

Polyphenylglyoxamide-based Amphiphilic Small Molecular Peptidomimetics as Antibacterial Agents with Anti-biofilm Activity

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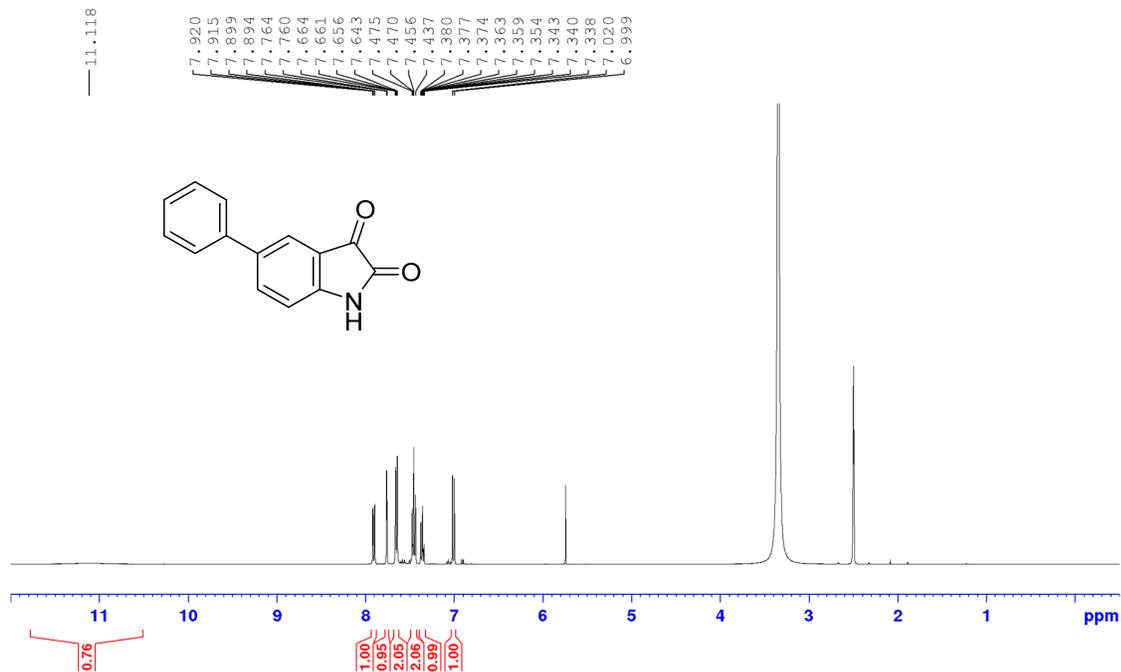
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^1H NMR and ^{13}C NMR spectra of synthesised compounds

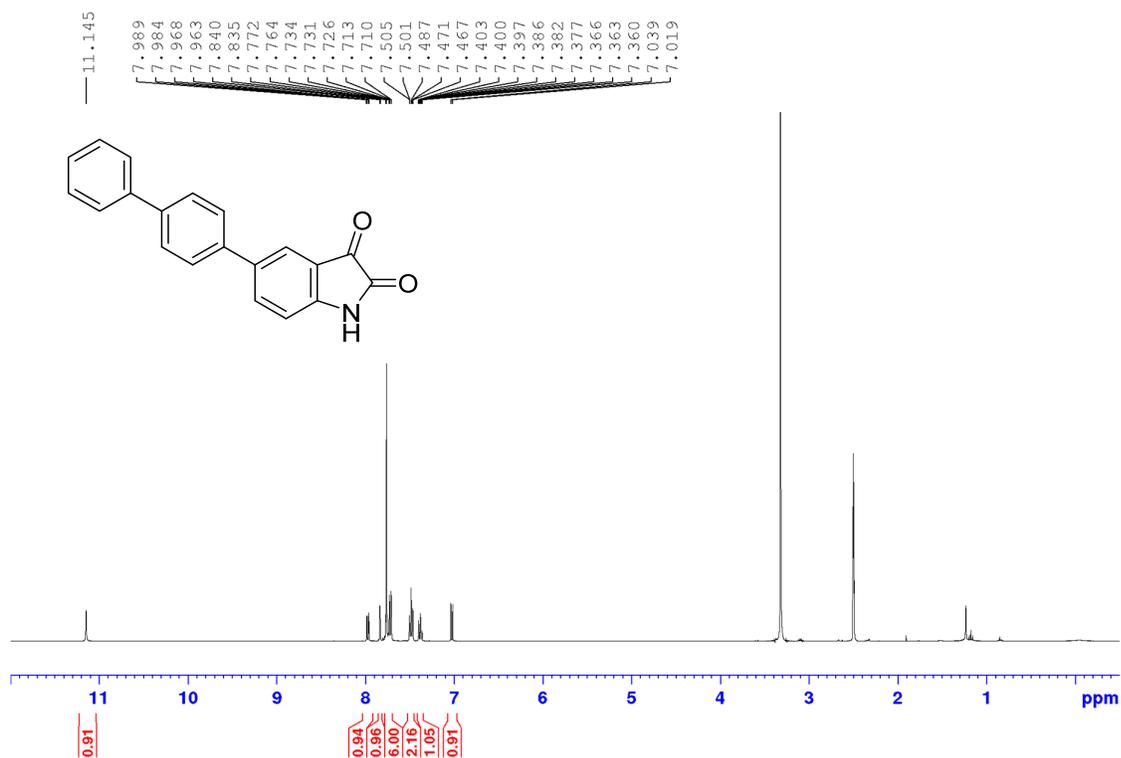
5-Phenylindoline-2,3-dione (4)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):



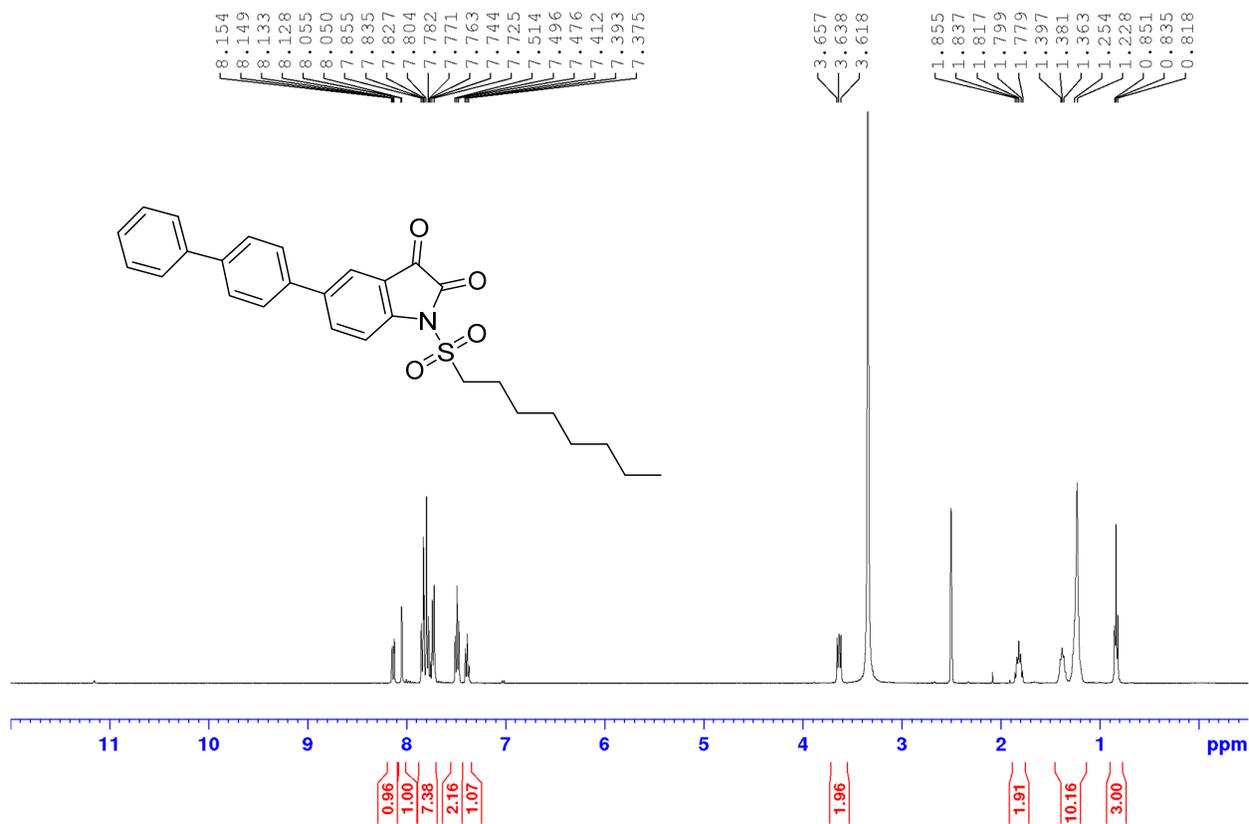
5-([1,1'-Biphenyl]-4-yl)indoline-2,3-dione (5)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

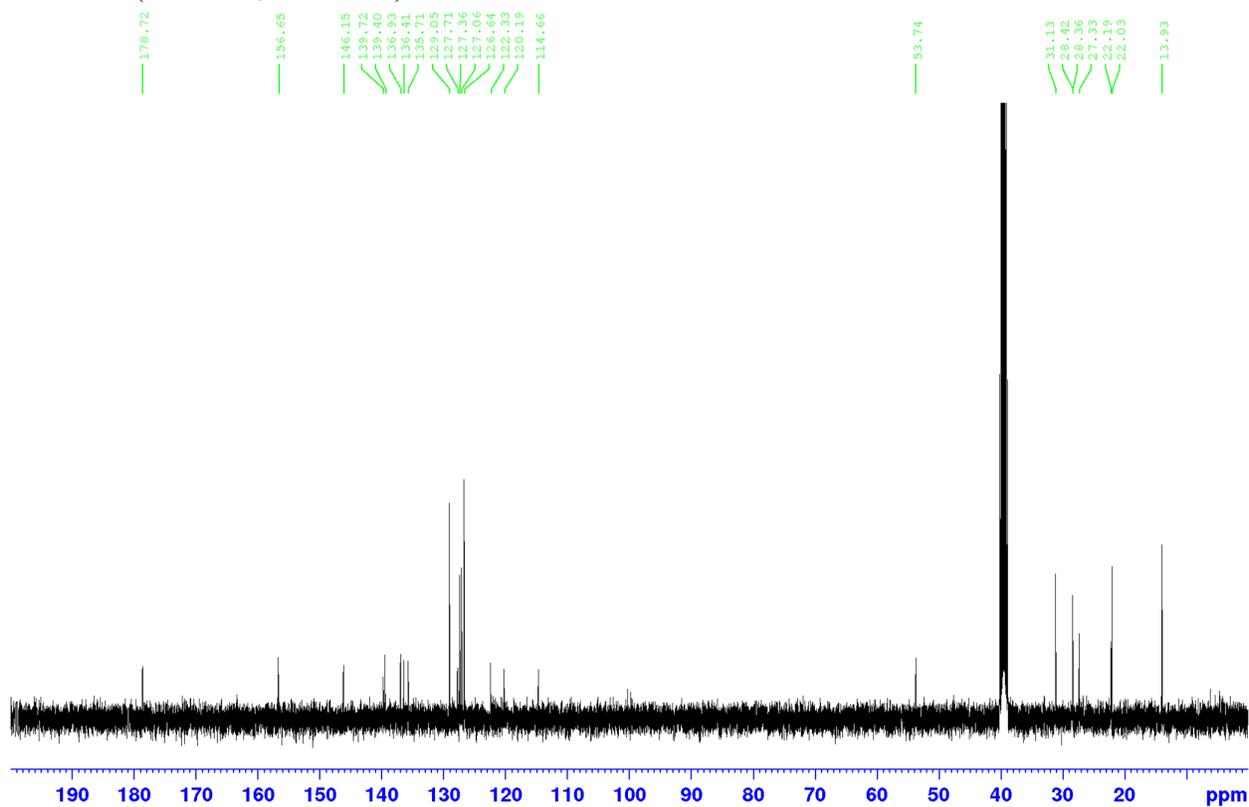


5-([1,1'-Biphenyl]-4-yl)-1-(octylsulfonyl)indoline-2,3-dione (**7d**)

¹H NMR (400 MHz, DMSO-*d*₆):

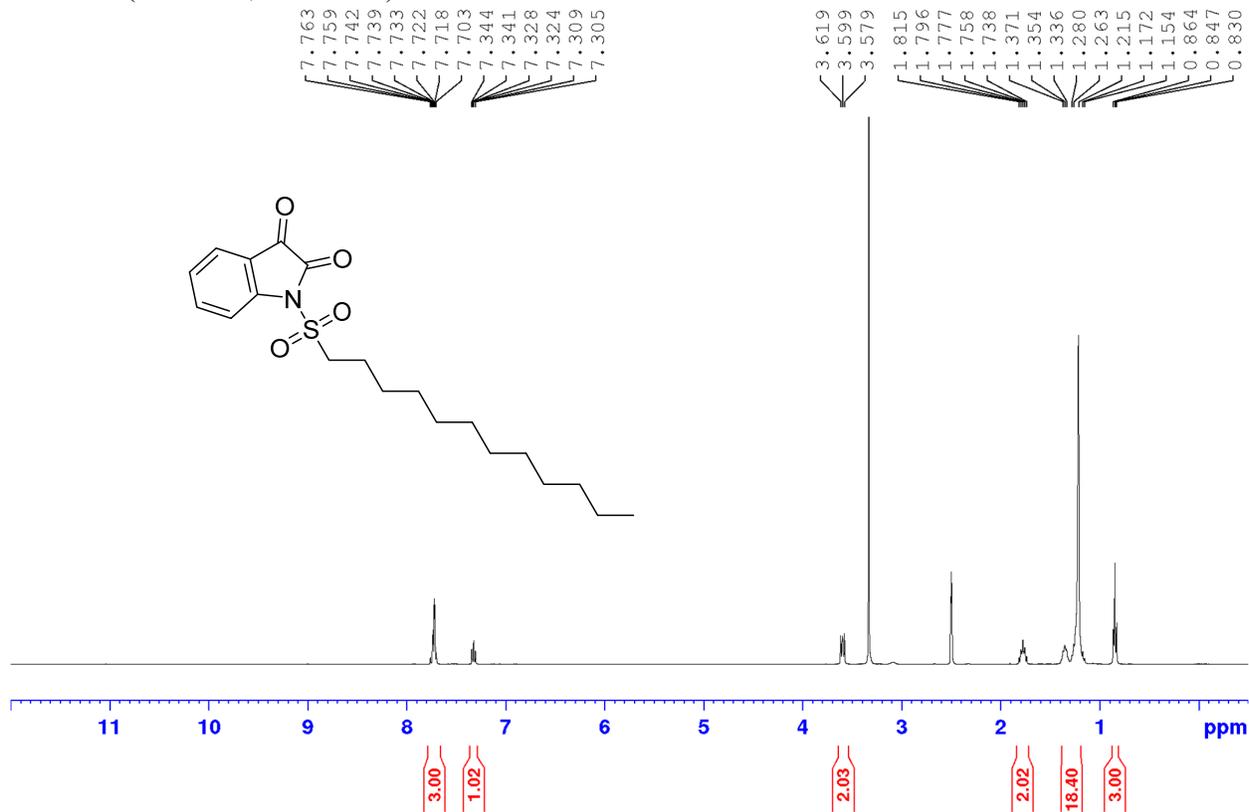


¹³C NMR (100 MHz, DMSO-*d*₆):

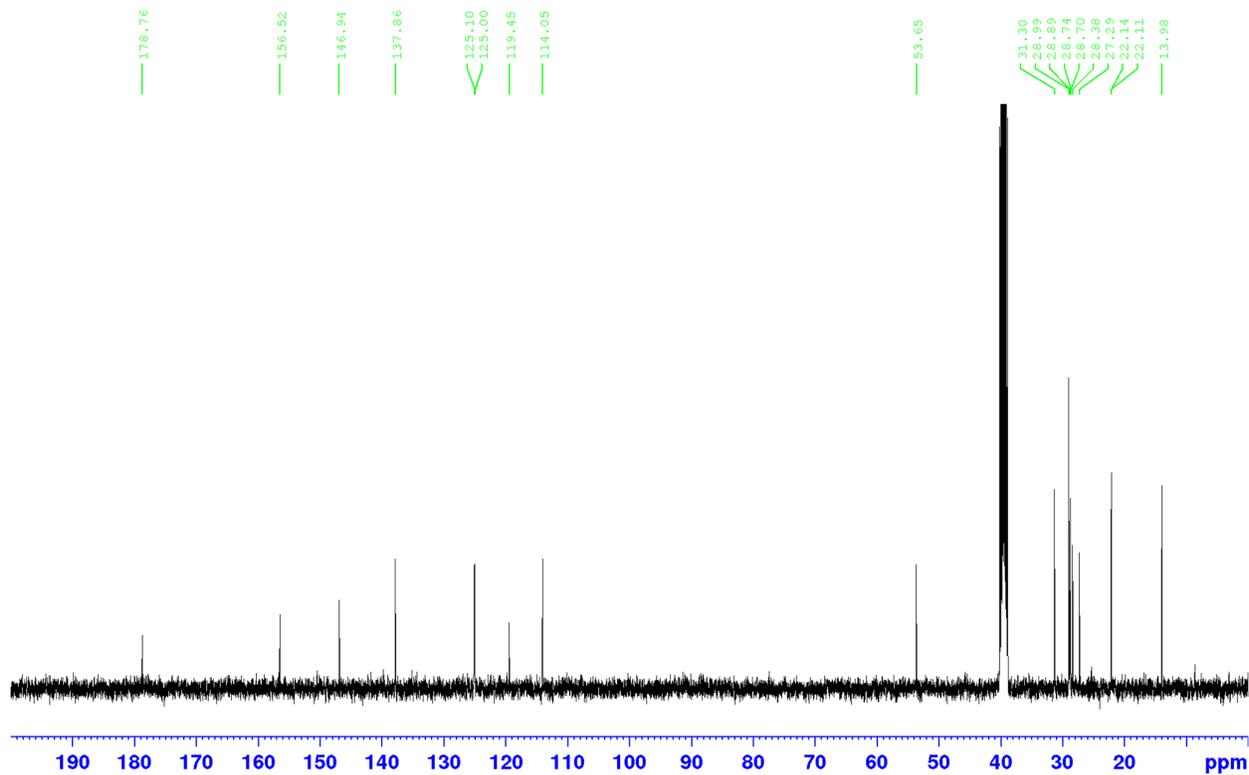


1-(Dodecylsulfonyl)indoline-2,3-dione (**8a**)

¹H NMR (400 MHz, DMSO-*d*₆):

