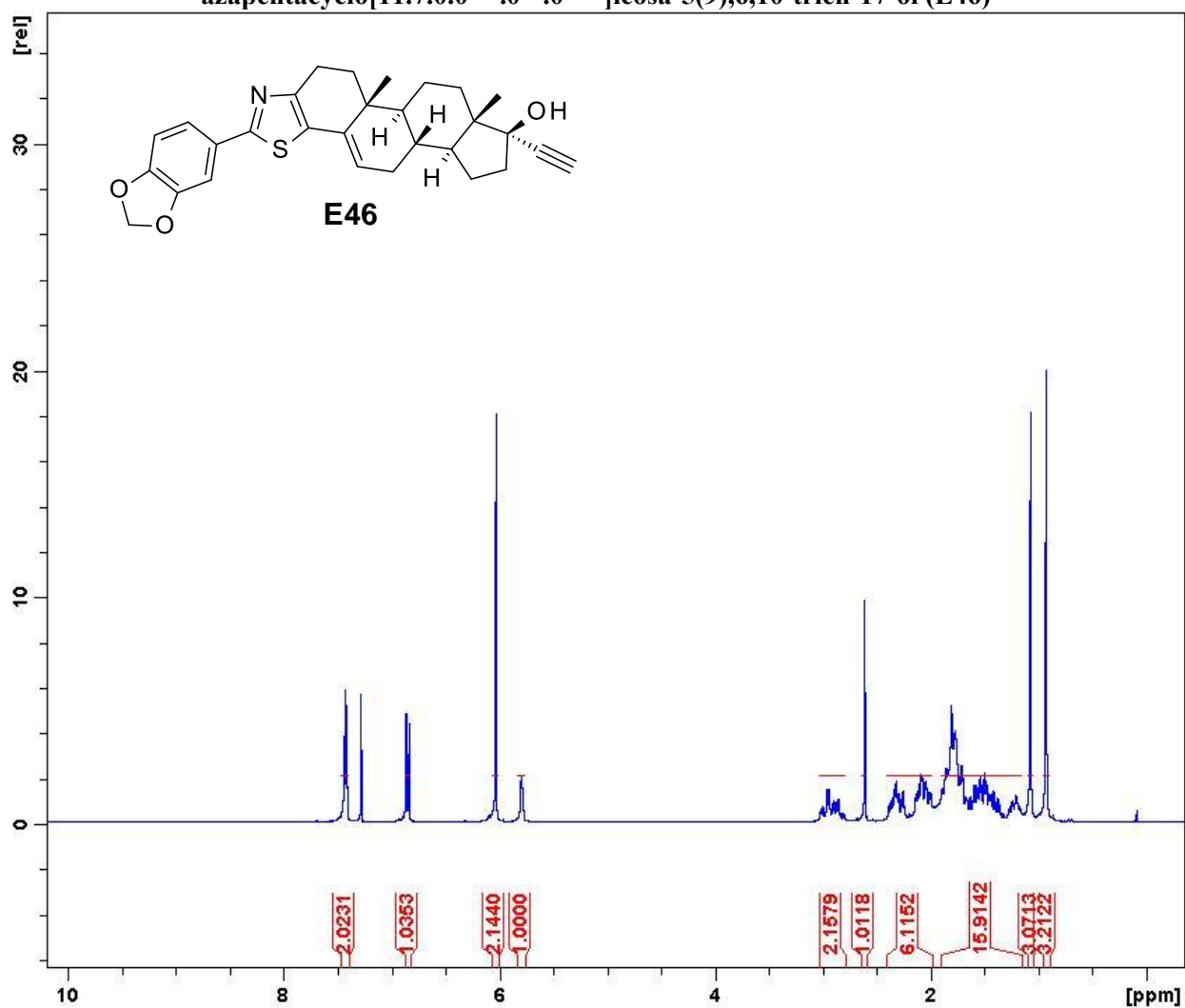


Figure S-78: ¹H NMR spectrum of compound E46 in CDCl₃

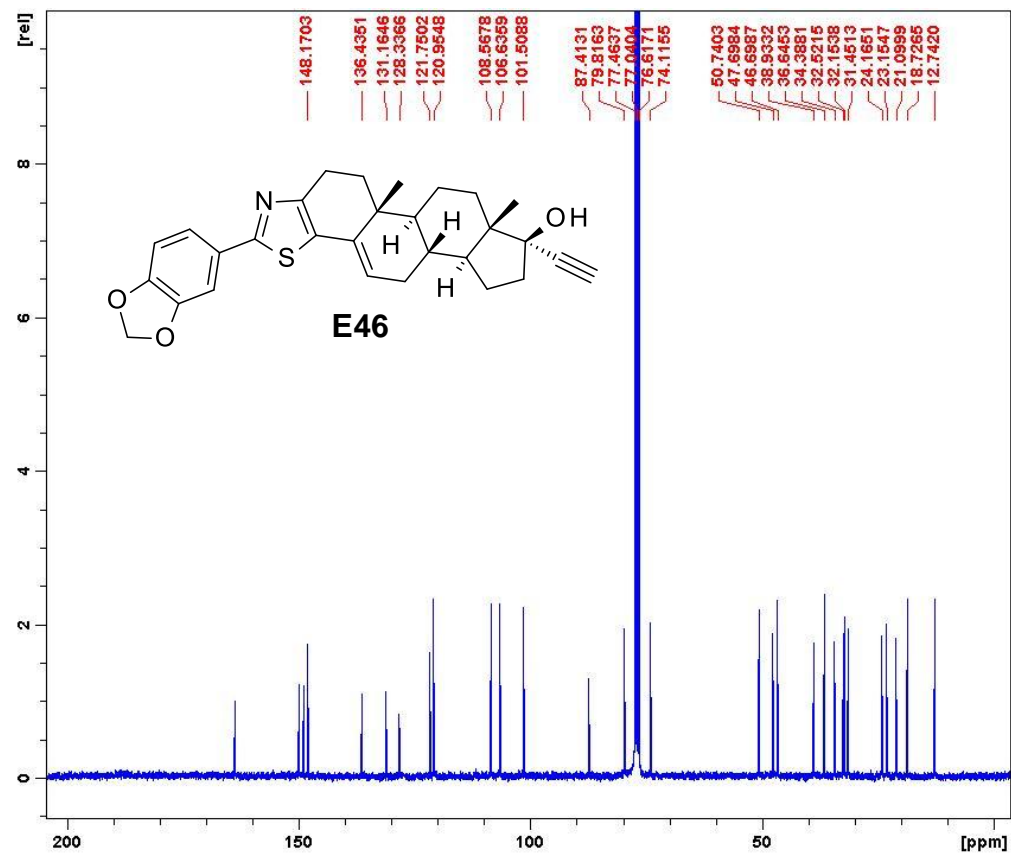


Figure S-79: ¹³C NMR spectrum of compound **E46** in CDCl₃

