

Click synthesis of triazole–linked polyazamacrocycles through selective isopimaric acid transformations

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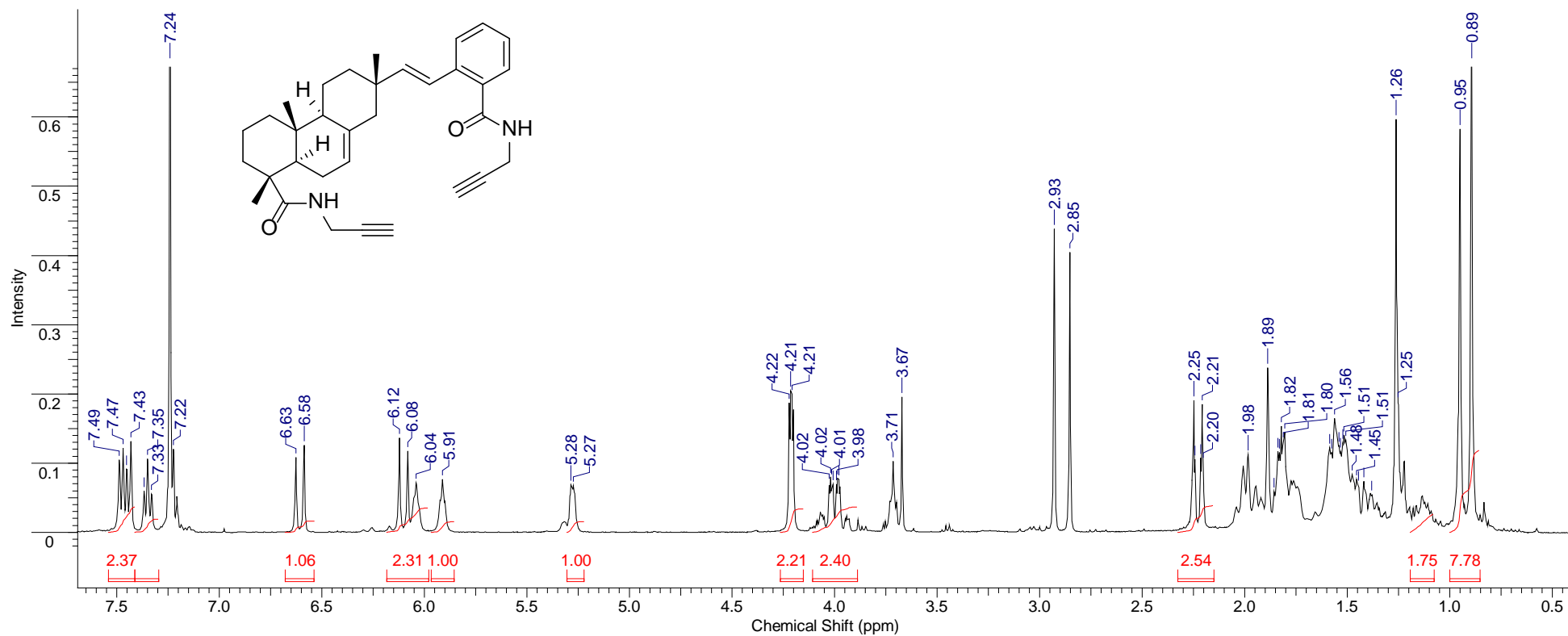
Supporting information