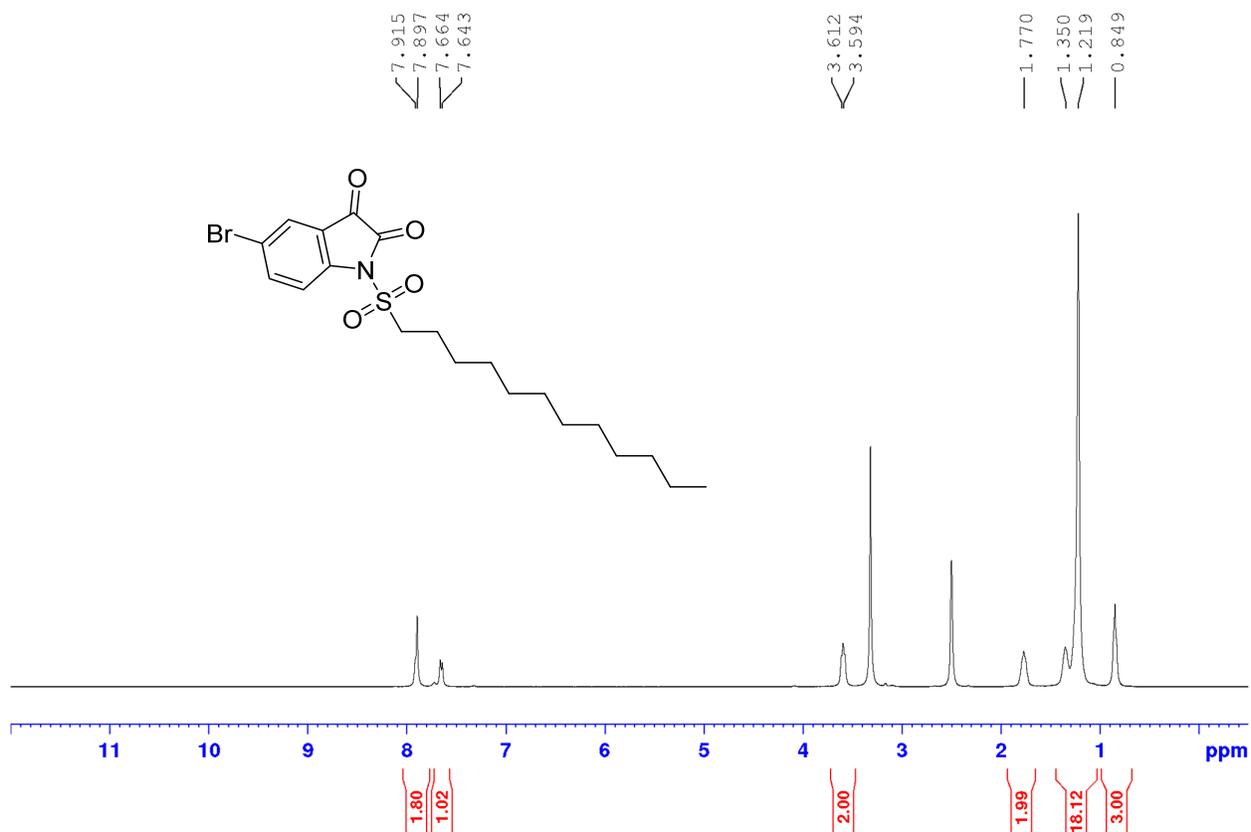


¹³C NMR (100 MHz, DMSO-*d*₆):

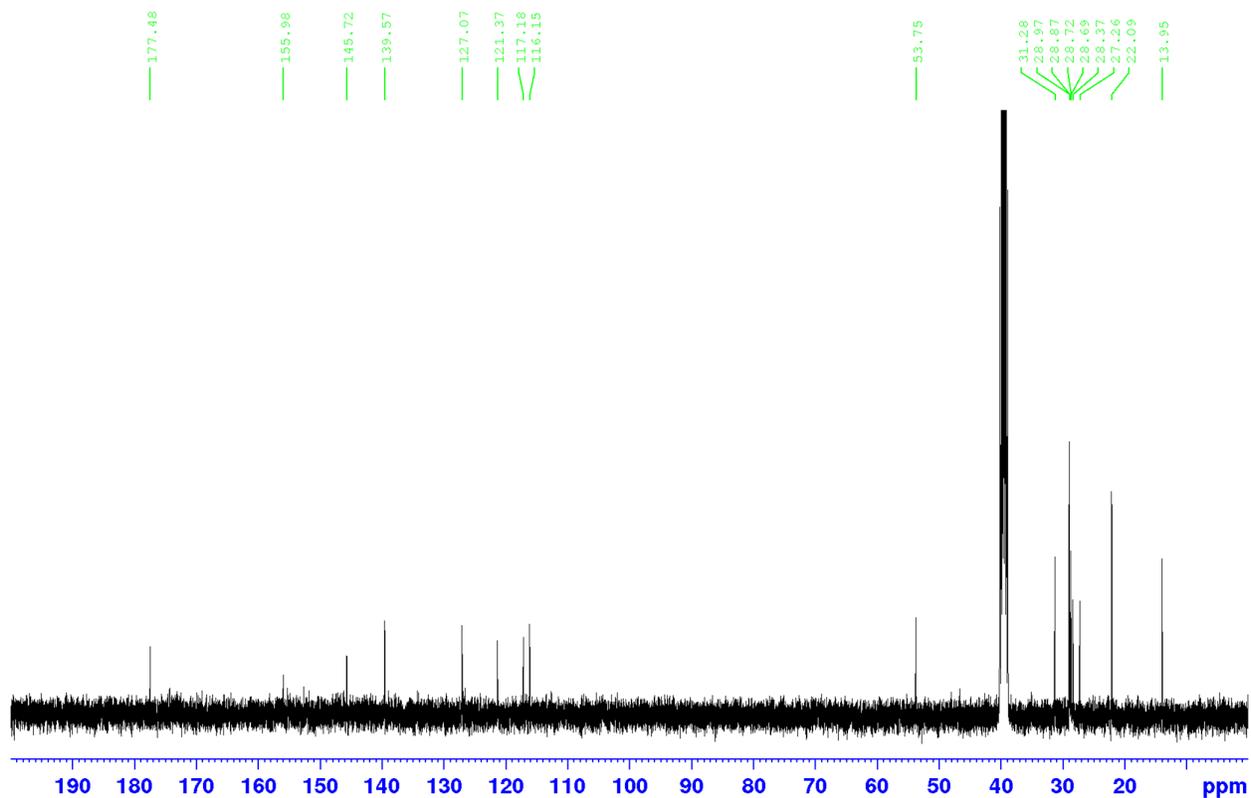


5-Bromo-1-(dodecylsulfonyl)indoline-2,3-dione (**8b**)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

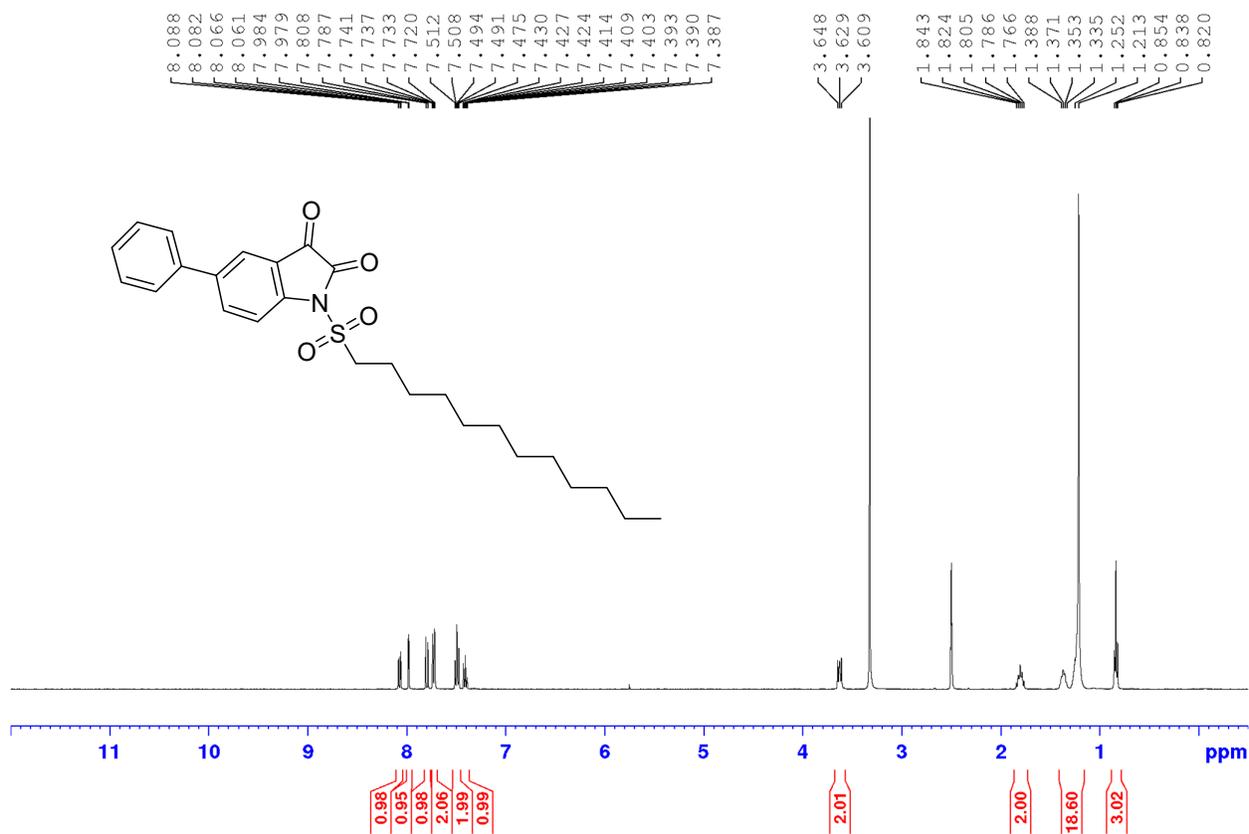


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):

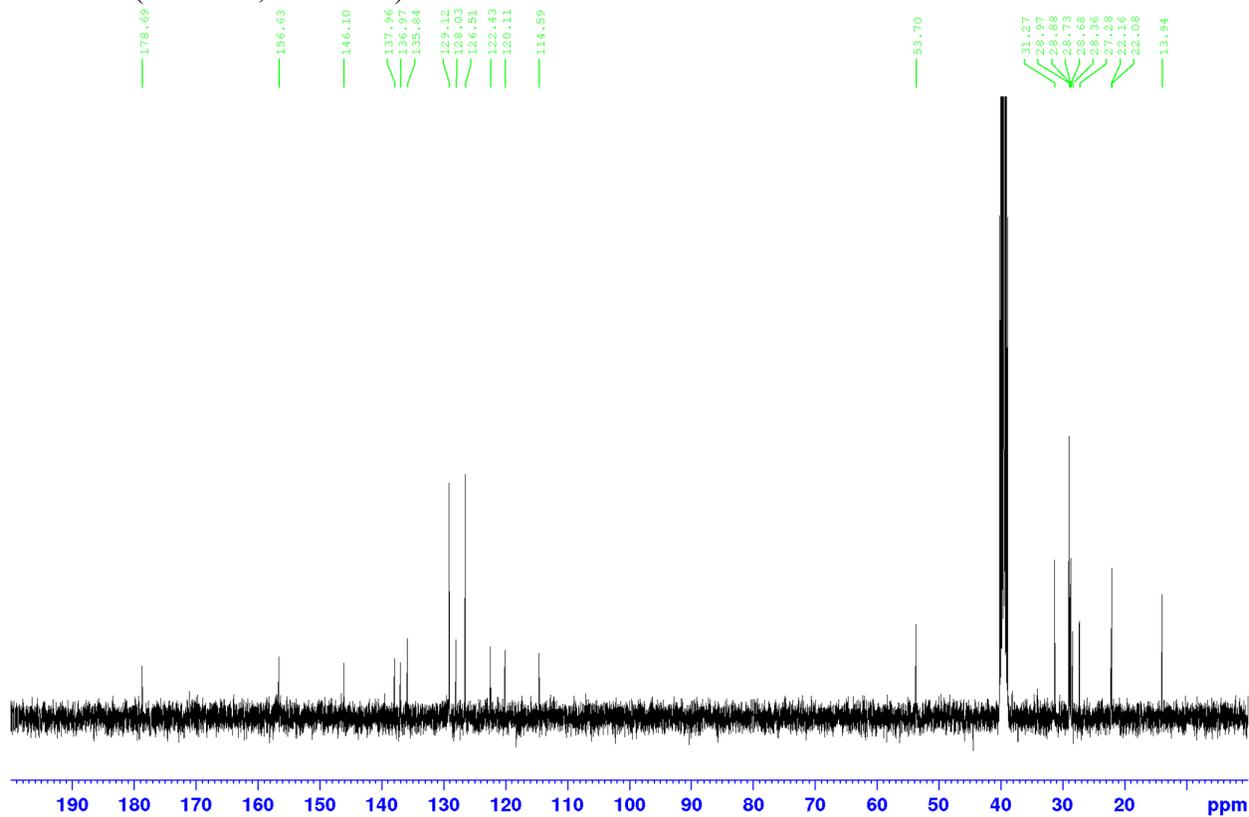


1-(Dodecylsulfonyl)-5-phenylindoline-2,3-dione (**8c**)

¹H NMR (400 MHz, DMSO-*d*₆):

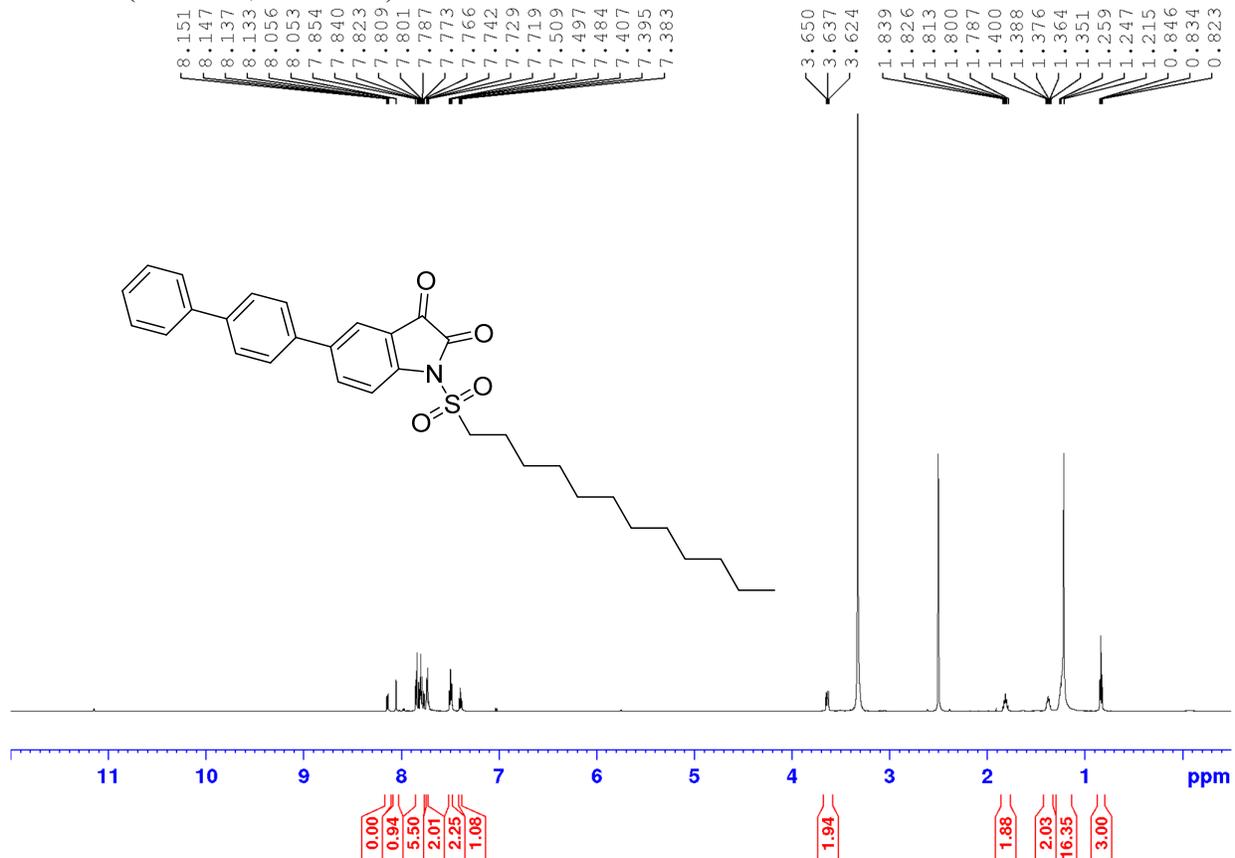


¹³C NMR (100 MHz, DMSO-*d*₆):

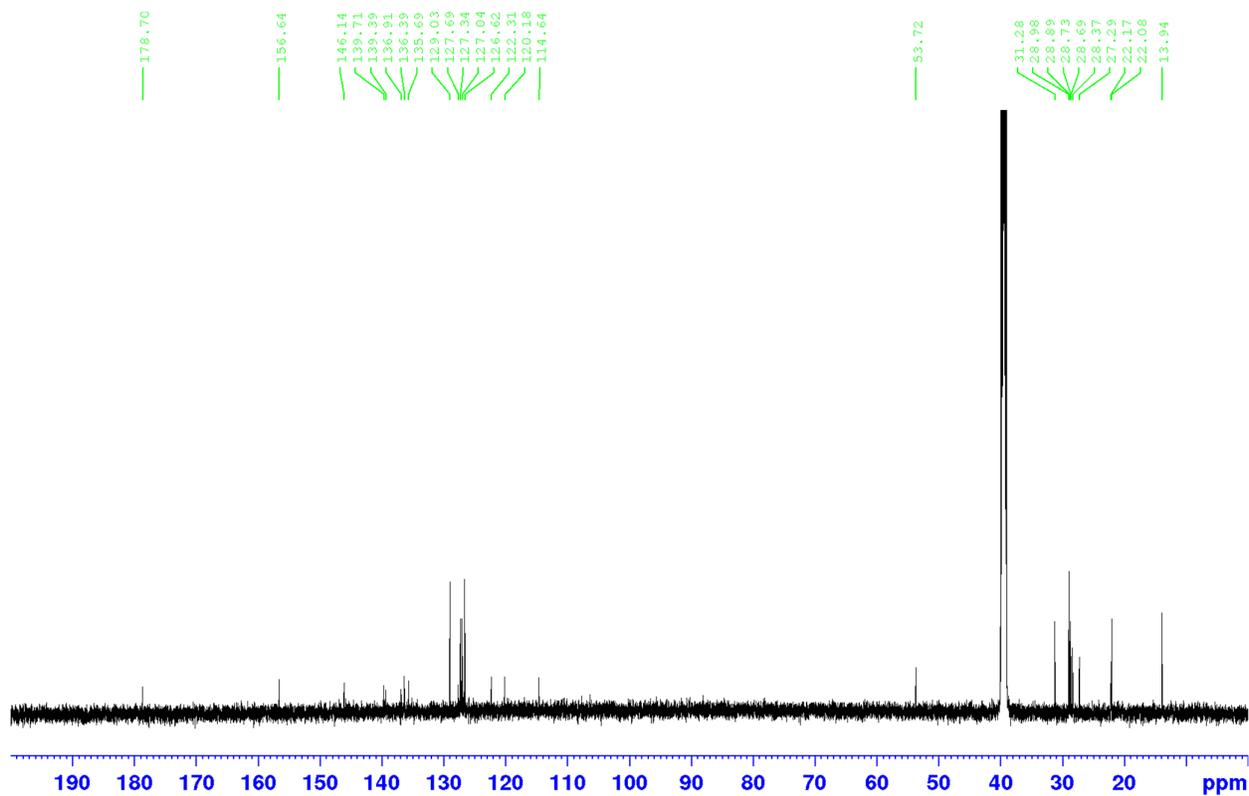


5-([1,1'-Biphenyl]-4-yl)-1-(dodecylsulfonyl)indoline-2,3-dione (**8d**)