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-27
 Sample id#: 5205
 Instrument: Shimadzu IT-TOF

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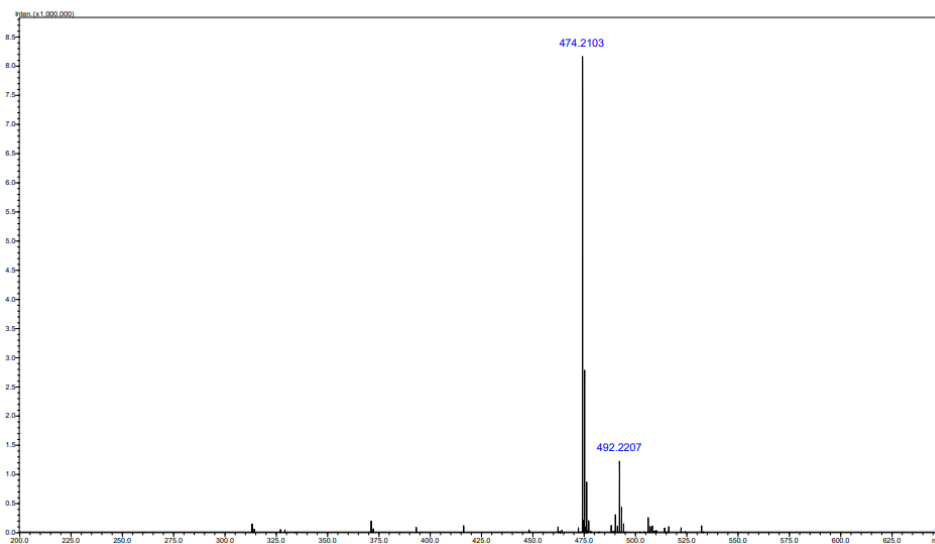