NMR spectra of compounds 6, 8a-d, 9

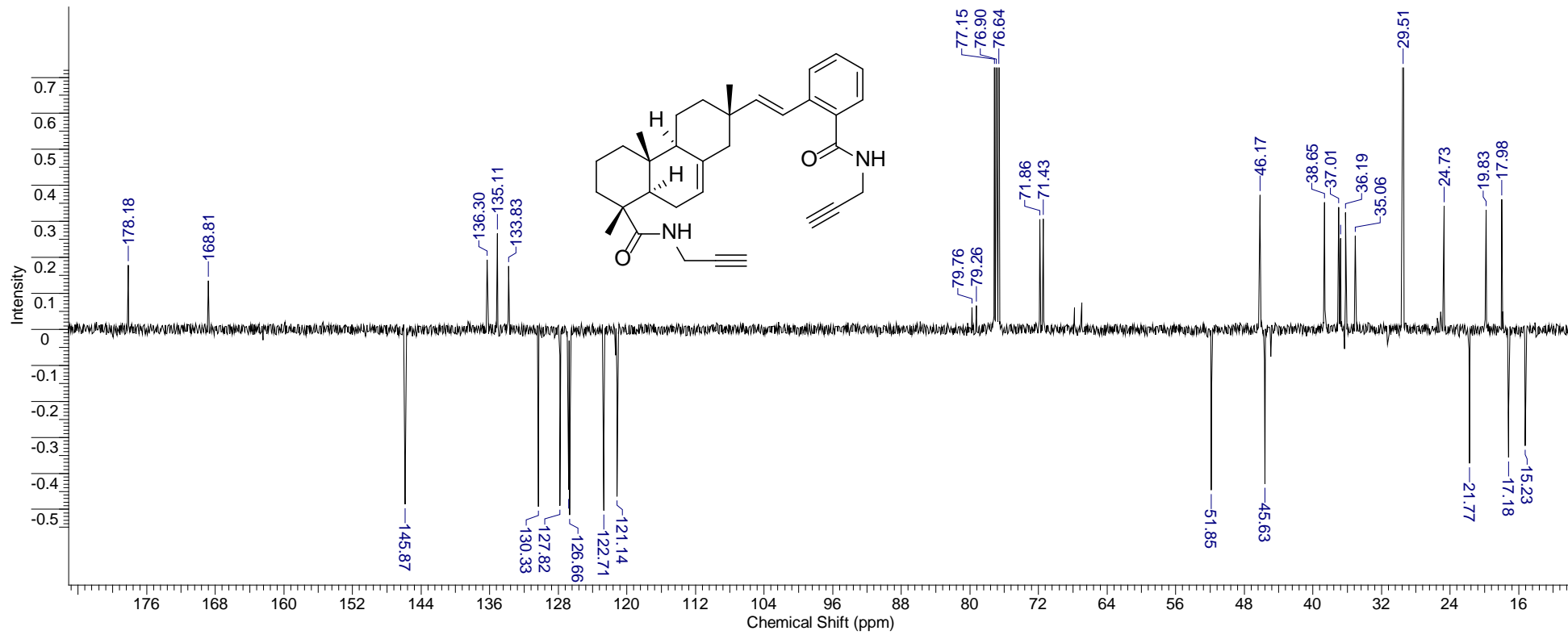
(1R,4aR,4bS,7S,10aR)-1,4a,7-Trimethyl-N-(prop-2-yn-1-yl)-7-((E)-2-(prop-2-yn-1-ylcarbamoyl)styryl)-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydrophenanthrene-1-carboxamide 6	2
(12S,14aS,14bR,18R,18aR,110Z,84Z,174Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,171H-11,14-dioxa-6,19-diaza-8(4,1),17(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacycloicosaphan-2-ene-5,20-dione 8a	4
(12S,14aS,14bR,18R,18aR,110Z,84Z,154Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,151H-6,17-diaza-8(4,1),15(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacyclooctadecaphan-2-ene-5,18-dione 8b	6
12S,14aS,14bR,18R,18aR,110Z,84Z,144Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,141H-11-oxa-6,16-diaza-8(4,1),14(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacycloheptadecaphan-2-ene-5,17-dione 8c	10
(12S,14aS,14bR,18R,18aR,110Z,84Z,144Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,141H-6,16-diaza-8(4,1),14(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacycloheptadecaphan-2-ene-5,17-dione 8d	12
Dimeric compound 9	14

(1R,4aR,4bS,7S,10aR)-1,4a,7-Trimethyl-N-(prop-2-yn-1-yl)-7-((E)-2-(prop-2-yn-1-ylcarbamoyl)styryl)-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydrophenanthrene-1-carboxamide 6

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ ppm

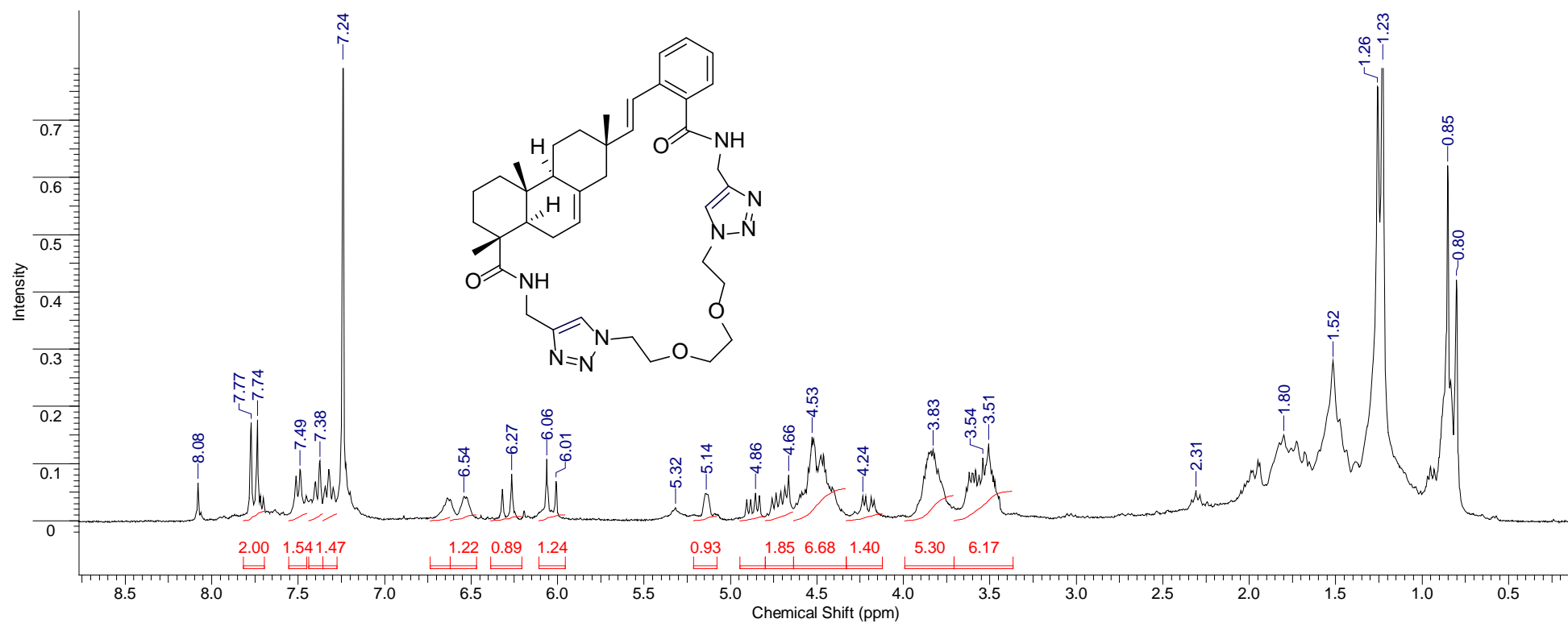


¹³C NMR (125-MHz, CDCl₃) δ (ppm)