¹H NMR (600 MHz, DMSO-*d*₆):

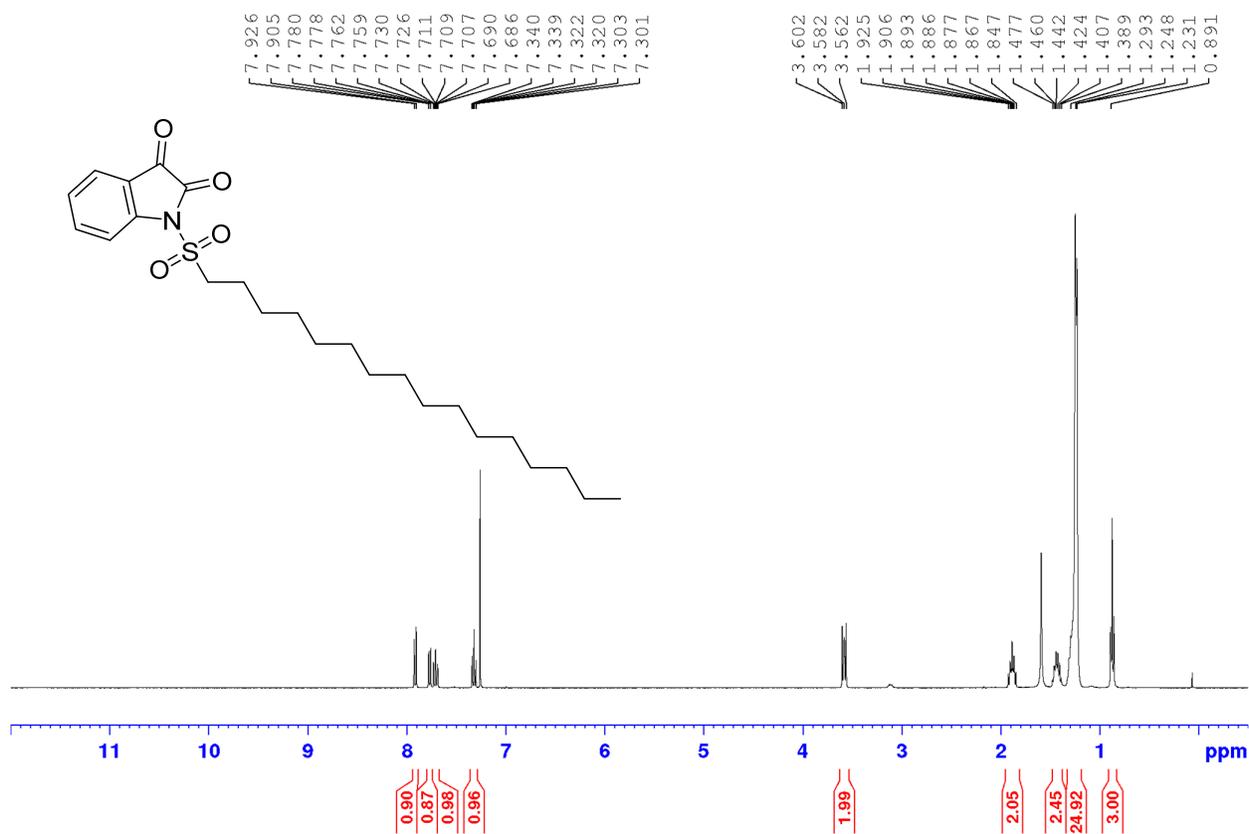


¹³C NMR (150 MHz, DMSO-*d*₆):

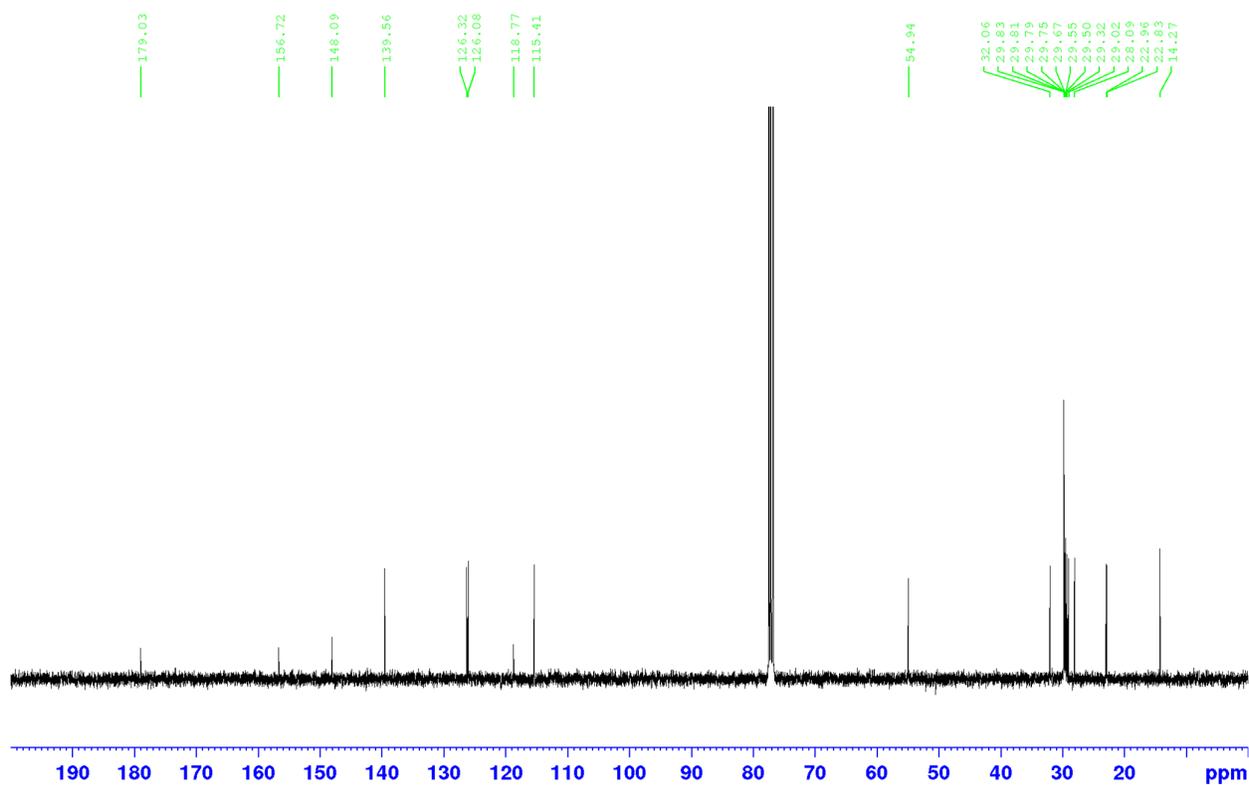


1-(Hexadecylsulfonyl)indoline-2,3-dione (**9a**)

^1H NMR (400 MHz, CDCl_3):

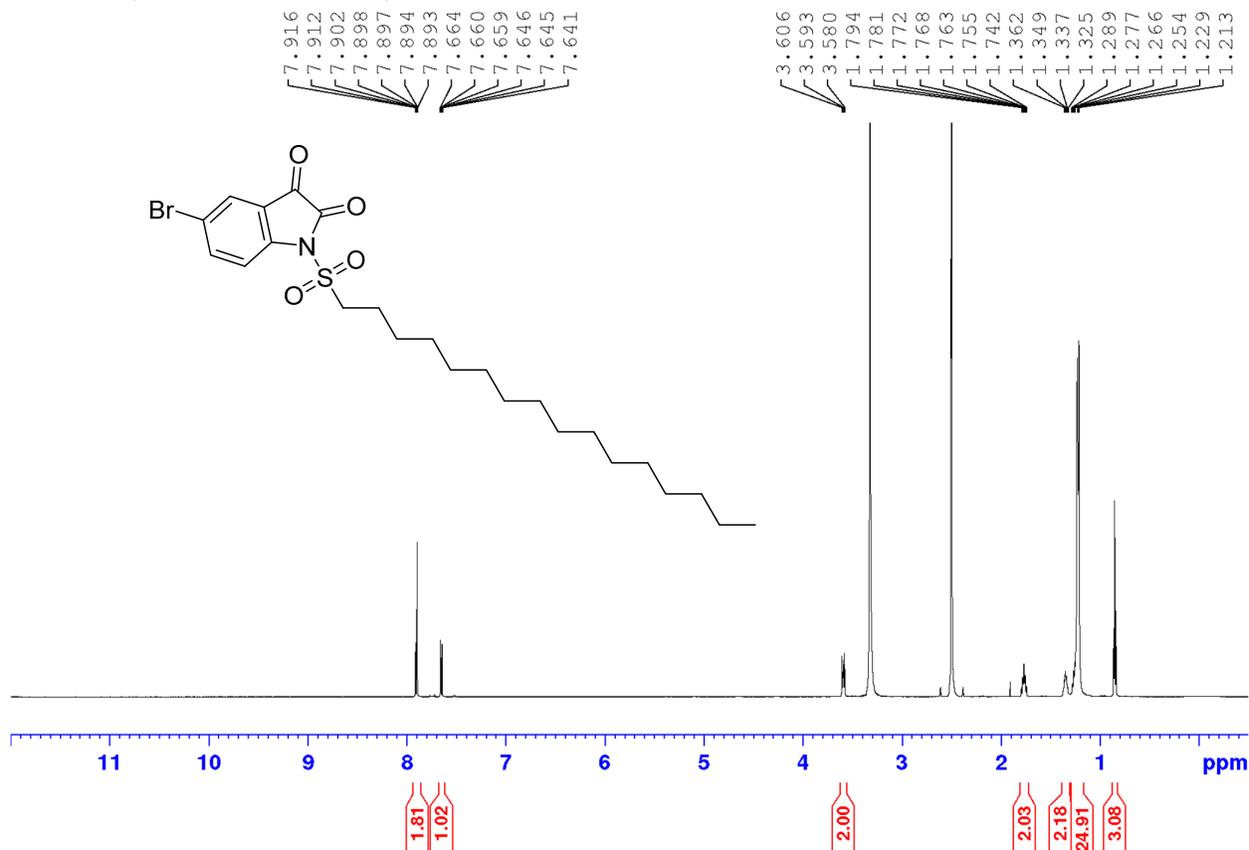


^{13}C NMR (100 MHz, CDCl_3):

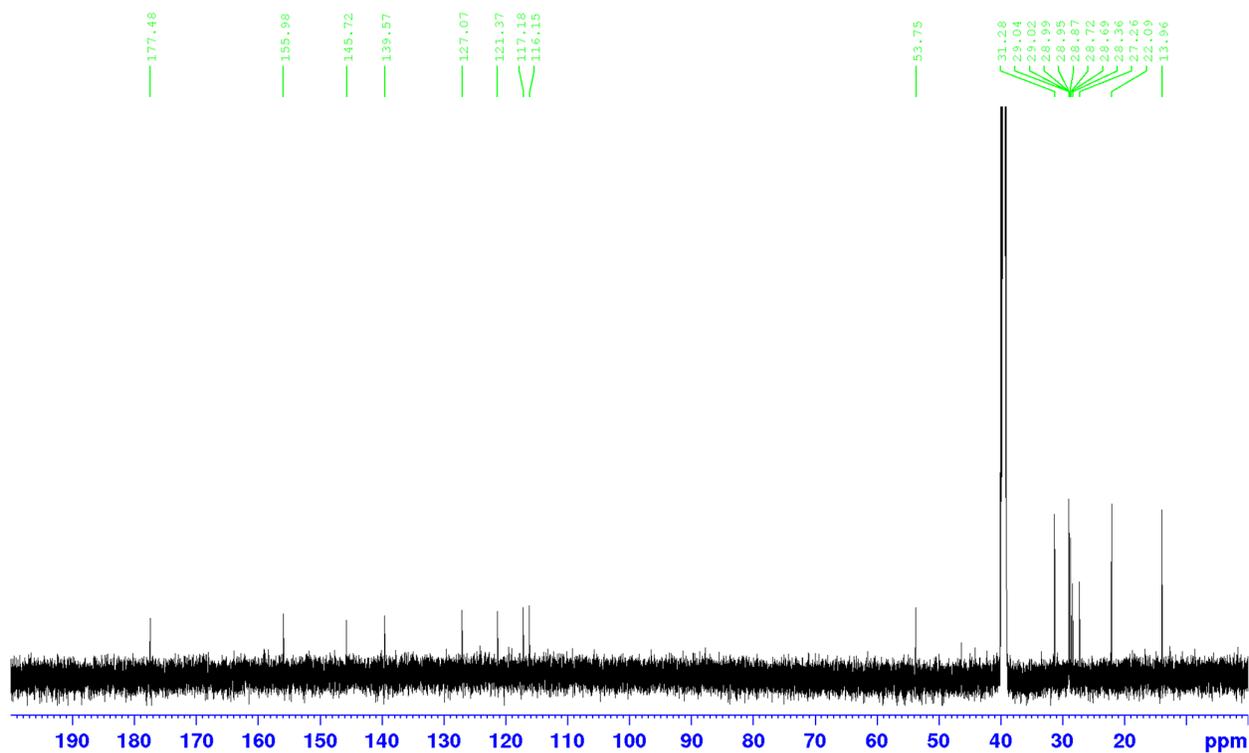


5-Bromo-1-(hexadecylsulfonyl)indoline-2,3-dione (**9b**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

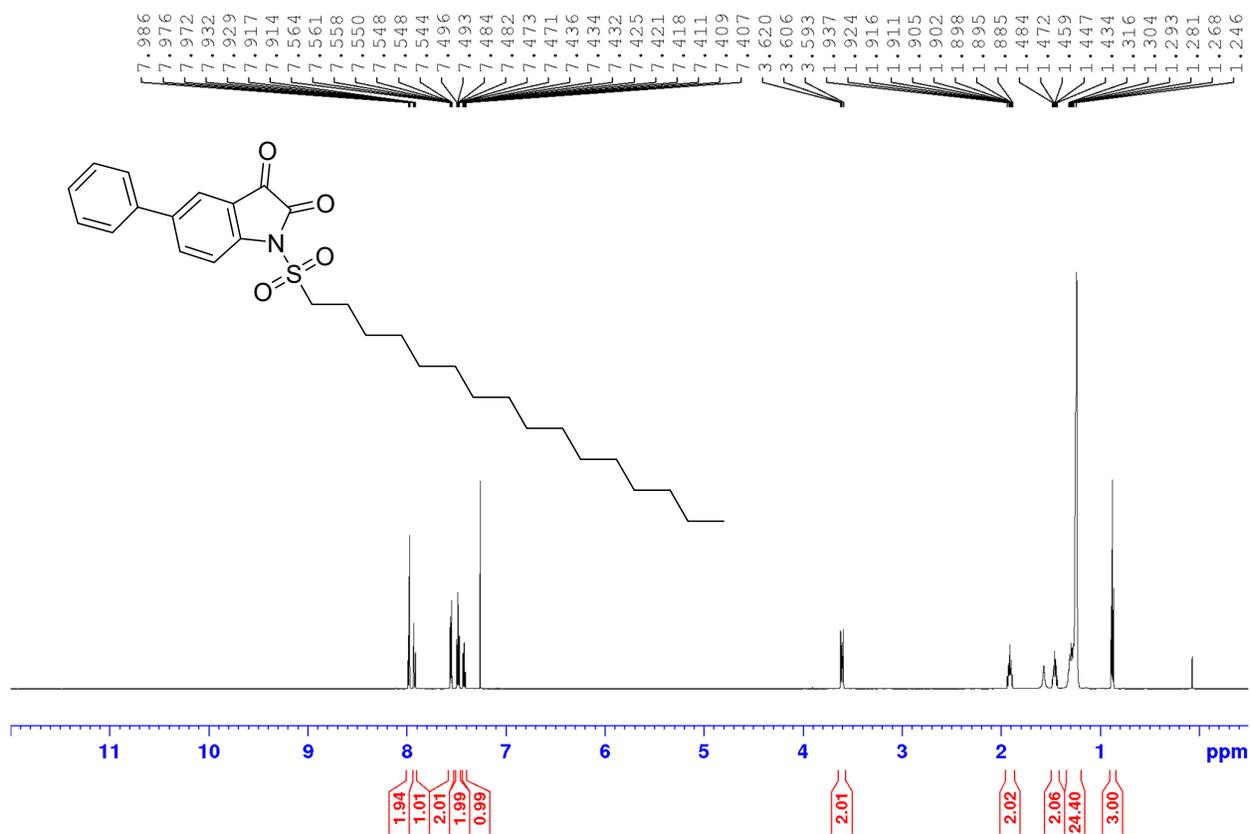


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

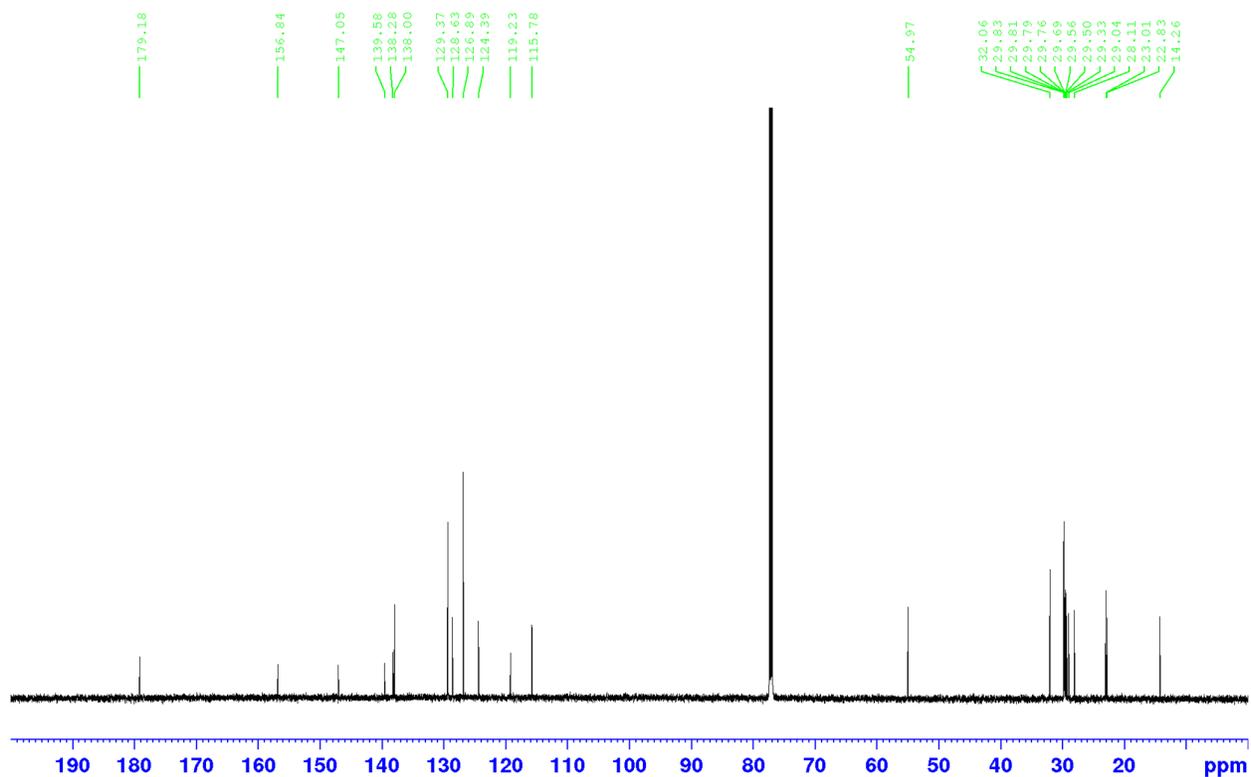


1-(Hexadecylsulfonyl)-5-phenylindoline-2,3-dione (9c)