Figure S-80: High-resolution mass spectrum of compound **E46**

4-[(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-17-hydroxy-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-7-yl]benzene-1,2-diol (E47)

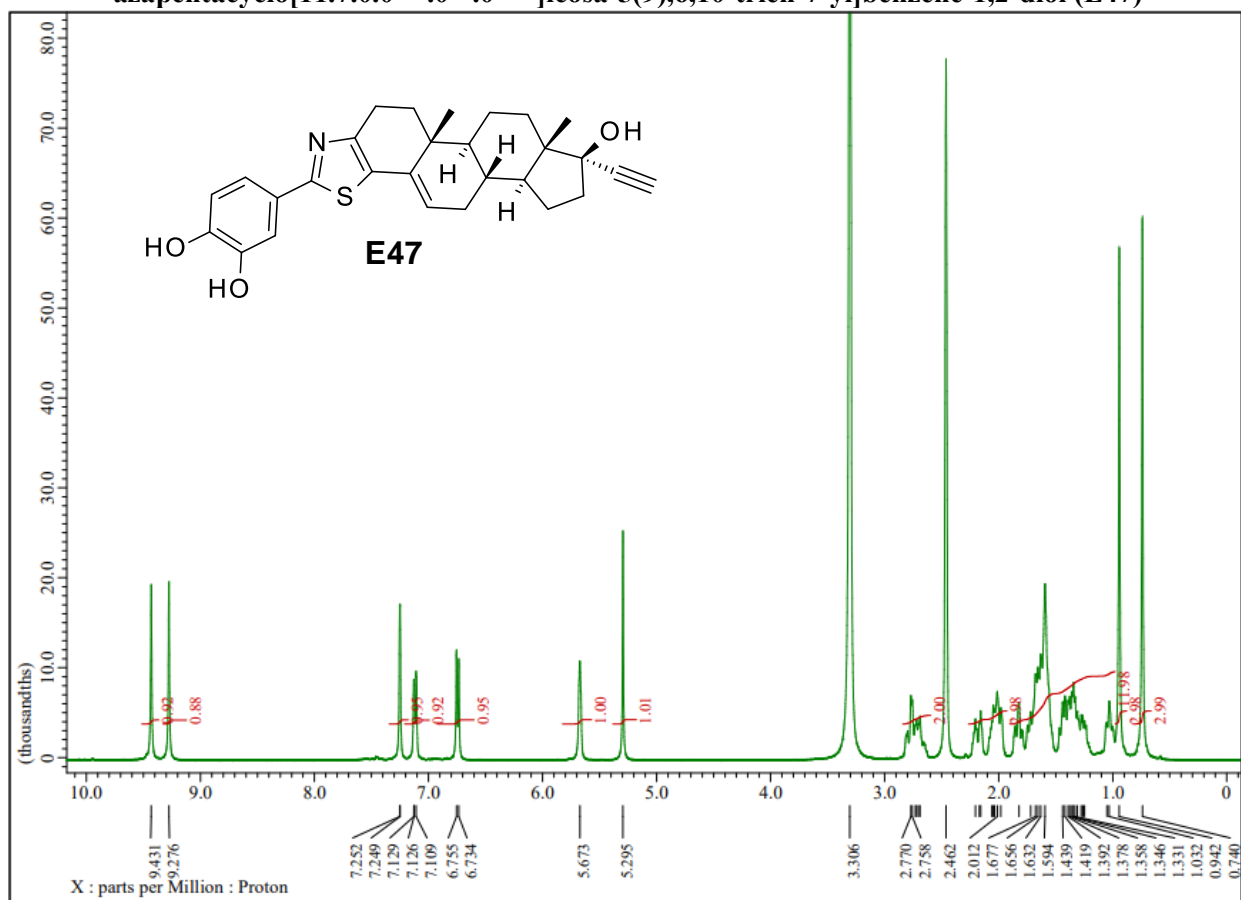


Figure S-81: ¹H NMR spectrum of compound E47 in DMSO-*d*₆

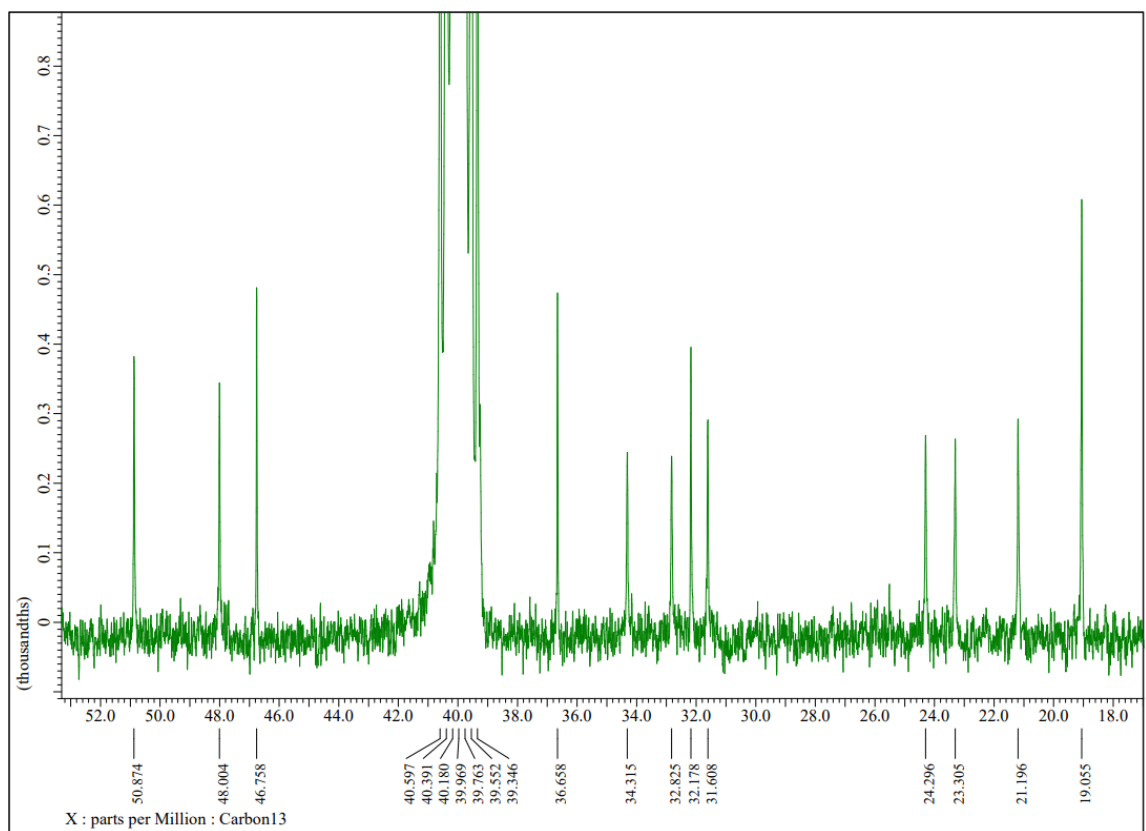
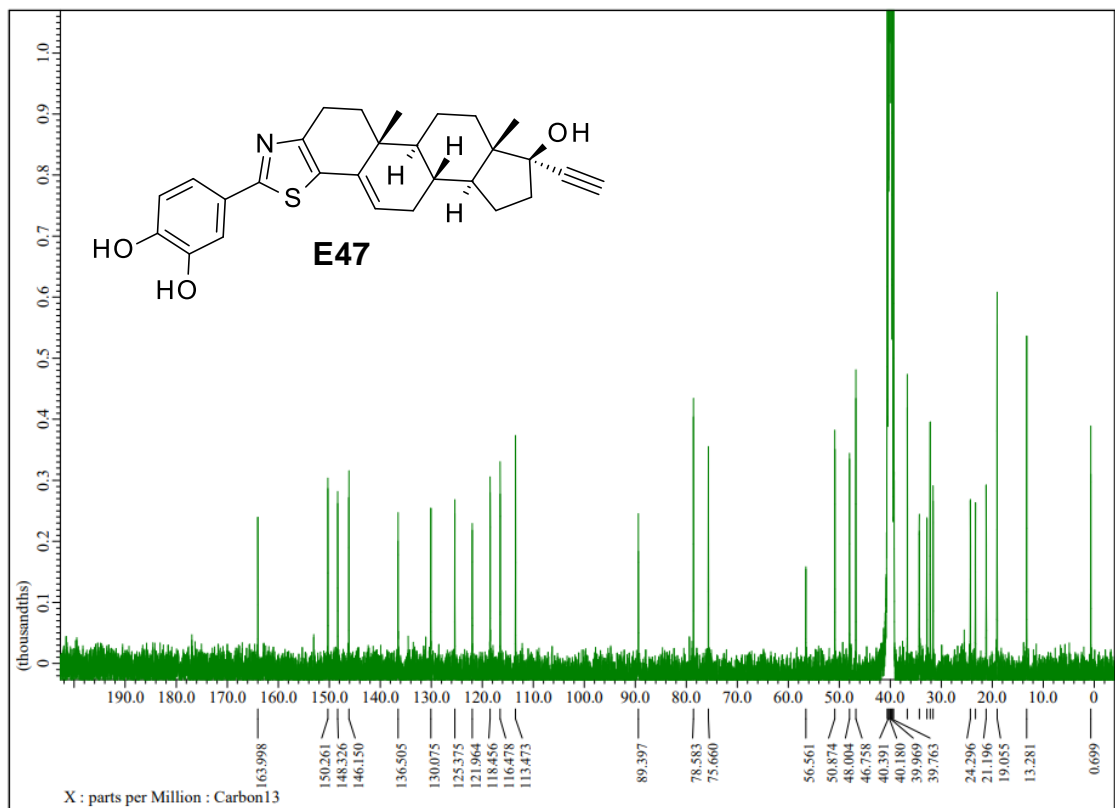