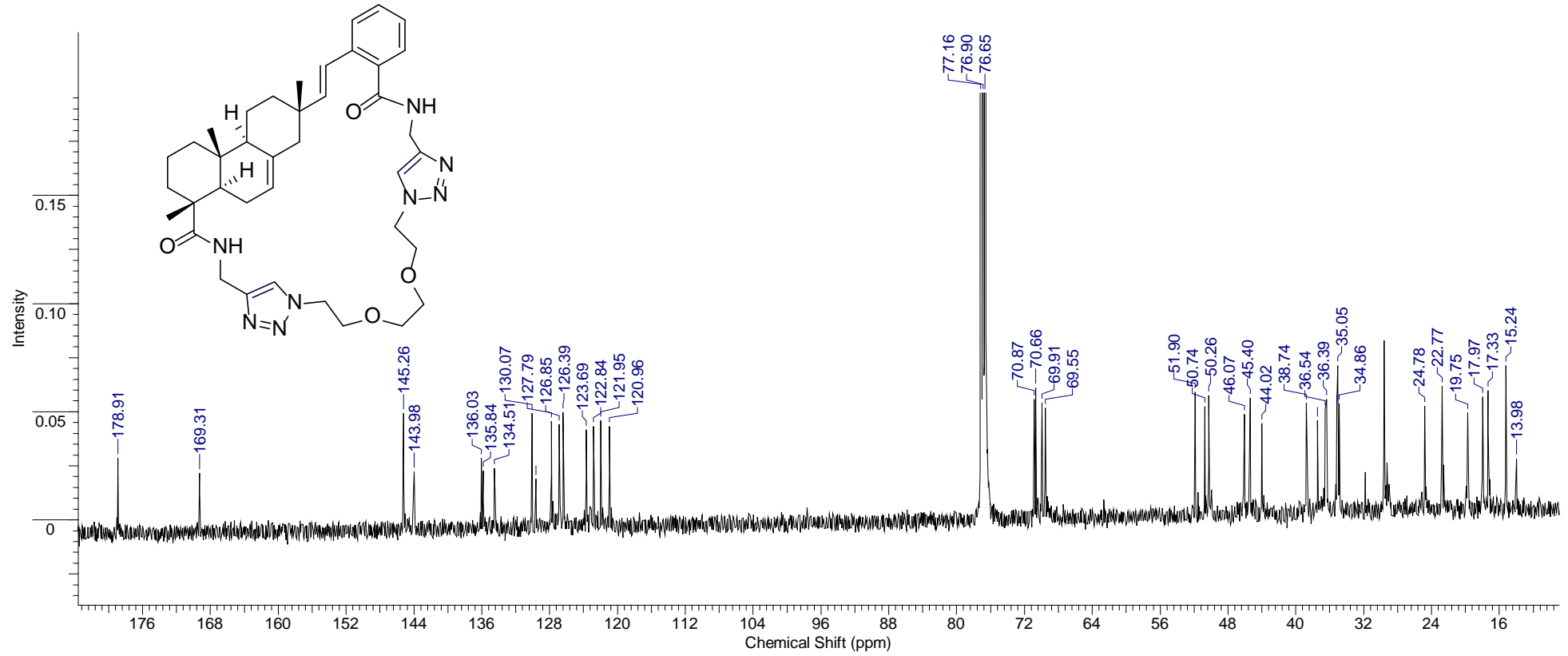


(12S,14aS,14bR,18R,18aR,110Z,84Z,174Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,171H-11,14-dioxa-6,19-diaza-8(4,1),17(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacycloicosaphan-2-ene-5,20-dione 8a