^1H NMR (600 MHz, CDCl_3):

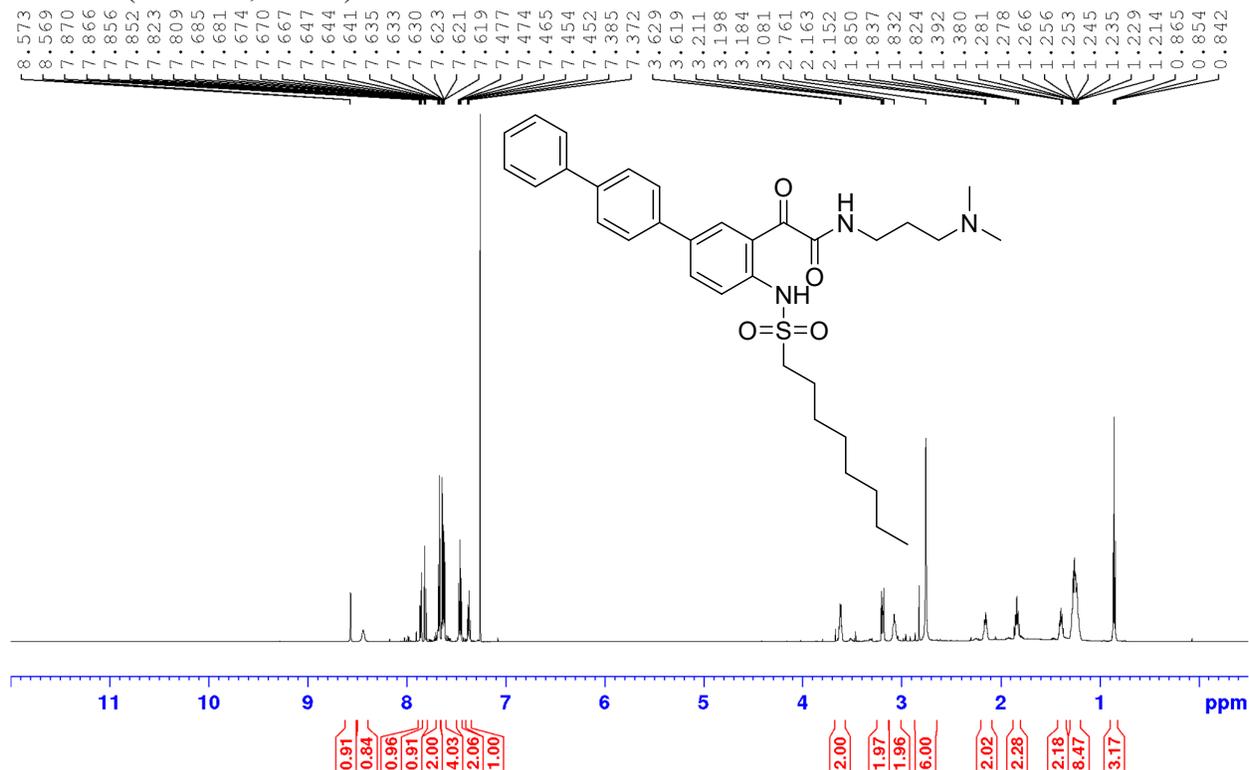


^{13}C NMR (150 MHz, CDCl_3):

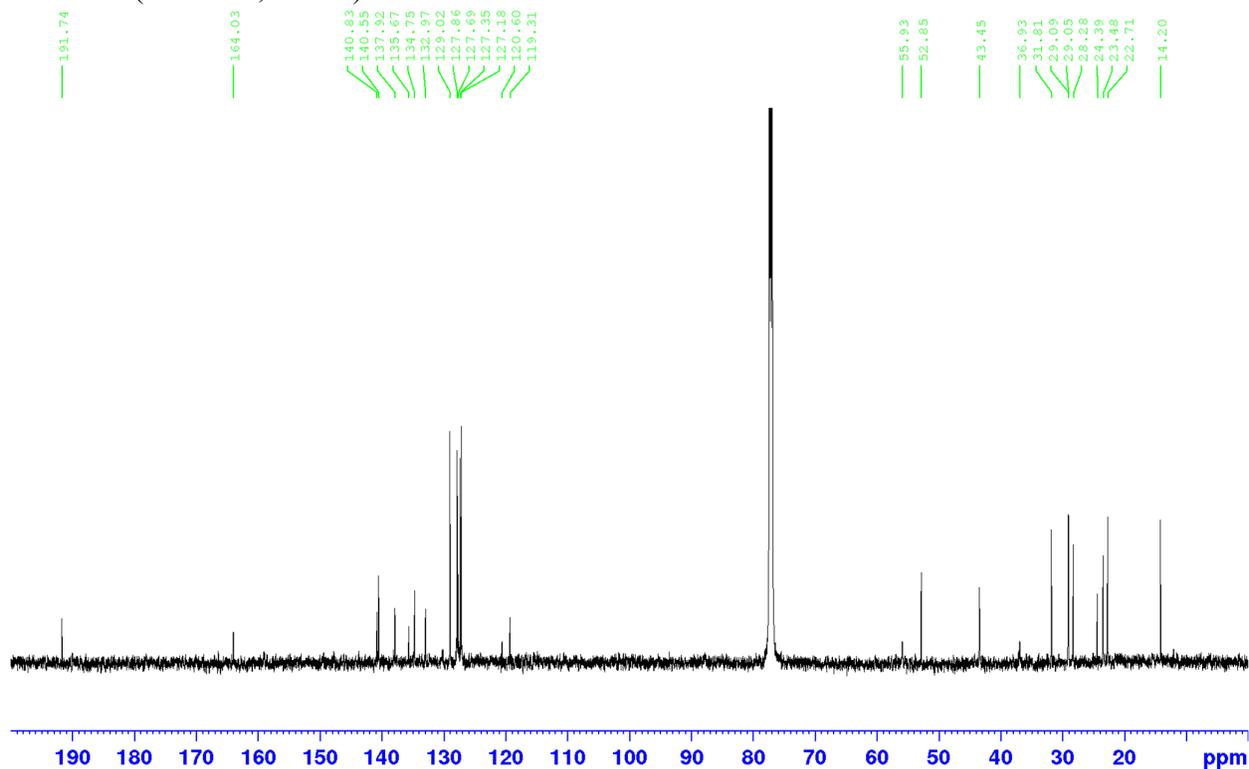


N-(3-(Dimethylamino)propyl)-2-(4-(octylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamide
(10d)

¹H NMR (600 MHz, CDCl₃):

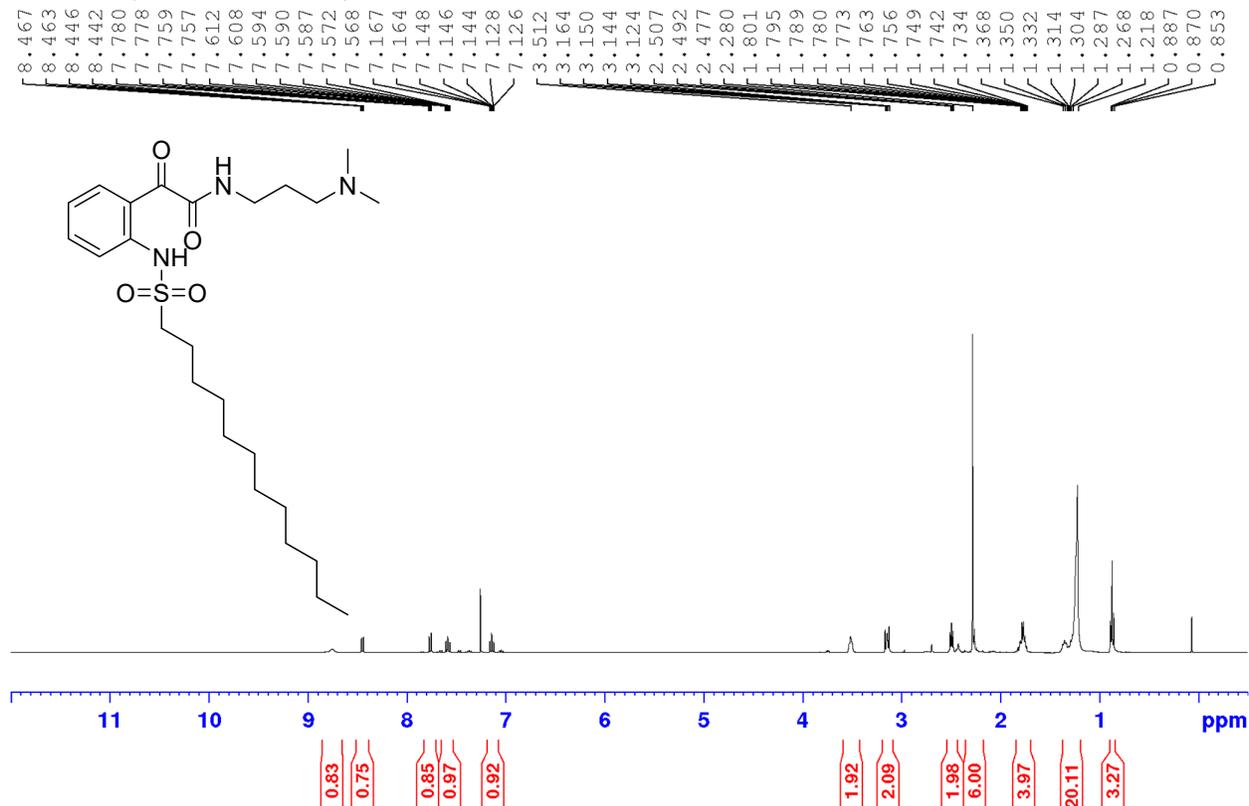


¹³C NMR (150 MHz, CDCl₃):

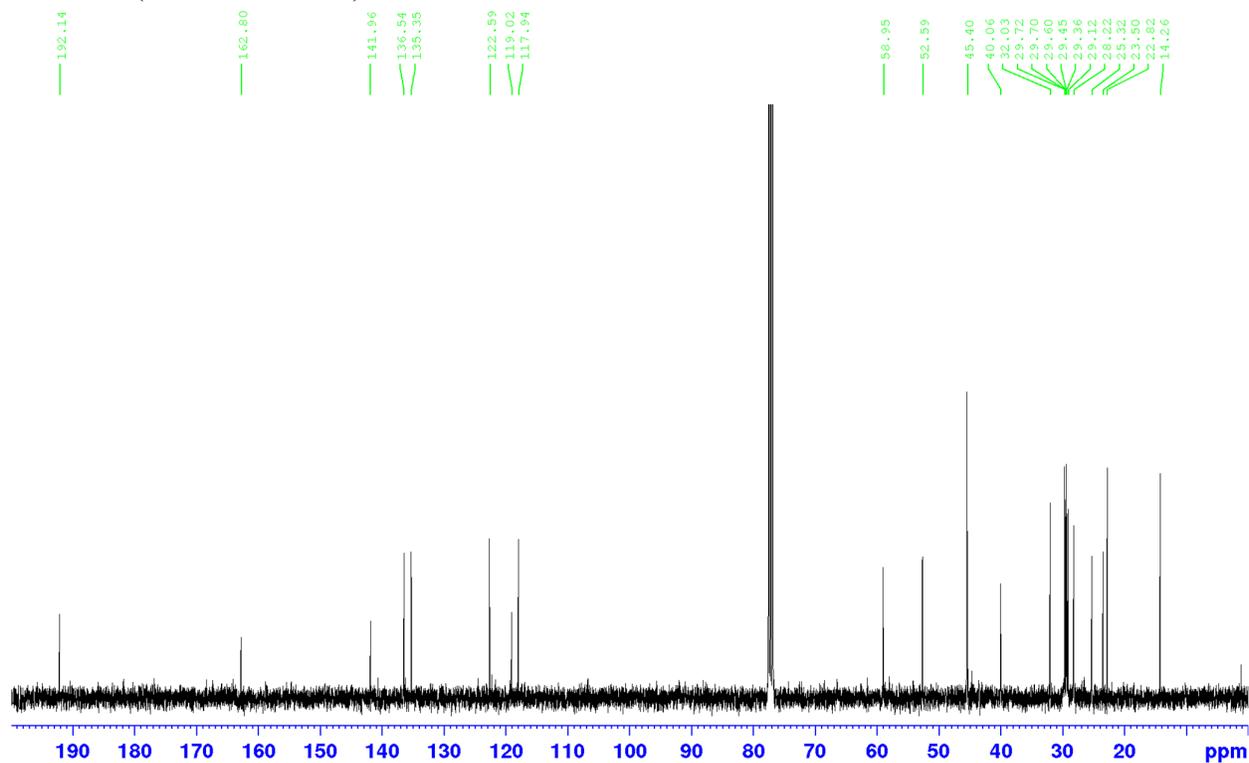


N-(3-(Dimethylamino)propyl)-2-(2-(dodecylsulfonamido)phenyl)-2-oxoacetamide (**11a**)

^1H NMR (400 MHz, CDCl_3):

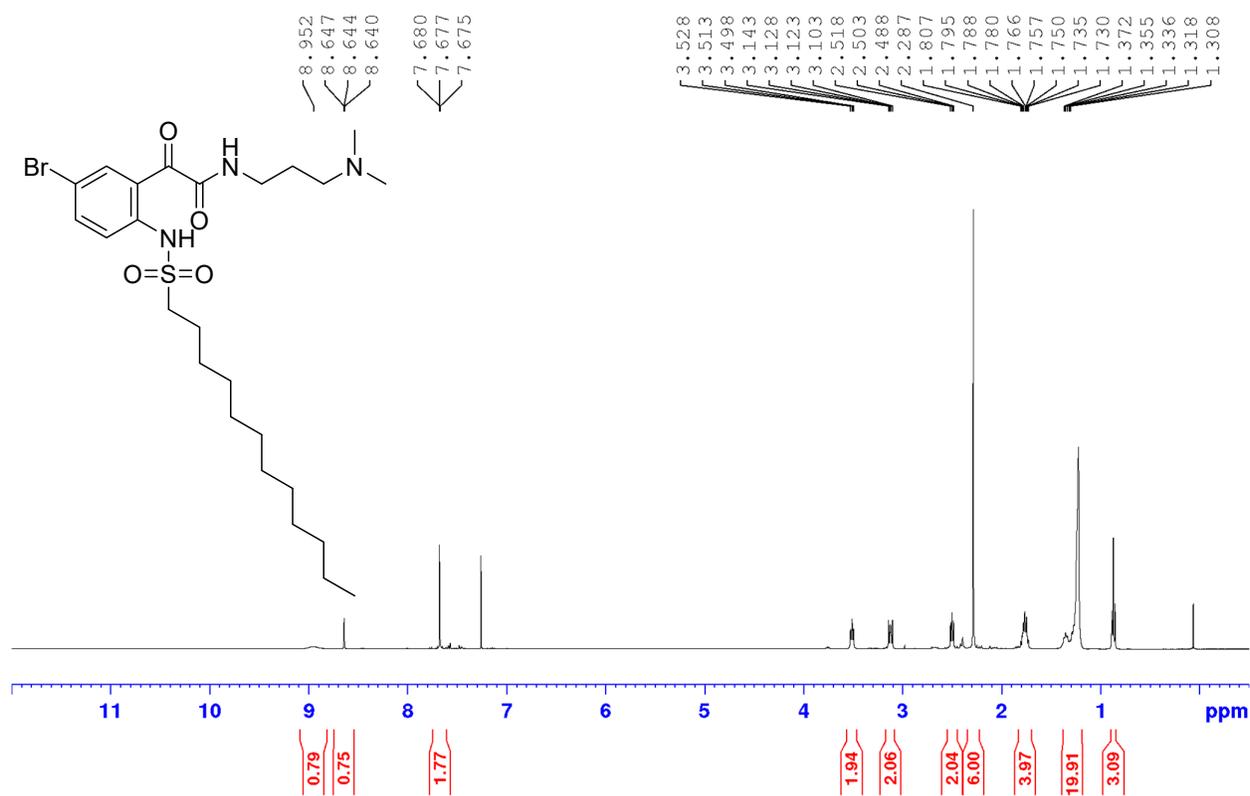


^{13}C NMR (100 MHz, CDCl_3):