Figure S-82: ^{13}C NMR spectrum of compound **E47** in $\text{DMSO-}d_6$

Arkansas Statewide Mass Spectrometry Facility

ESI high-res Mass Spectrum

Sample Name: E-28
Sample id#: S206
Instrument: Shimadzu IT-TOF

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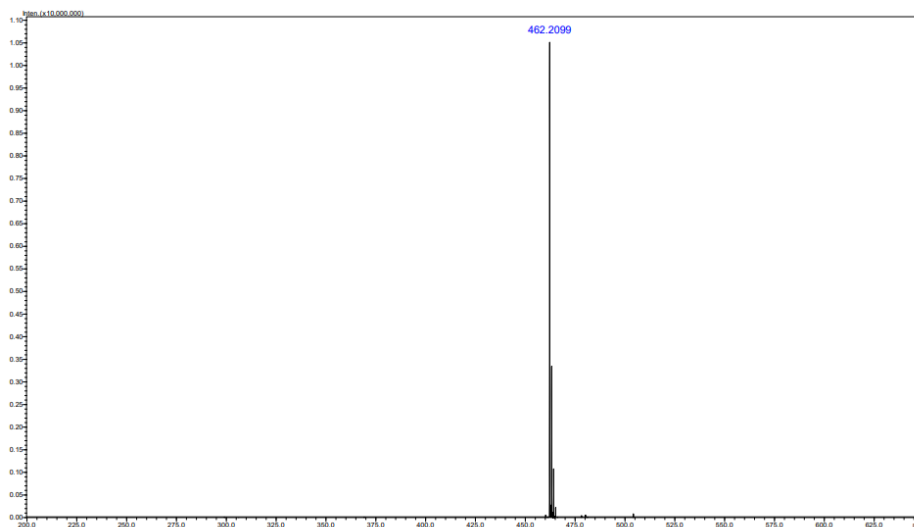


Figure S-83: High-resolution mass spectrum of compound E47

(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-Ethynyl-2,18-dimethyl-7-(4-pyridyl)-8-thia-6-azapentacyclo[11.7.0.0^{2,10}.0^{5,9}.0^{14,18}]icosa-5(9),6,10-trien-17-ol (E50)