$^1\text{H NMR}$ (CDCl_3 , 300 MHz) δ ppm

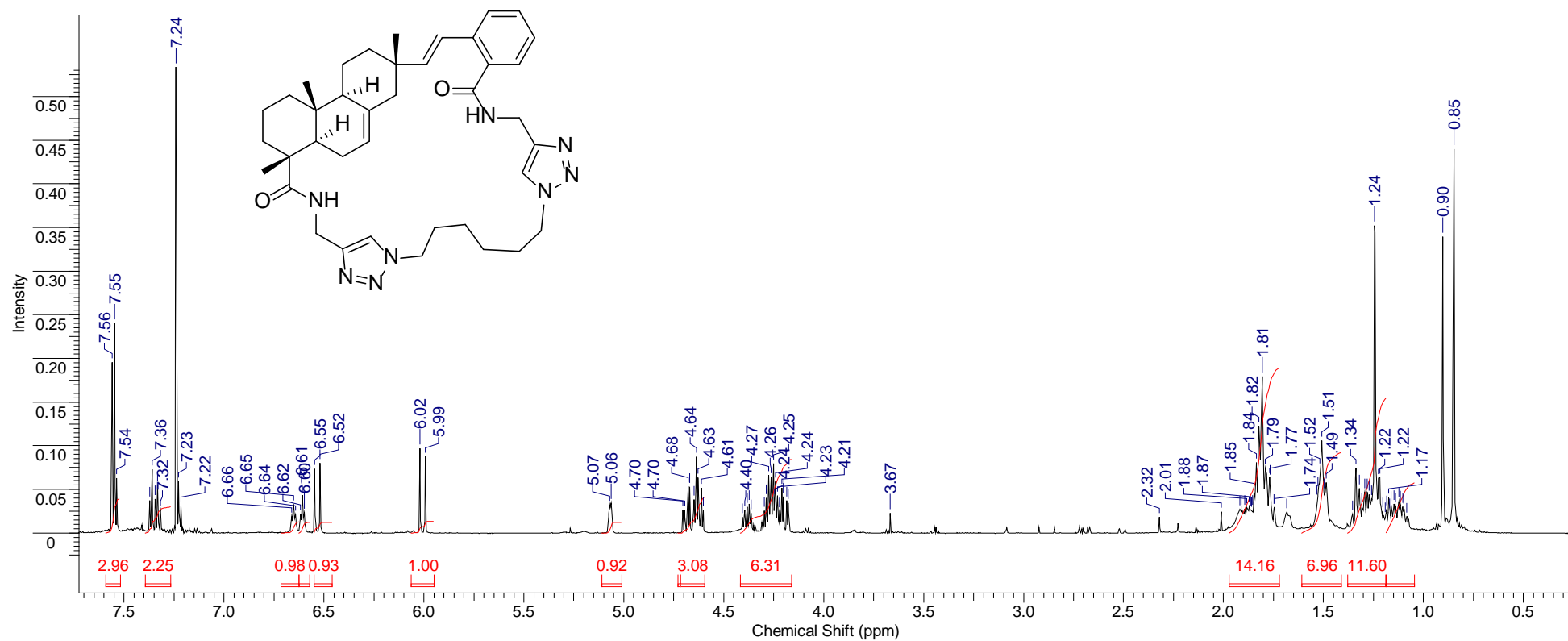


¹³C NMR (125-MHz, CDCl₃) δ (ppm)

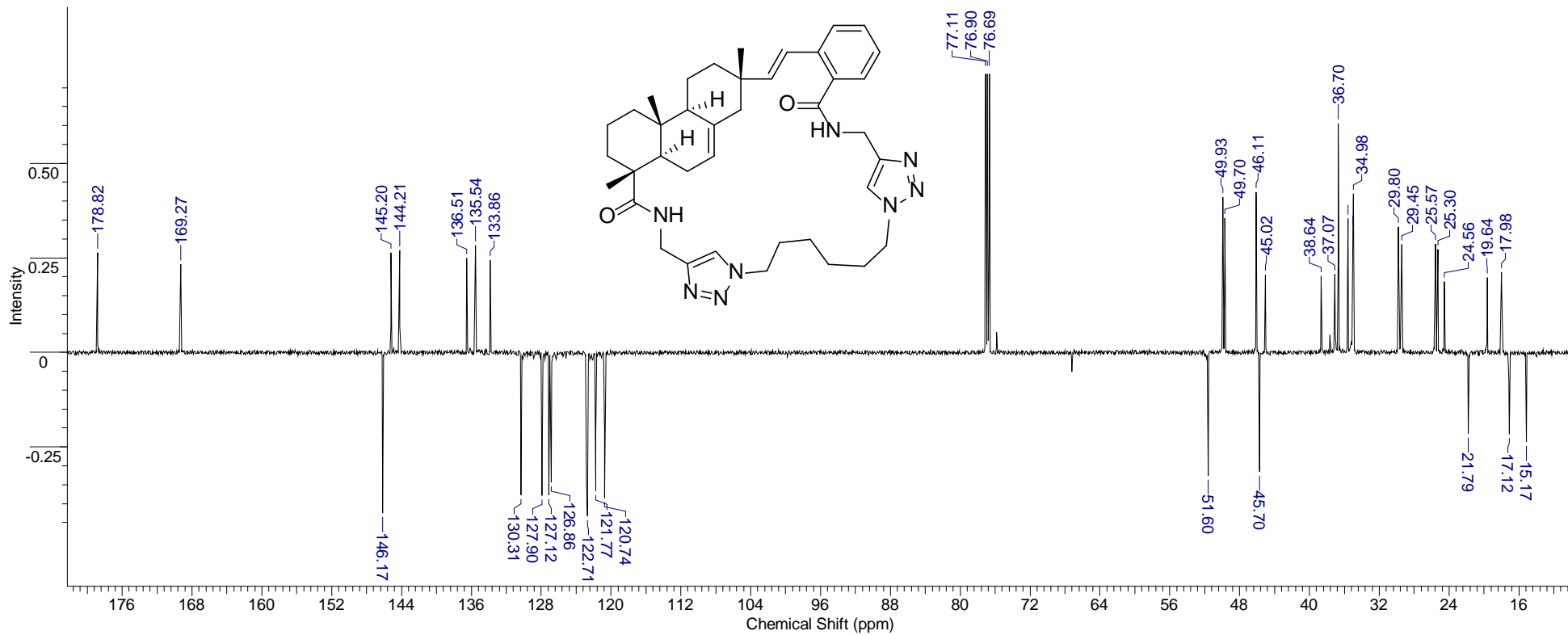


(12S,14aS,14bR,18R,18aR,110Z,84Z,154Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,151H-6,17-diaza-8(4,1),15(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacyclooctadecaphan-2-ene-5,18-dione 8b