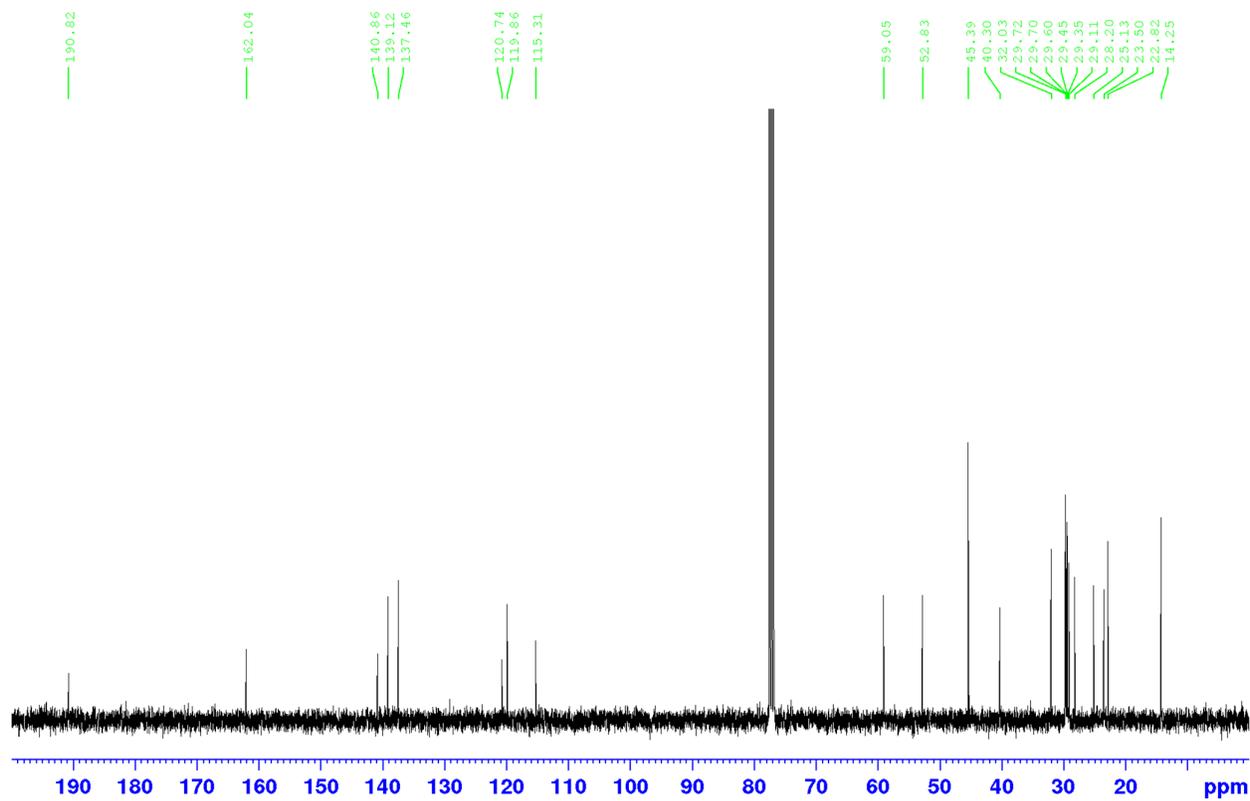


2-(5-Bromo-2-(dodecylsulfonamido)phenyl)-*N*-(3-(dimethylamino)propyl)-2-oxoacetamide (**11b**)

¹H NMR (400 MHz, CDCl₃):

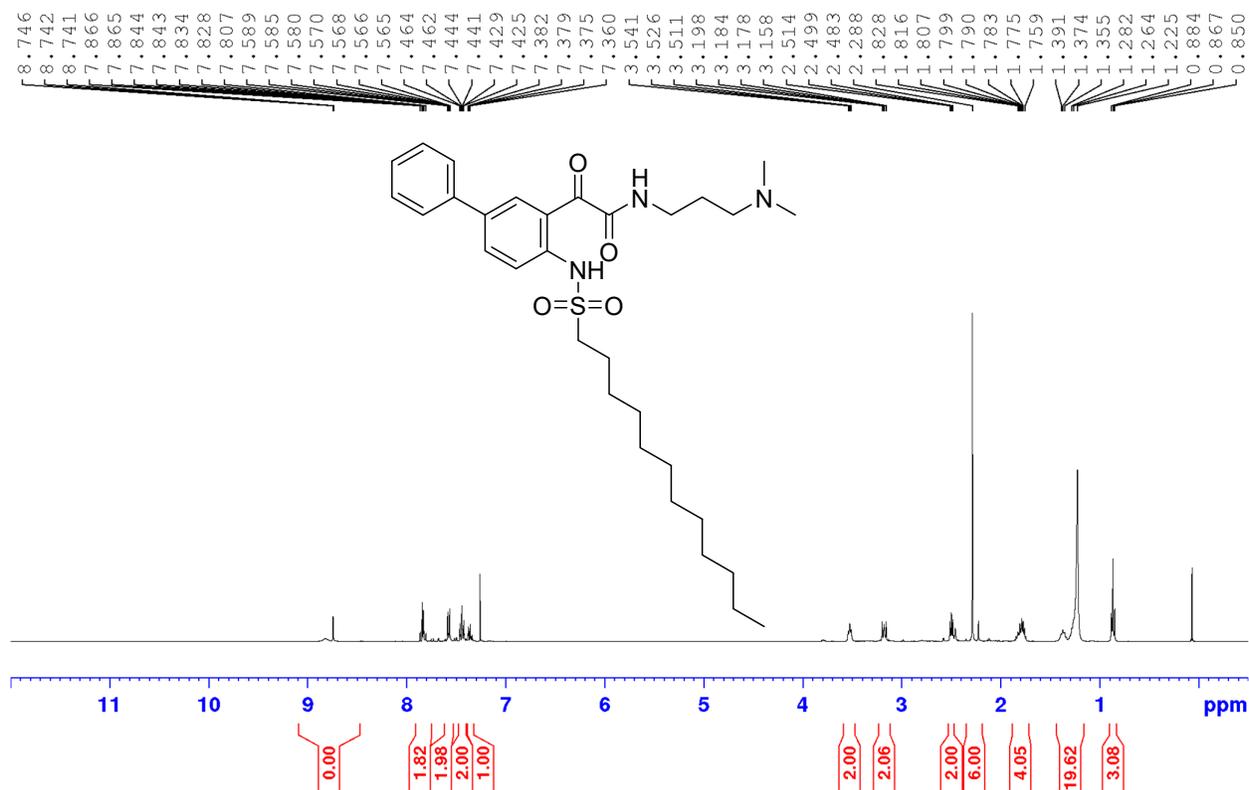


¹³C NMR (100 MHz, CDCl₃):

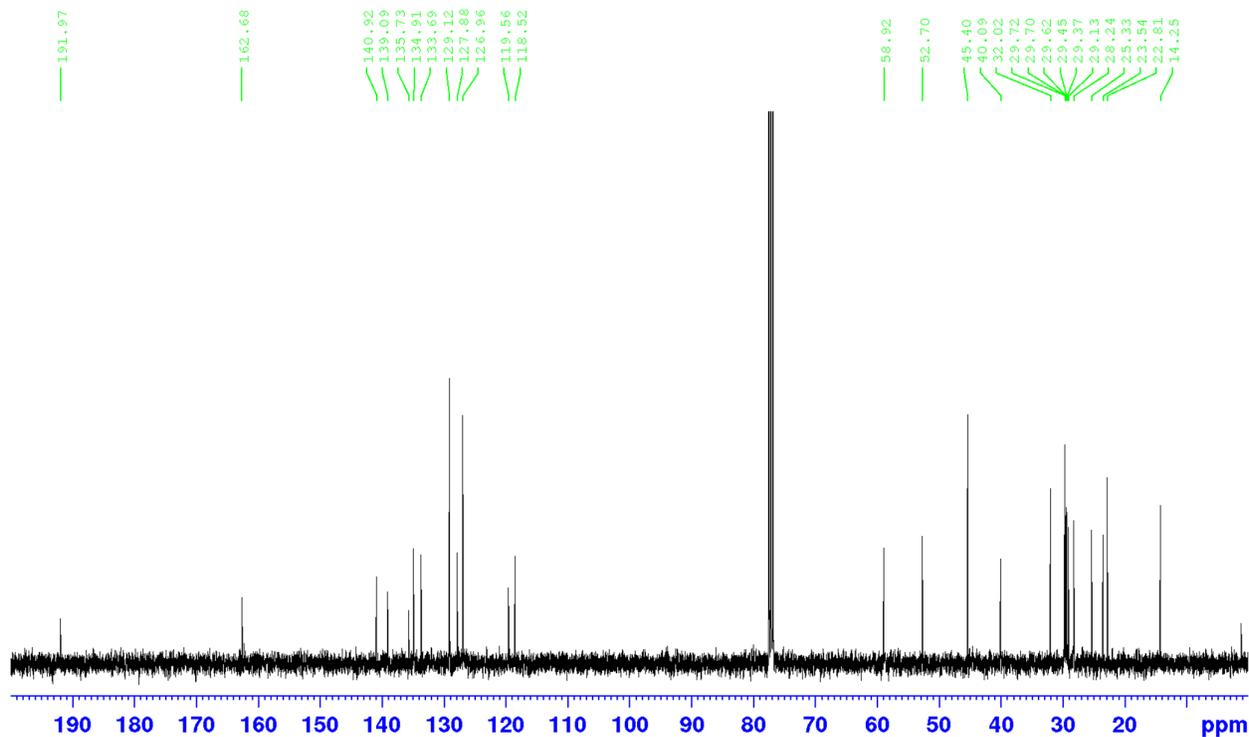


N-(3-(Dimethylamino)propyl)-2-(4-(dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamide (**11c**)

¹H NMR (400 MHz, CDCl₃):

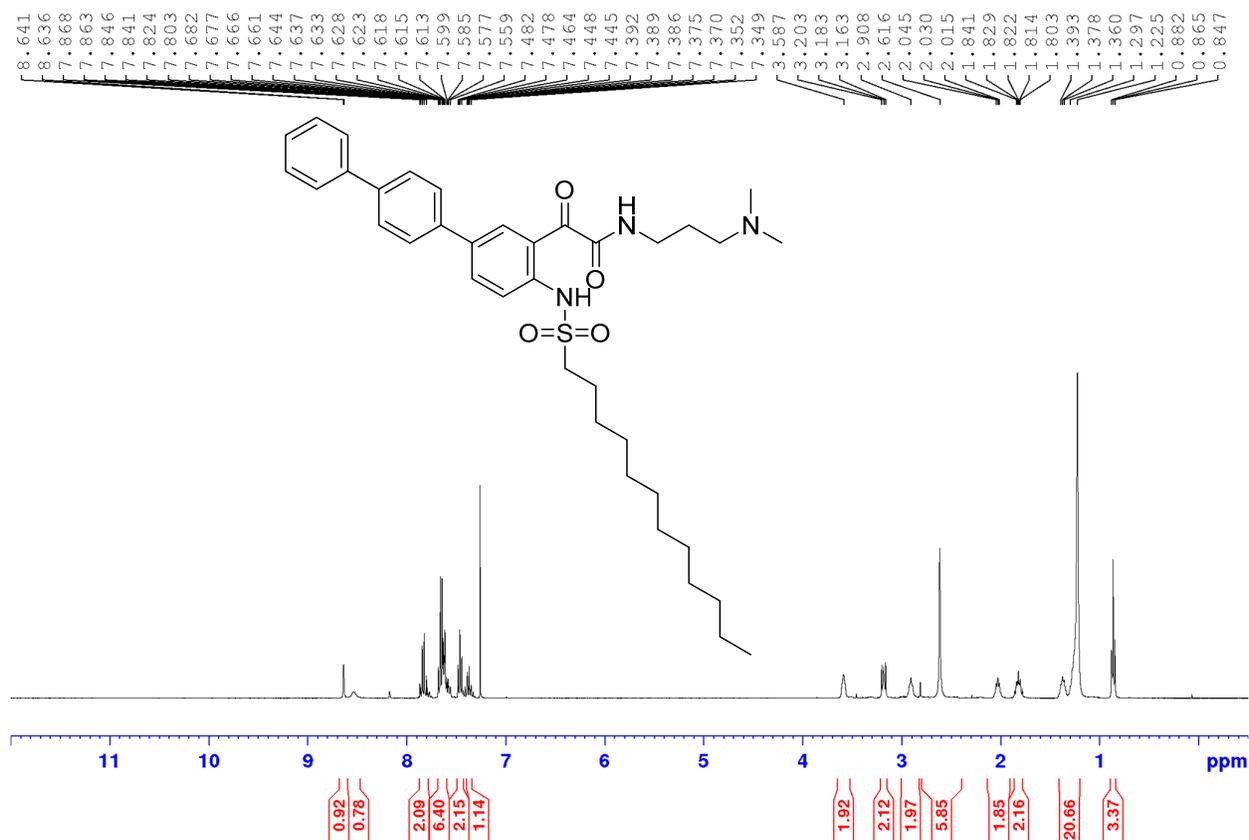


¹³C NMR (100 MHz, CDCl₃):

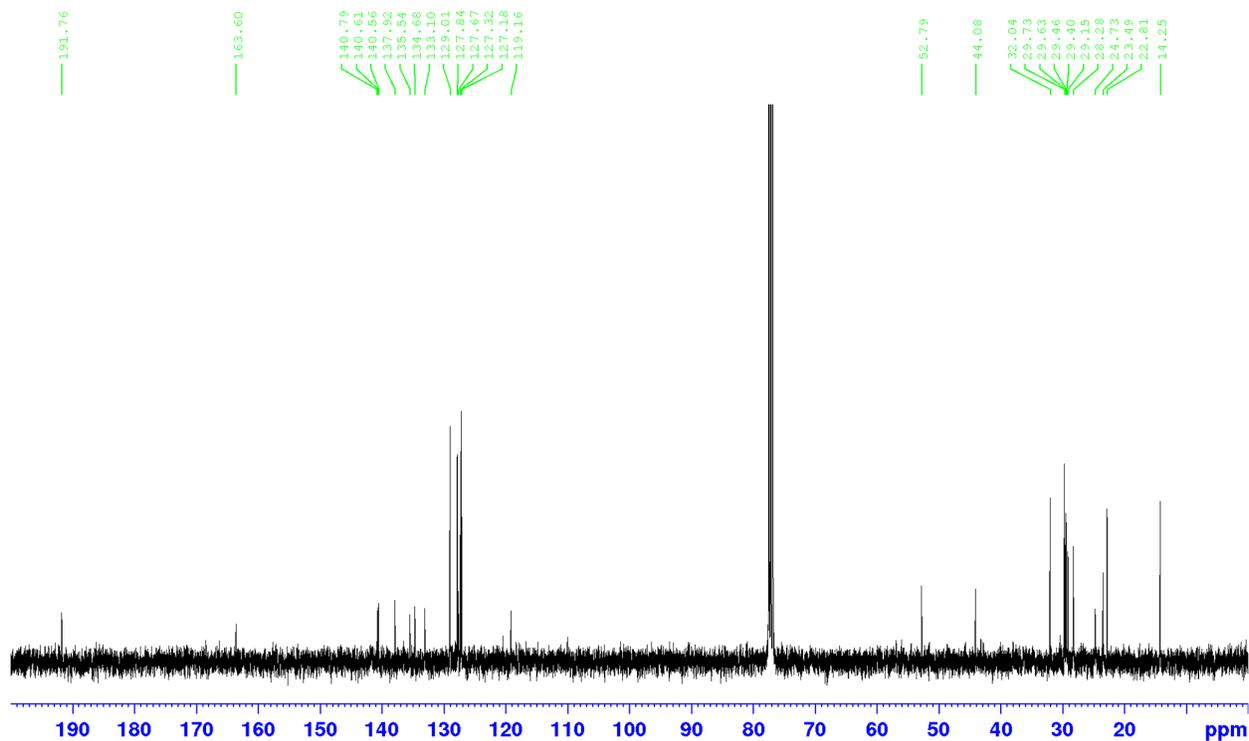


N-(3-(Dimethylamino)propyl)-2-(4-(dodecylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamide
(11d)

^1H NMR (400 MHz, CDCl_3):

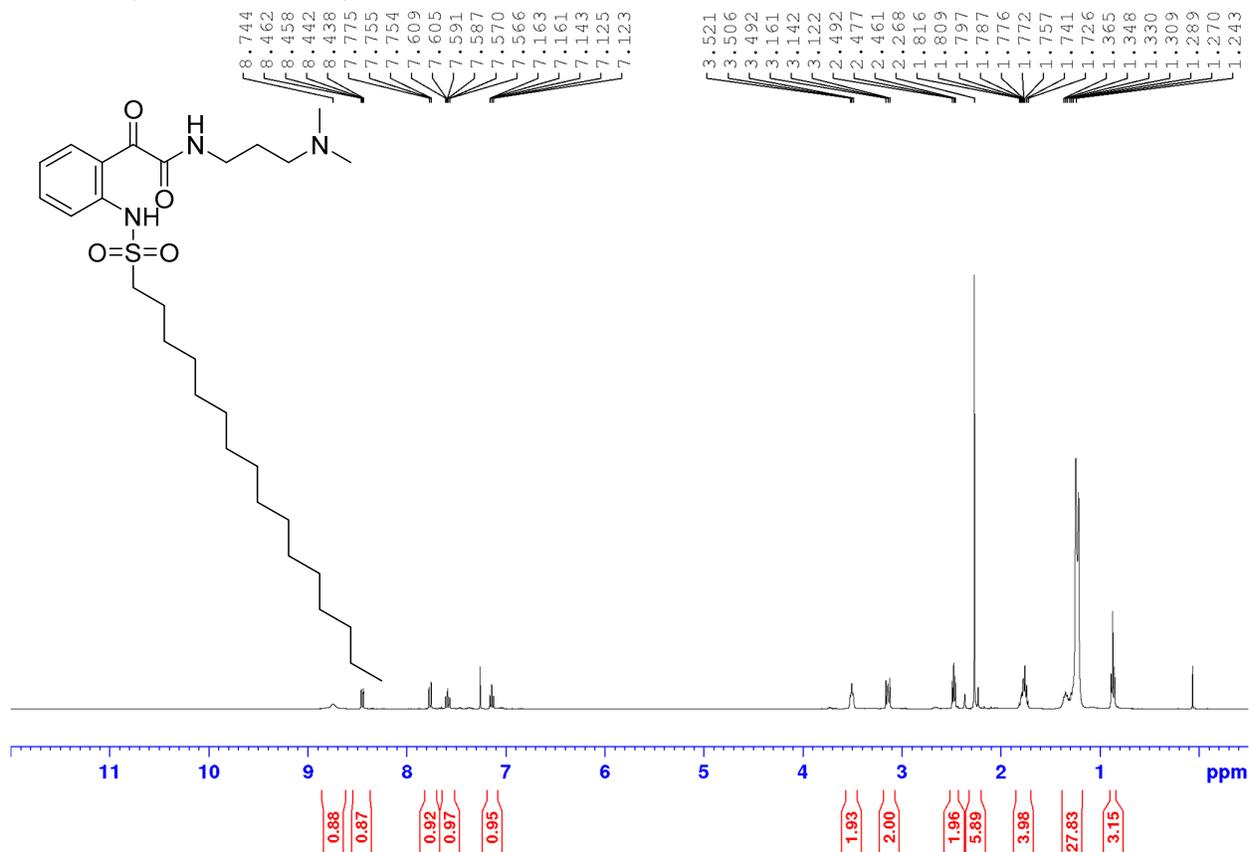


^{13}C NMR (100 MHz, CDCl_3):