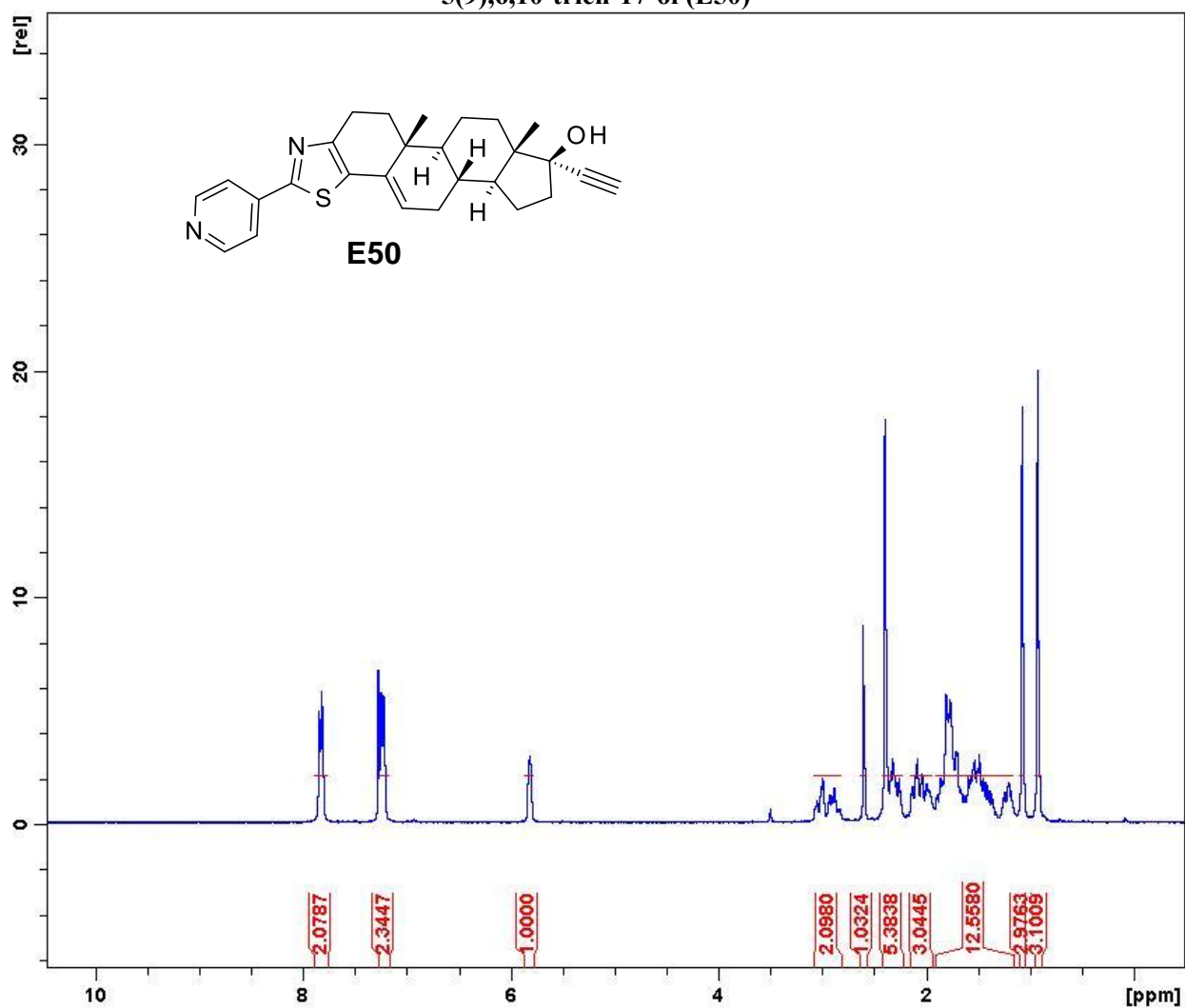


Figure S-84: ¹H NMR spectrum of compound E50 in CDCl₃

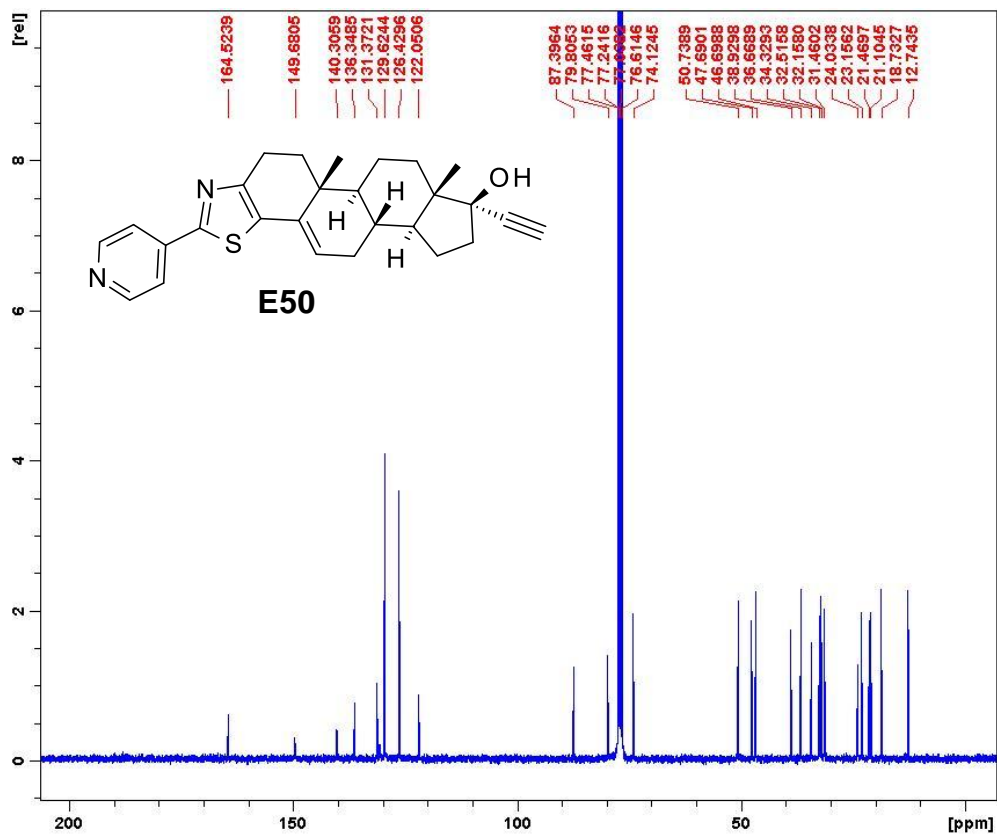


Figure S-85: ^{13}C NMR spectrum of compound **E50** in CDCl_3