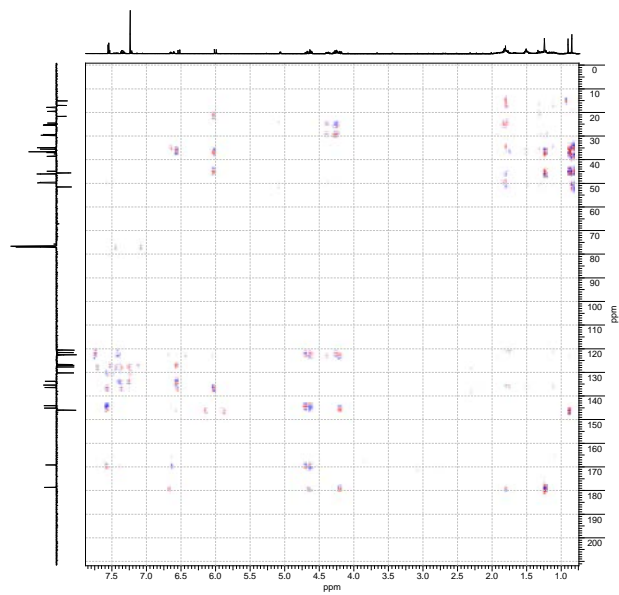
$^1\text{H NMR}$ (CDCl_3 , 600 MHz) δ ppm



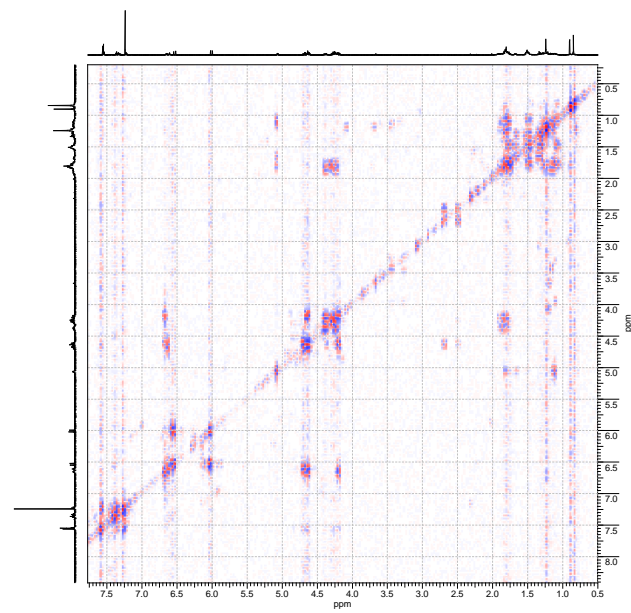
¹³C NMR (150.95 MHz, CDCl₃) (ppm)