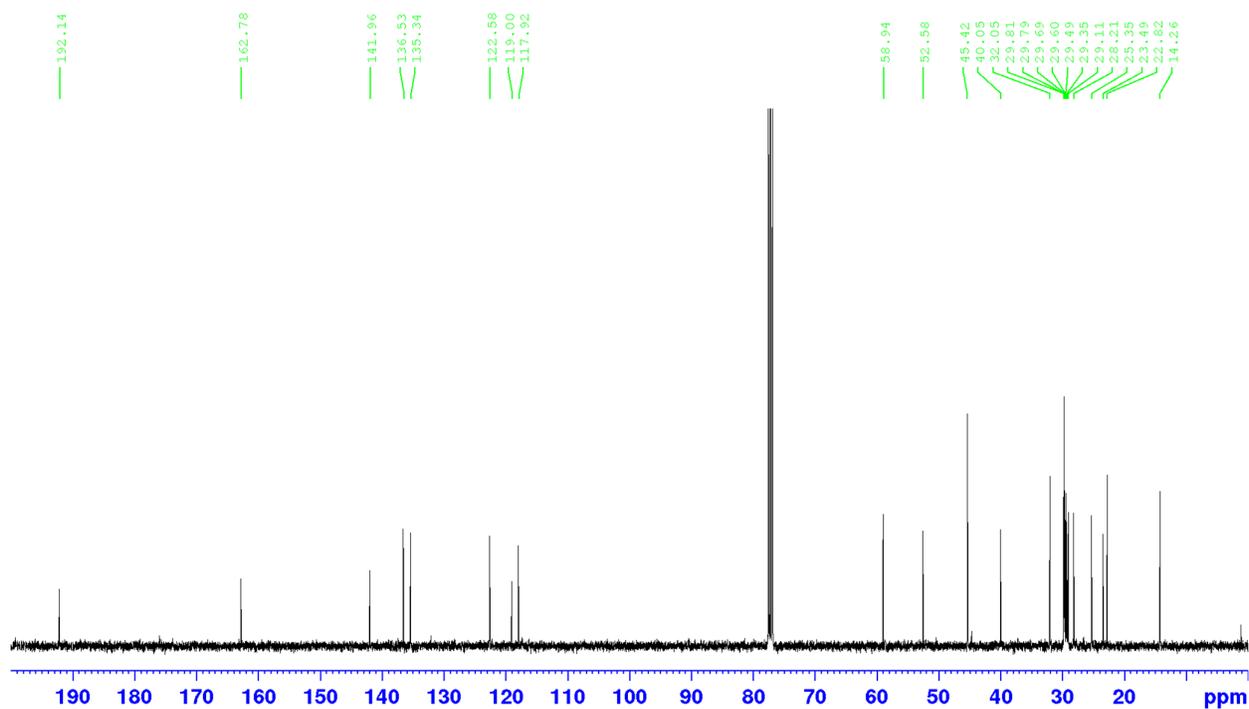


N-(3-(Dimethylamino)propyl)-2-(2-(hexadecylsulfonamido)phenyl)-2-oxoacetamide (**12a**)

¹H NMR (400 MHz, CDCl₃):

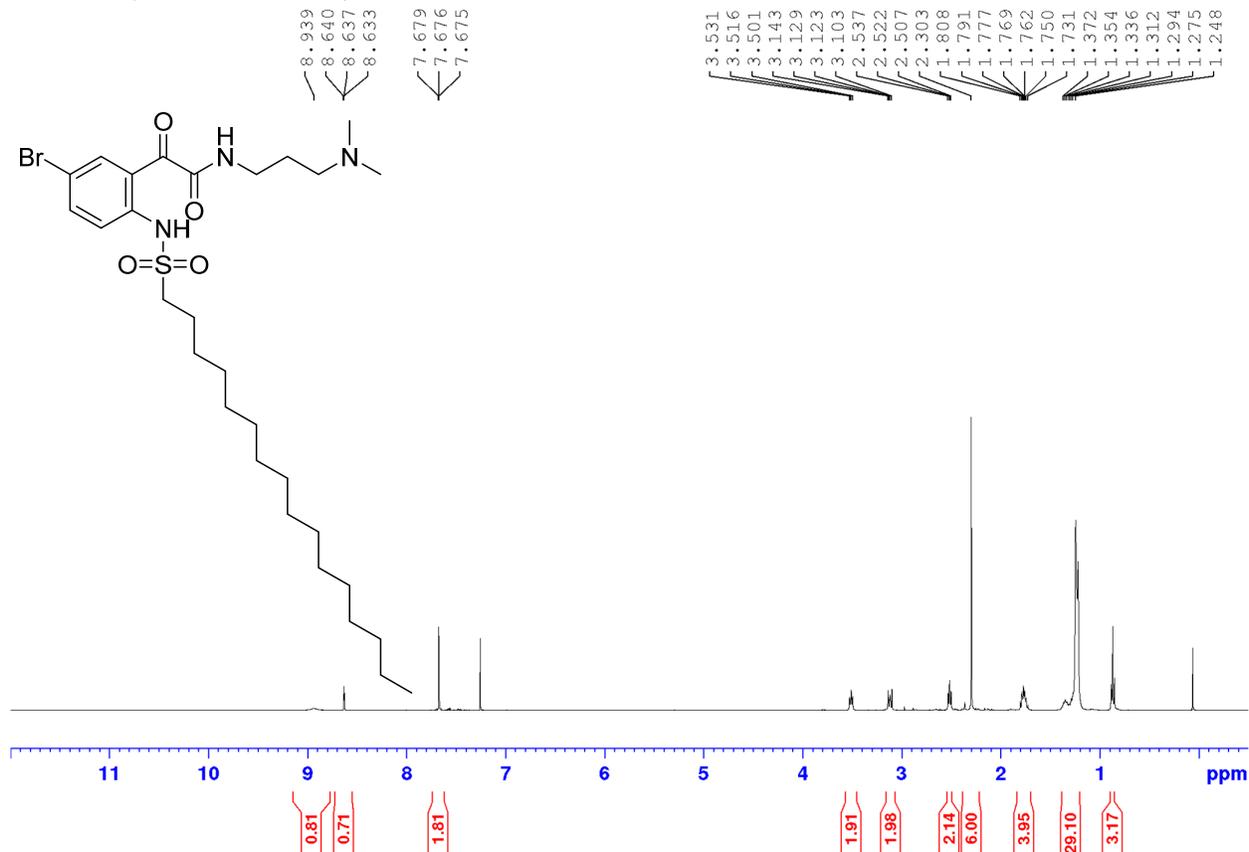


¹³C NMR (100 MHz, CDCl₃):

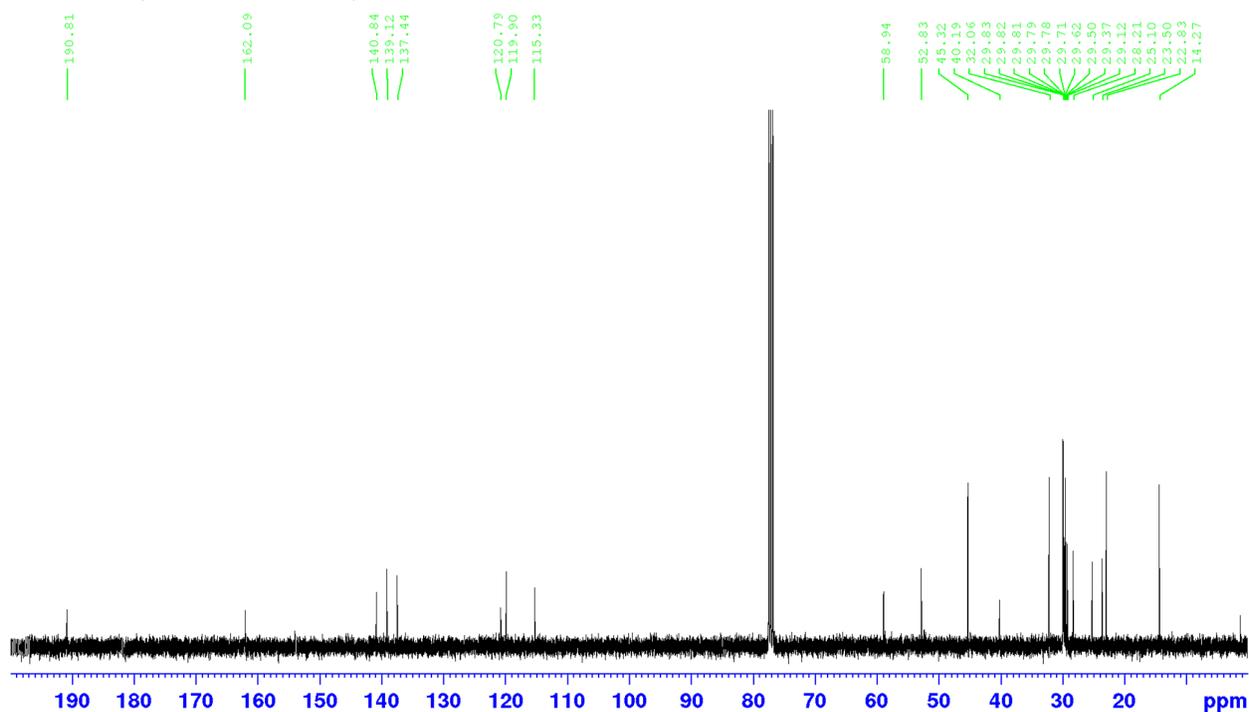


2-(5-Bromo-2-(hexadecylsulfonamido)phenyl)-*N*-(3-(dimethylamino)propyl)-2-oxoacetamide (**12b**)

^1H NMR (400 MHz, CDCl_3):

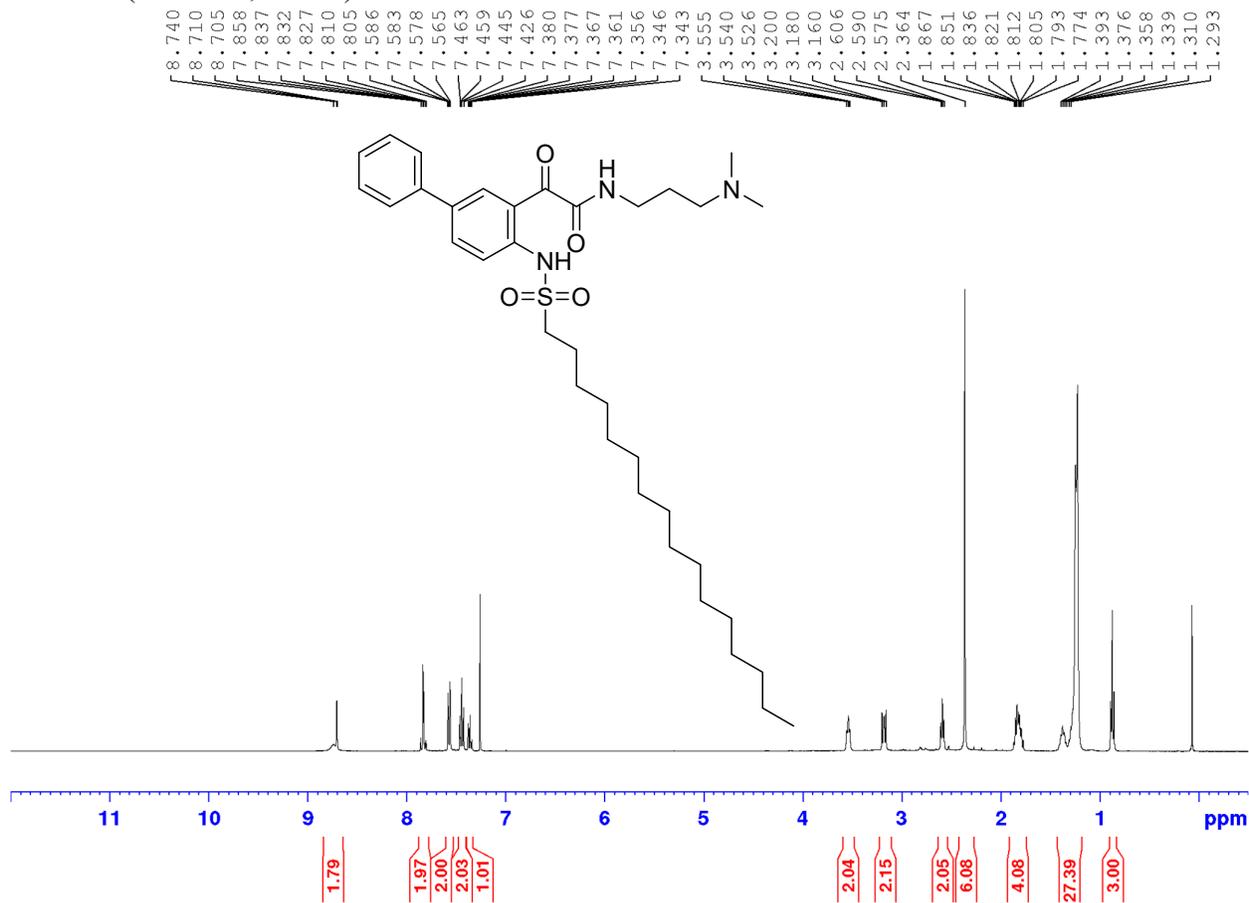


^{13}C NMR (100 MHz, CDCl_3):

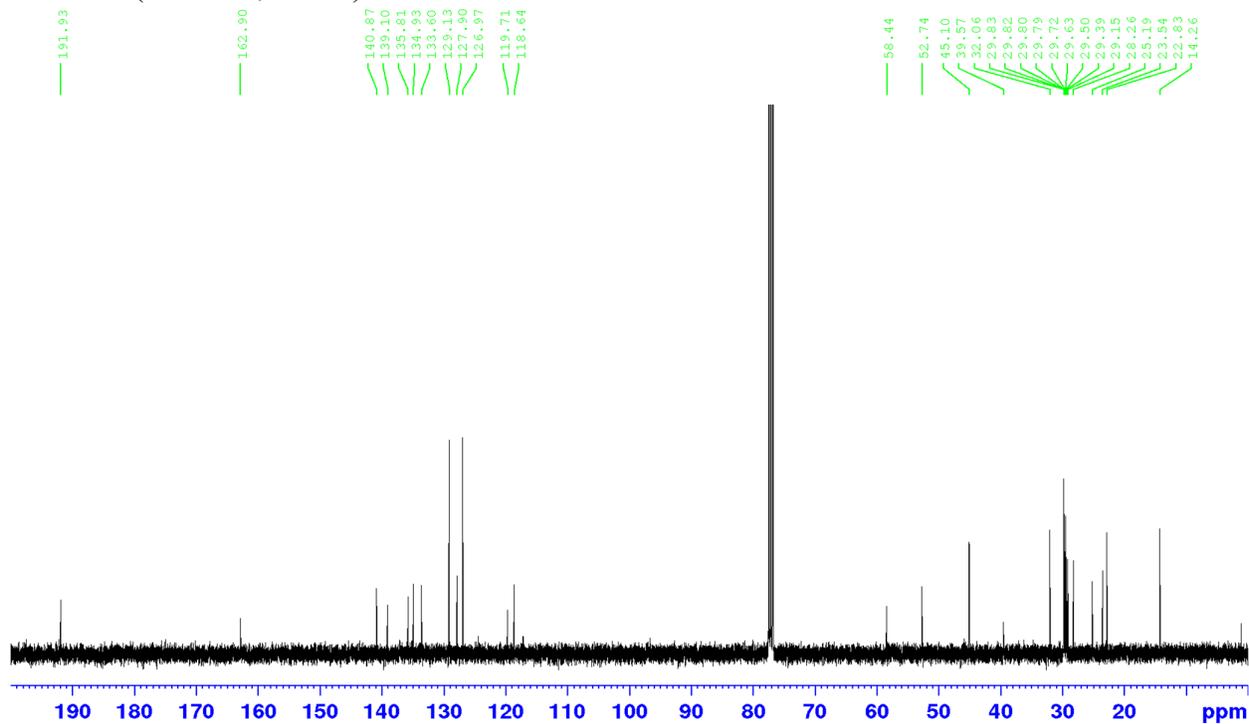


N-(3-(Dimethylamino)propyl)-2-(4-(hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamide
(12c)

¹H NMR (400 MHz, CDCl₃):

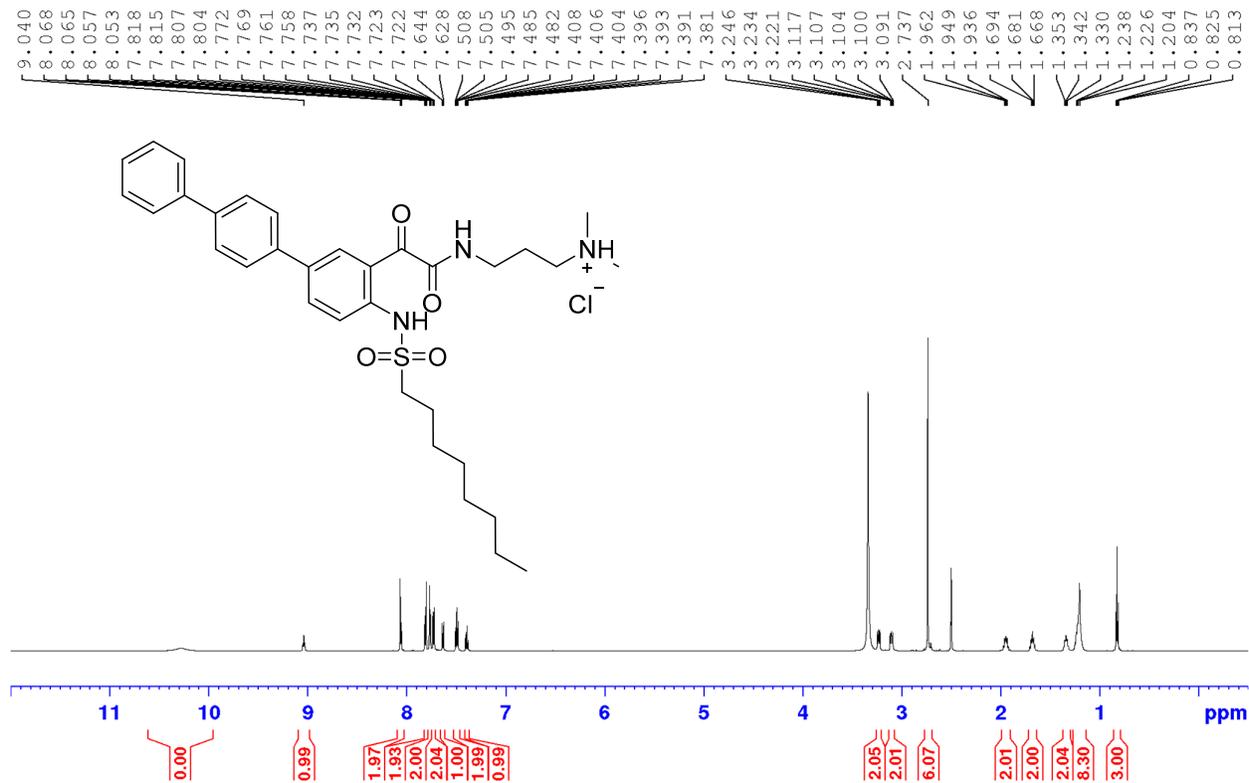


¹³C NMR (100 MHz, CDCl₃):