Arkansas Statewide Mass Spectrometry Facility

ESI Mass Spectrum

Sample Name: E-2
 Sample id#: 5258
 Instrument: Shimadzu IT-TOF

11/8/2023

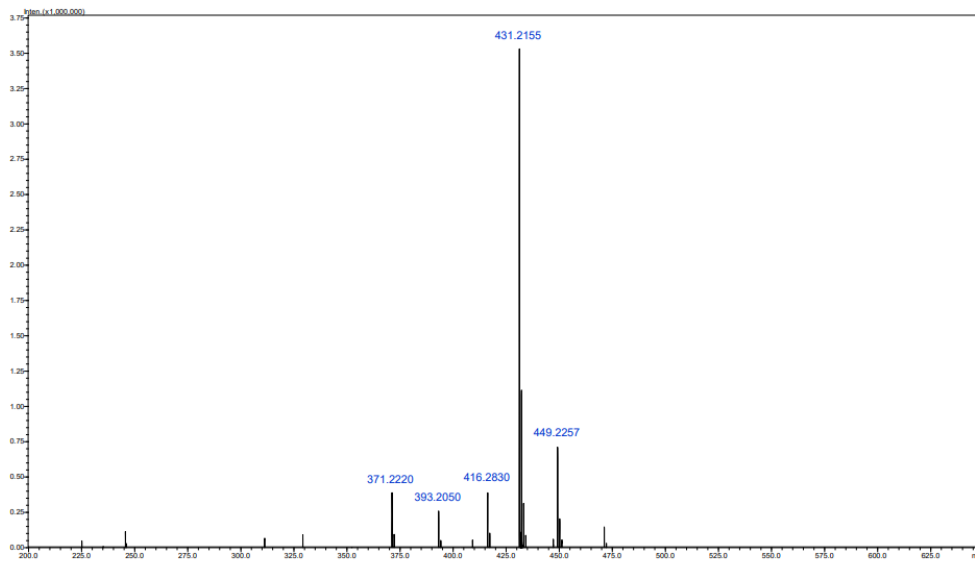


Figure S-86: High-resolution mass spectrum of compound **E50**