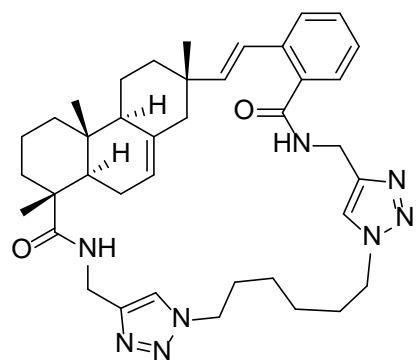


COLOC

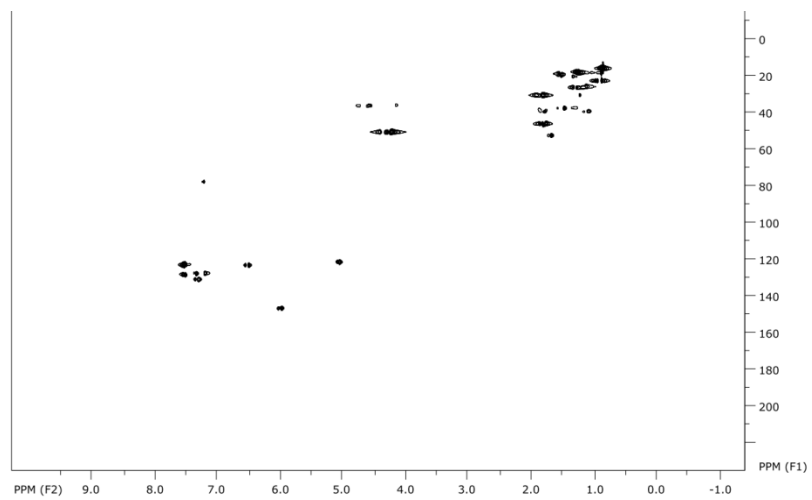


^1H - ^1H ! OSY



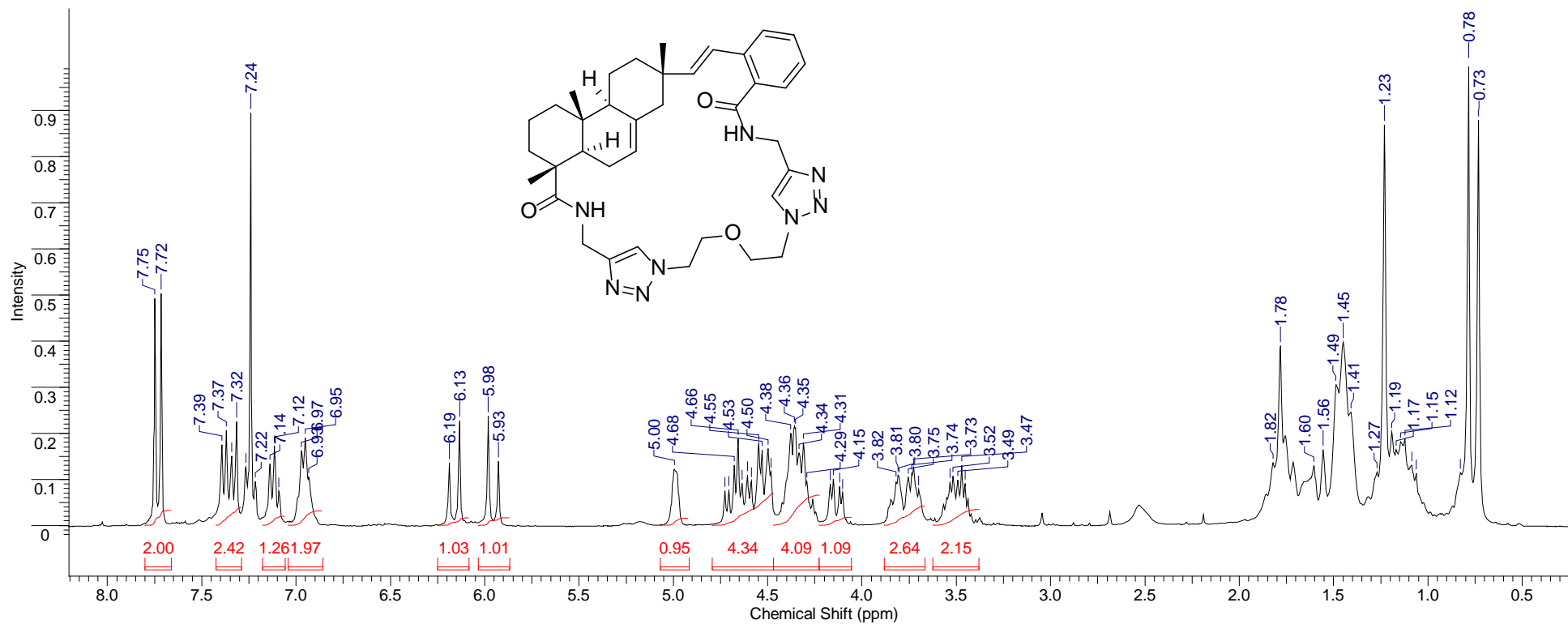


^{13}C - ^1H COXH

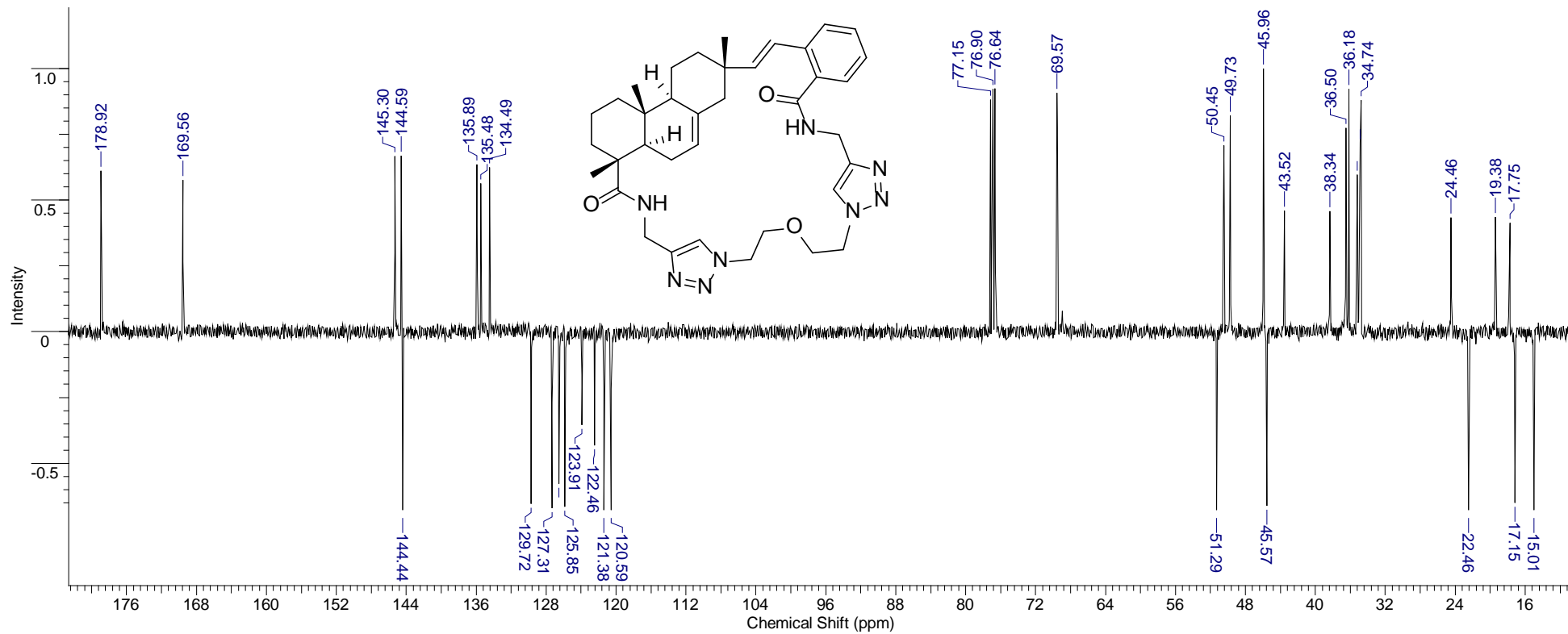


12S,14aS,14bR,18R,18aR,110Z,84Z,144Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,141H-11-oxa-6,16-diaza-8(4,1),14(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacycloheptadecaphan-2-ene-5,17-dione 8c