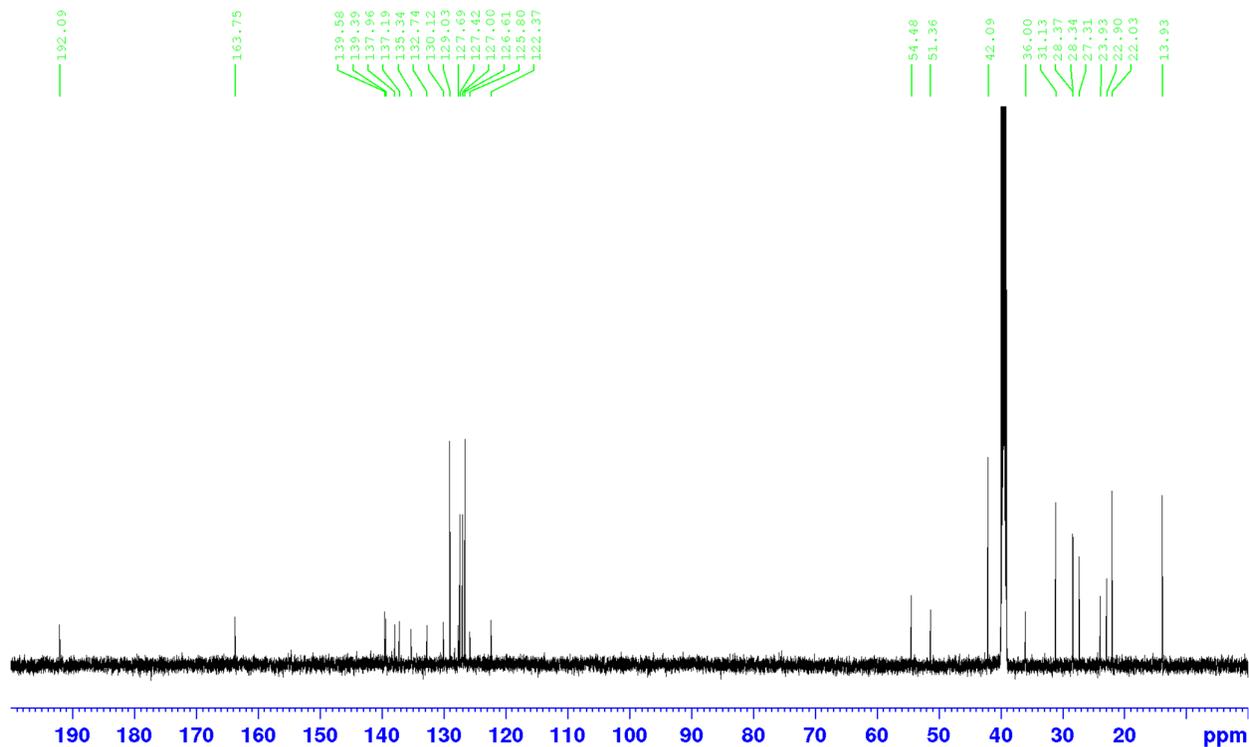


N,N-Dimethyl-3-(2-(4-(octylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamido)propan-1-aminium chloride (**13d**)

¹H NMR (600 MHz, DMSO-*d*₆):



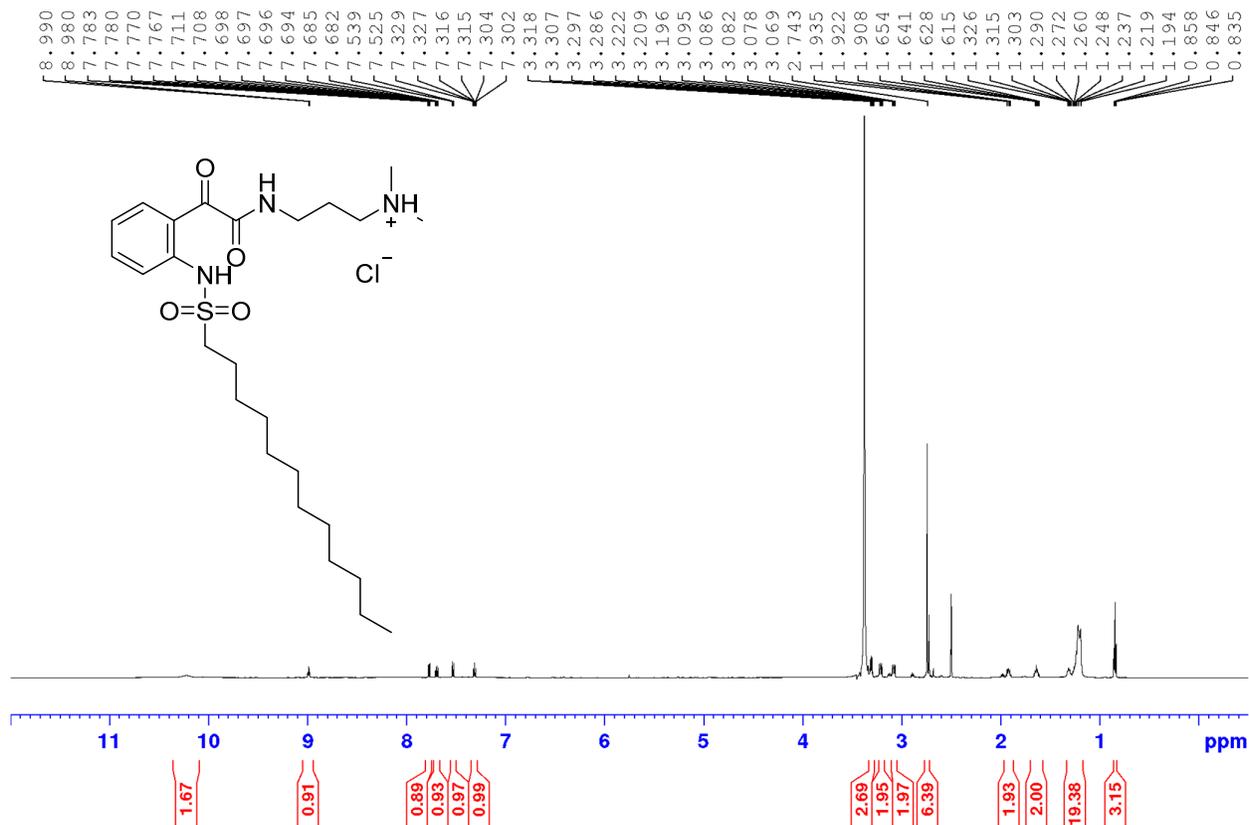
¹³C NMR (150 MHz, DMSO-*d*₆):



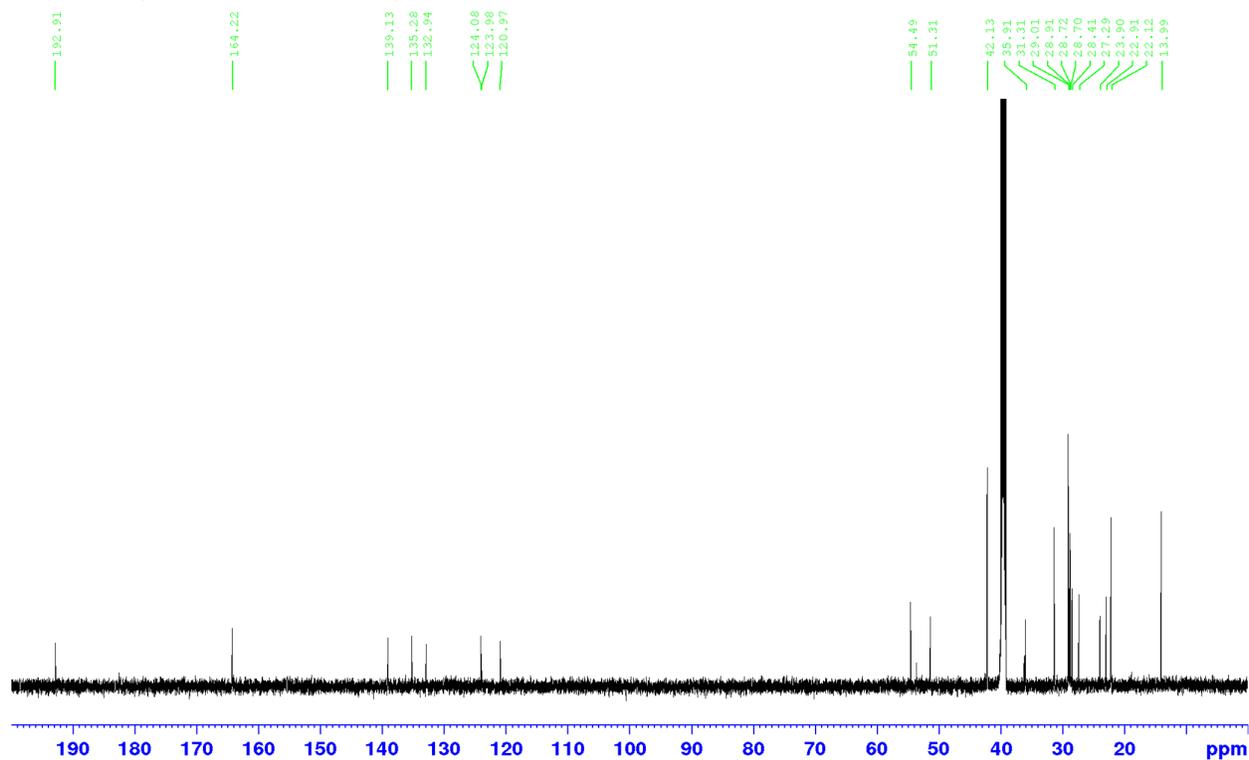
3-(2-(2-(Dodecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride

(14a)

¹H NMR (600 MHz, DMSO-*d*₆):

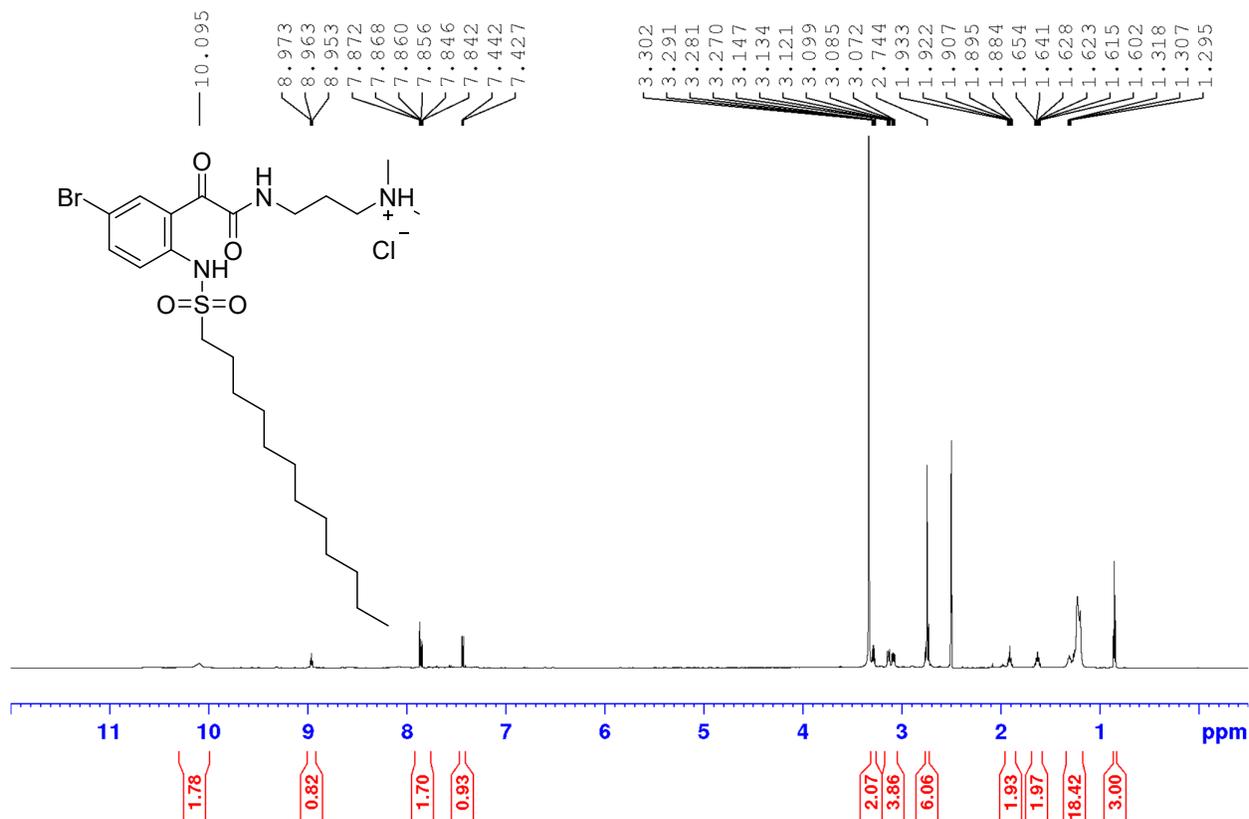


¹³C NMR (150 MHz, DMSO-*d*₆):

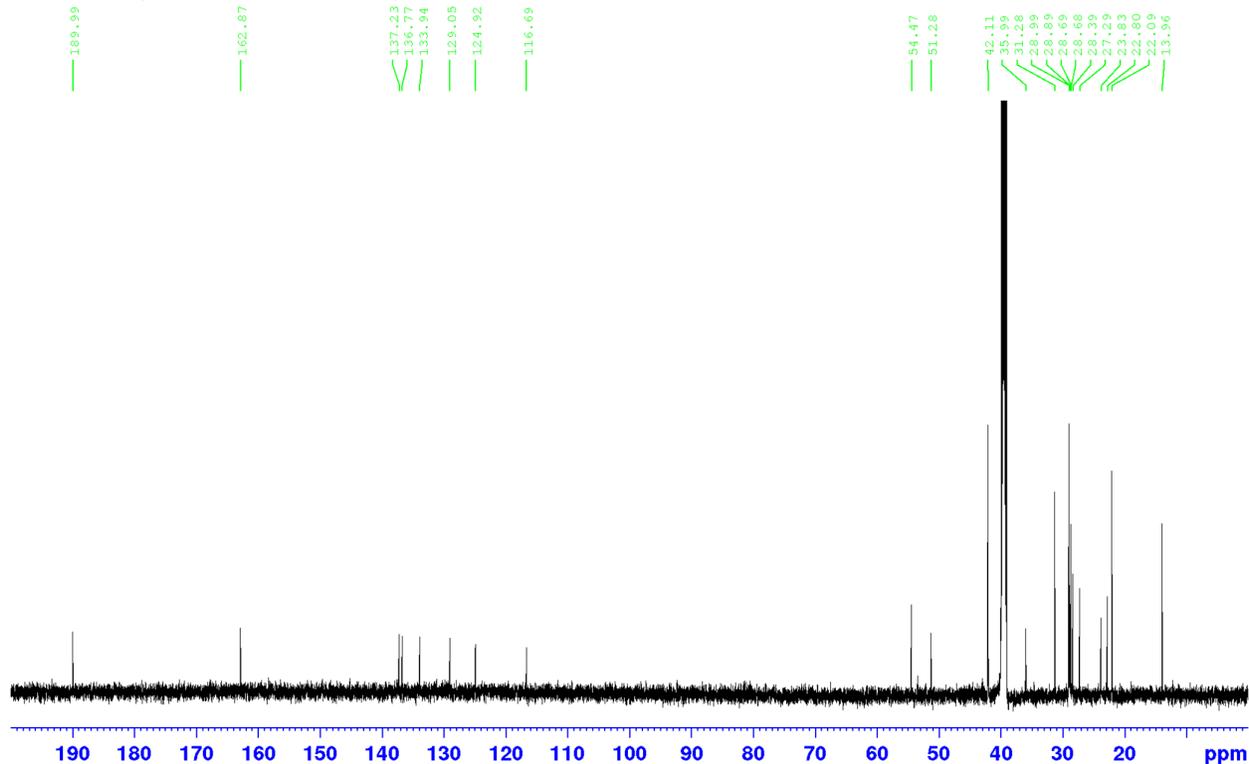


3-(2-(5-Bromo-2-(dodecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride (**14b**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

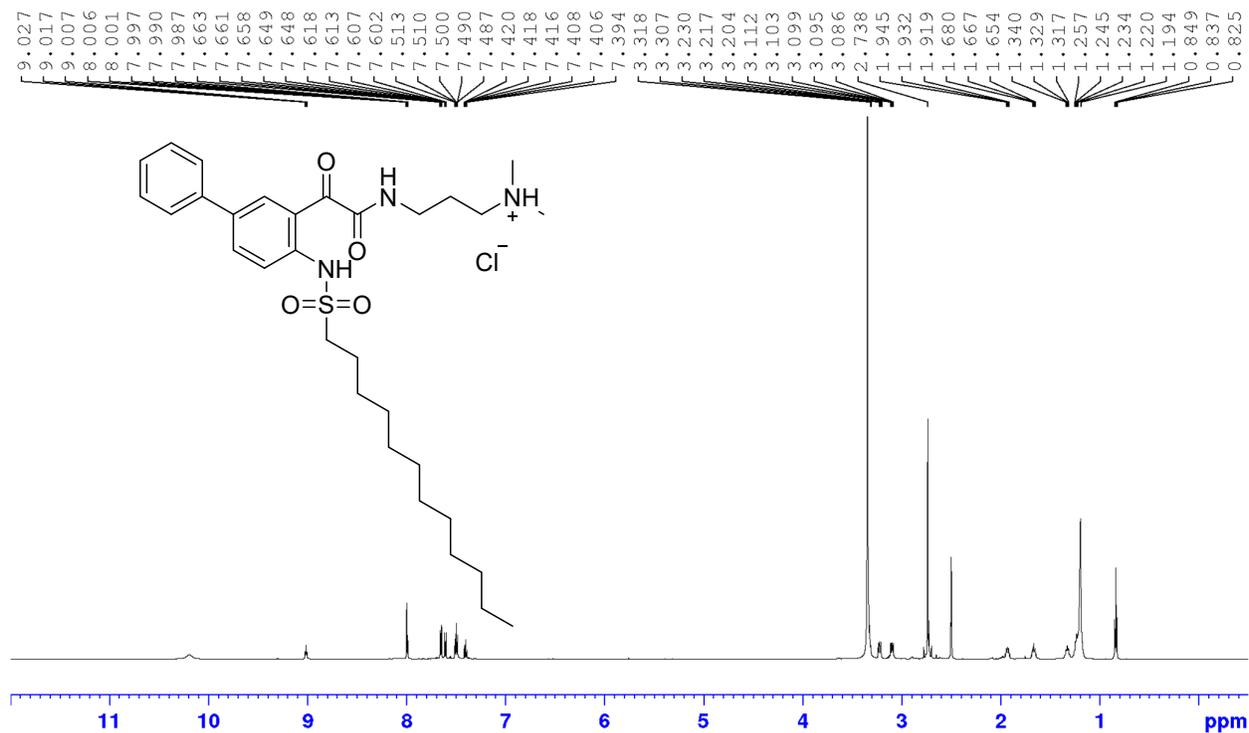


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

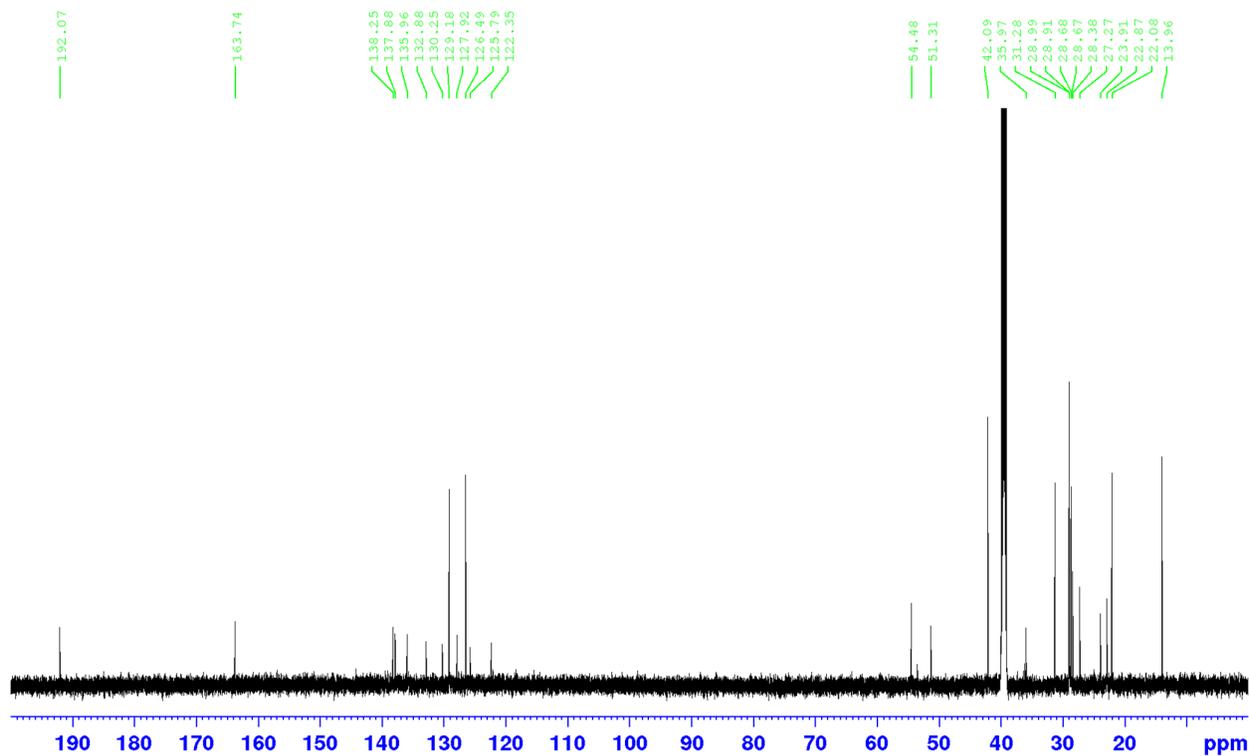


3-(2-(4-(Dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride (**14c**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