$^1\text{H NMR}$ (CDCl_3 , 300 MHz) δ ppm

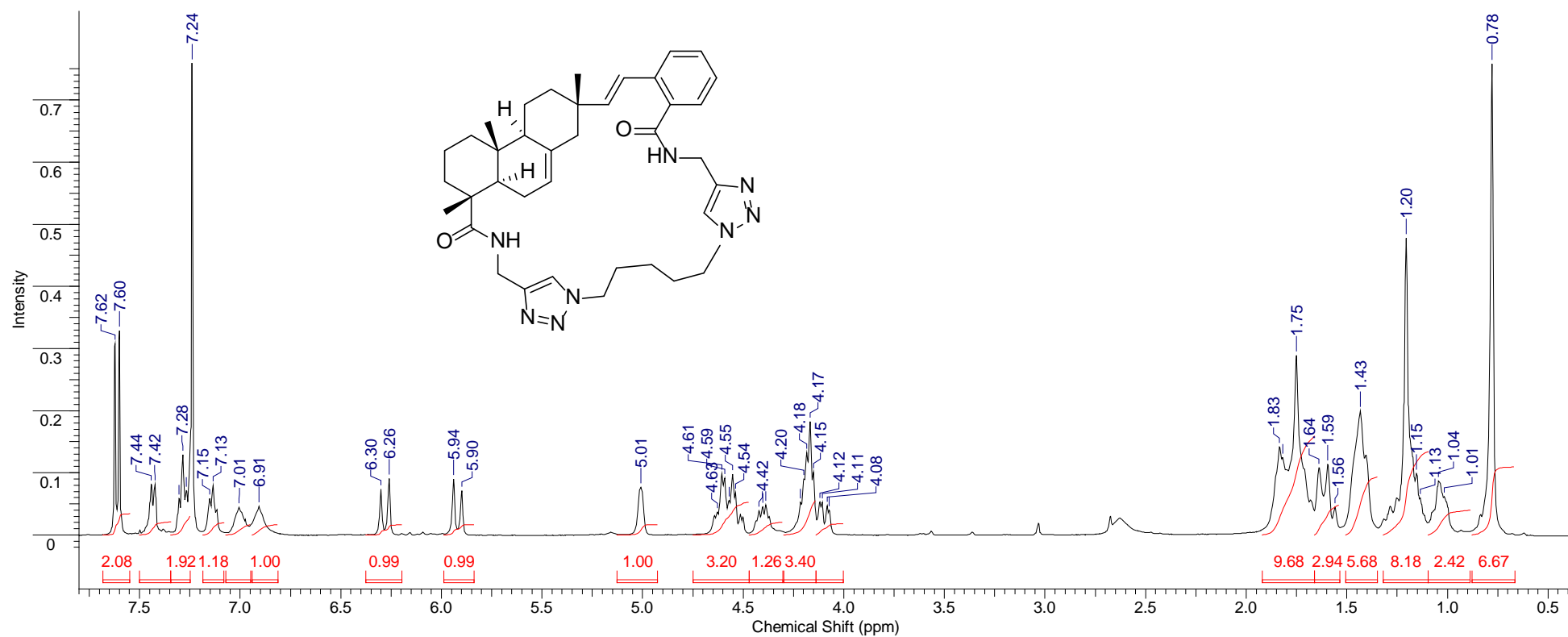


¹³C NMR (125.76 MHz, CDCl₃) δ (ppm)

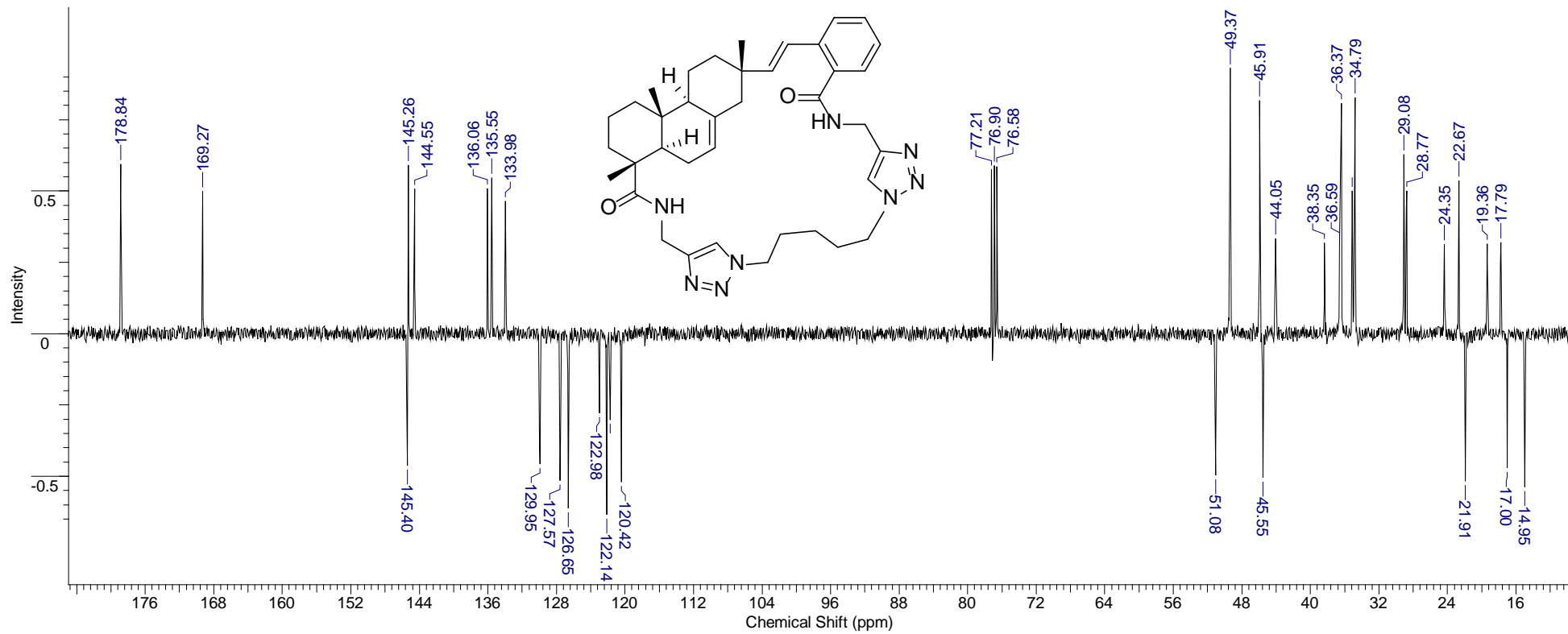


(12S,14aS,14bR,18R,18aR,110Z,84Z,144Z,2E)-12,14b,18-Trimethyl-11,12,13,14,14a,14b,15,16,17,18,18a,19-dodecahydro-81H,141H-6,16-diaza-8(4,1),14(1,4)-ditriazola-1(2,8)-phenanthrena-4(1,2)-benzenacycloheptadecaphan-2-ene-5,17-dione
8d

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ ppm

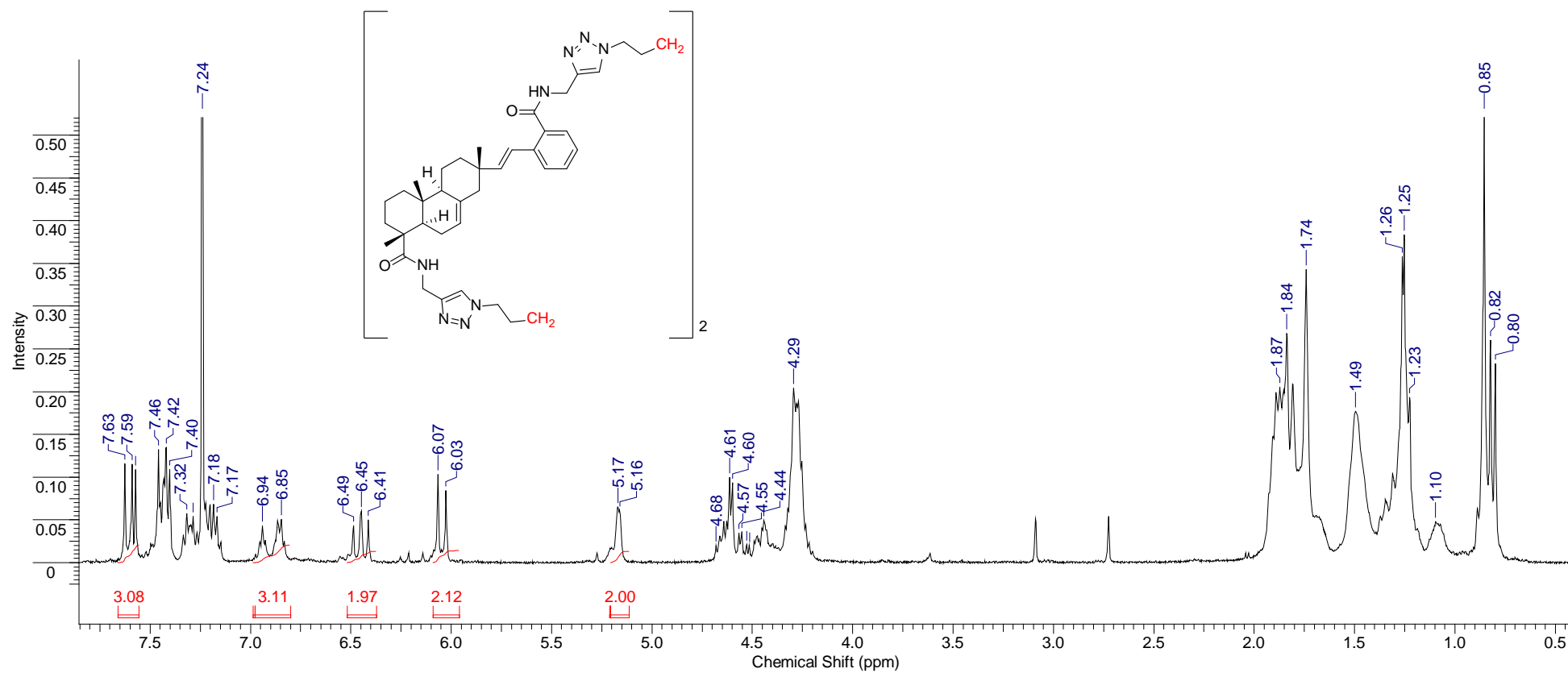


¹³C NMR (100.61 MHz, CDCl₃) (ppm)



Dimeric compound 9

^1H NMR (CDCl_3 , 400 MHz) δ ppm



¹³C NMR (150.95 MHz, CDCl₃) (ppm)