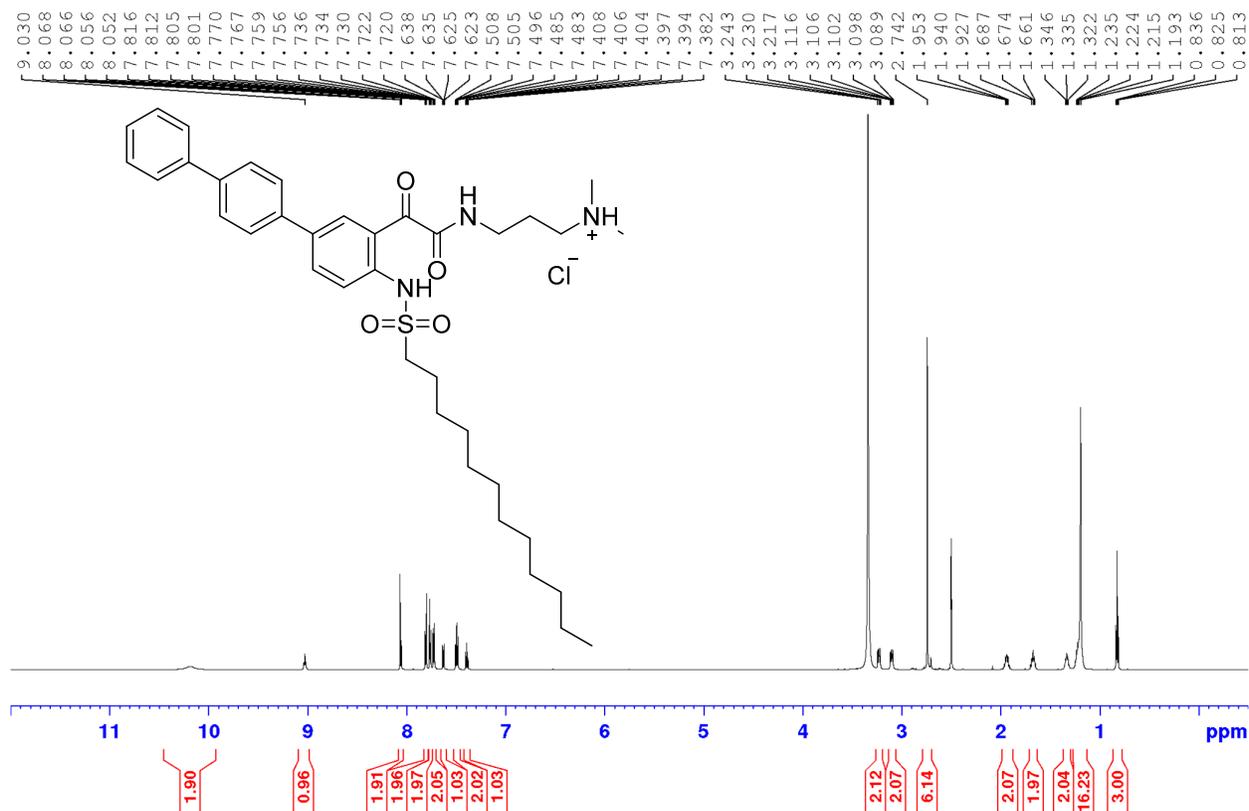


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

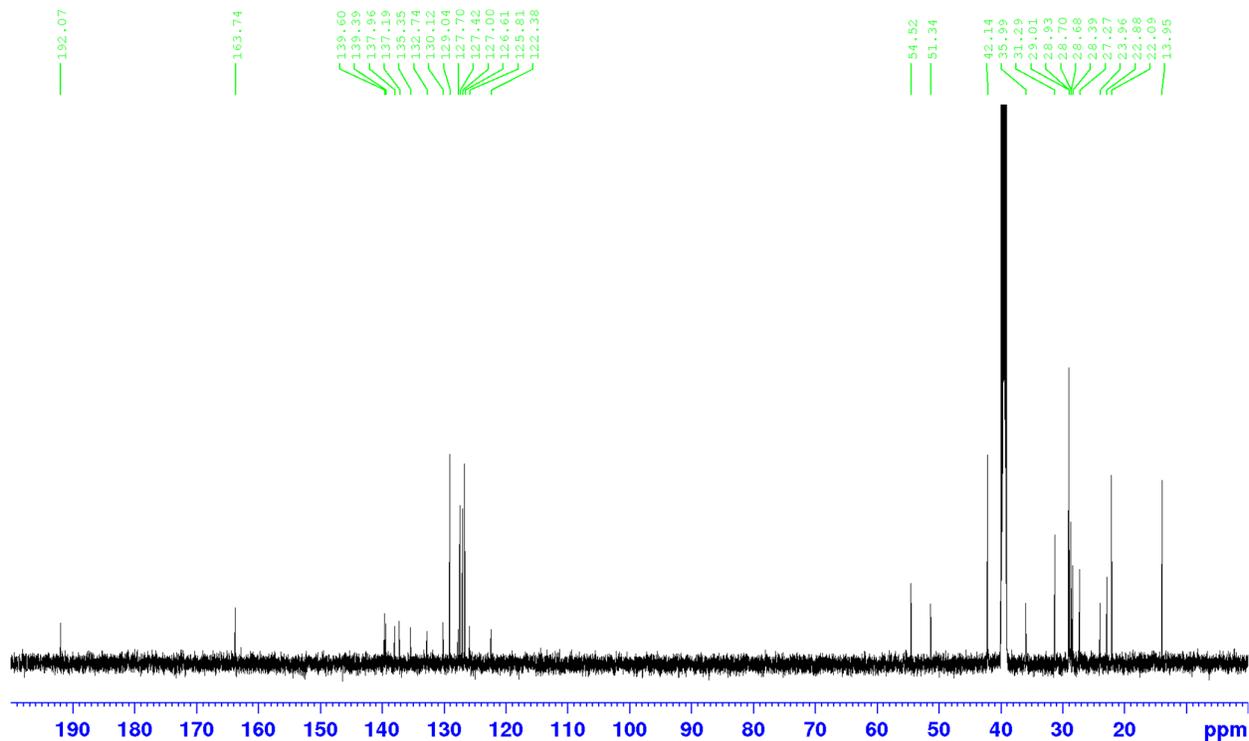


3-(2-(4-(Dodecylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride (**14d**)

¹H NMR (600 MHz, DMSO-*d*₆):

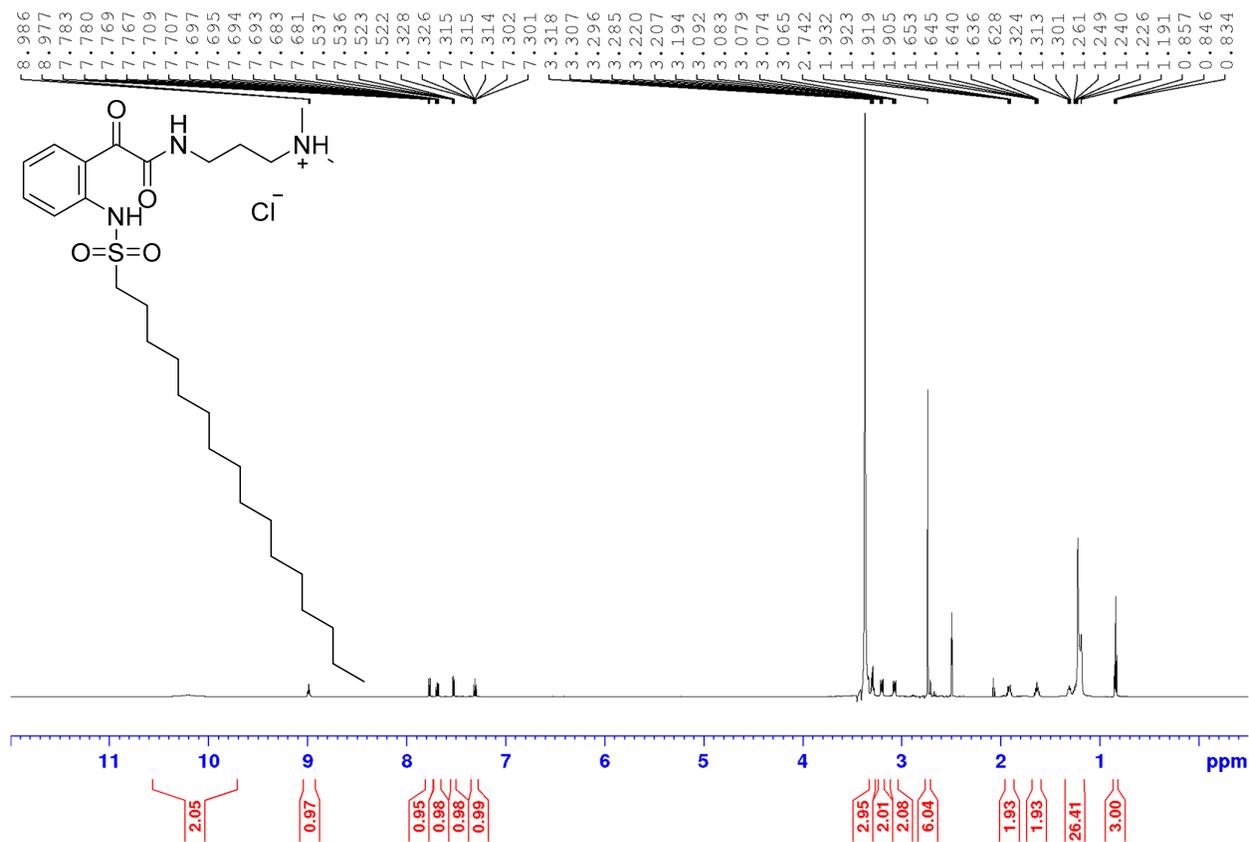


¹³C NMR (150 MHz, DMSO-*d*₆):

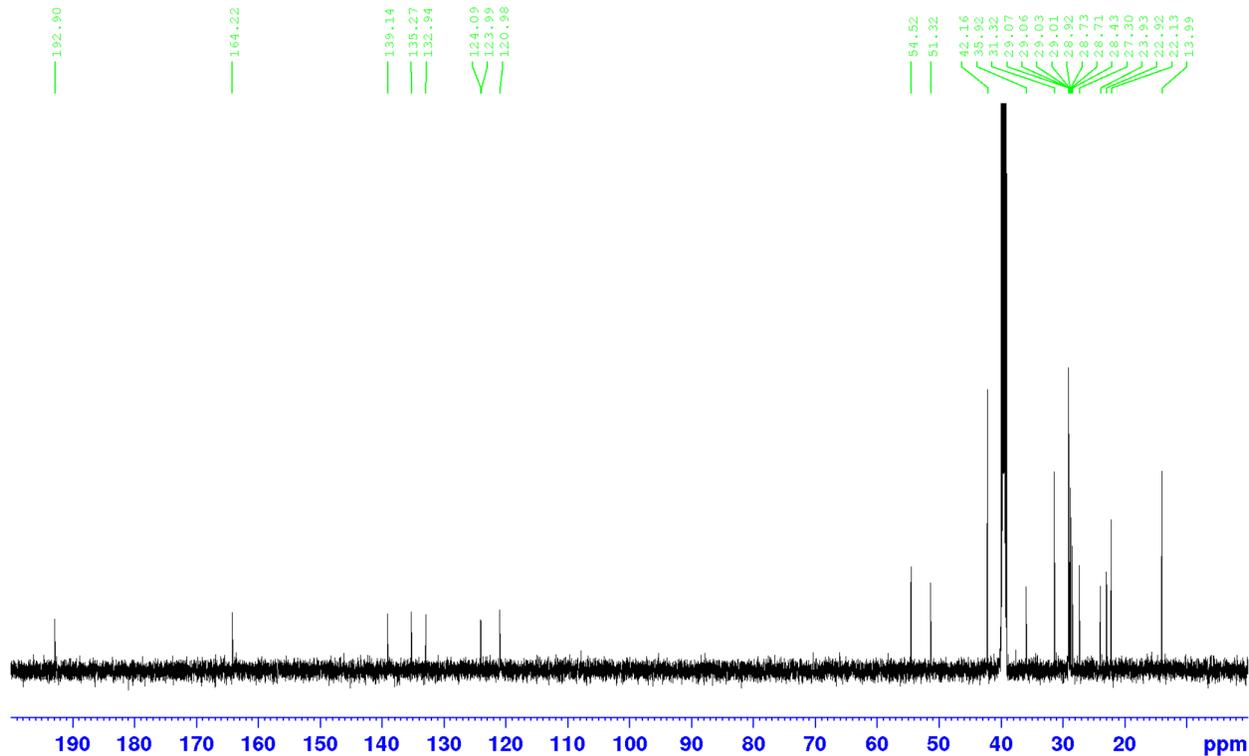


3-(2-(2-(Hexadecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride
(15a)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

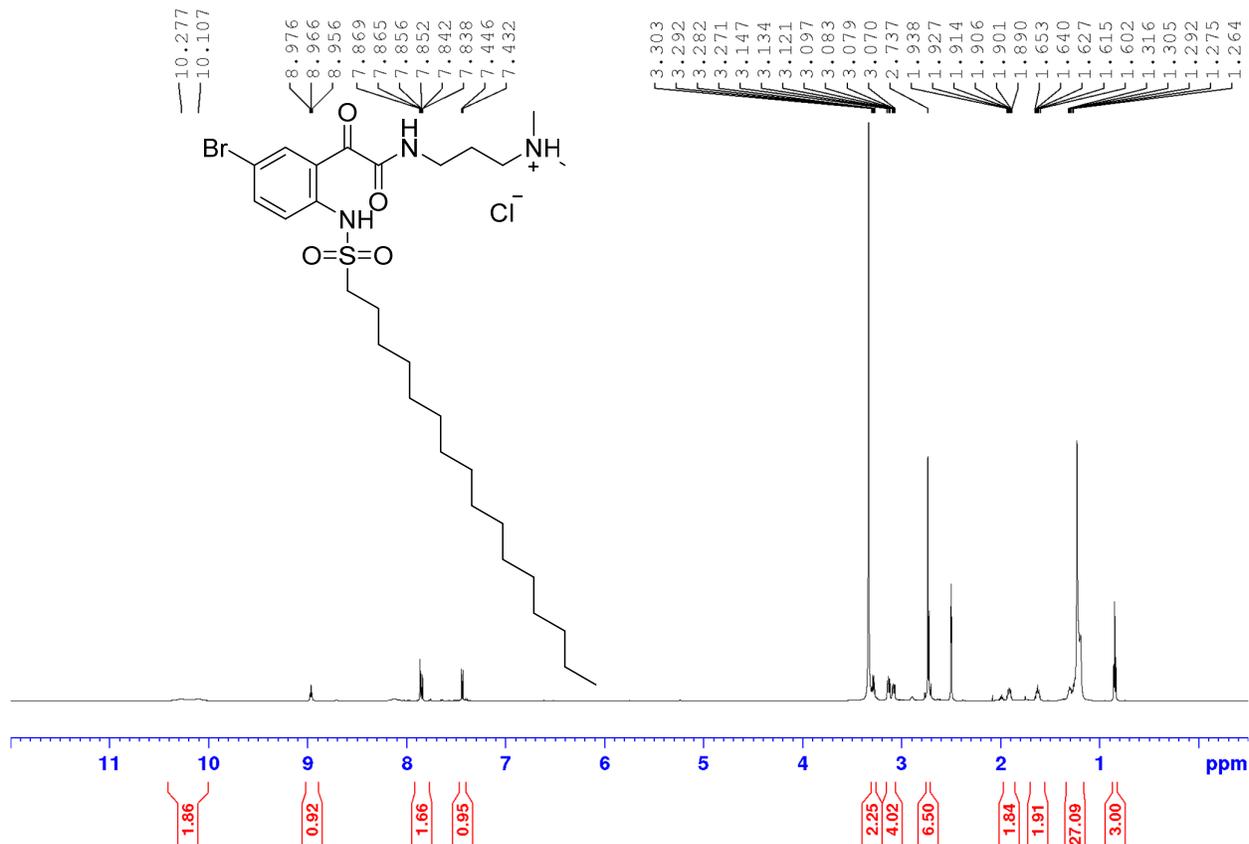


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

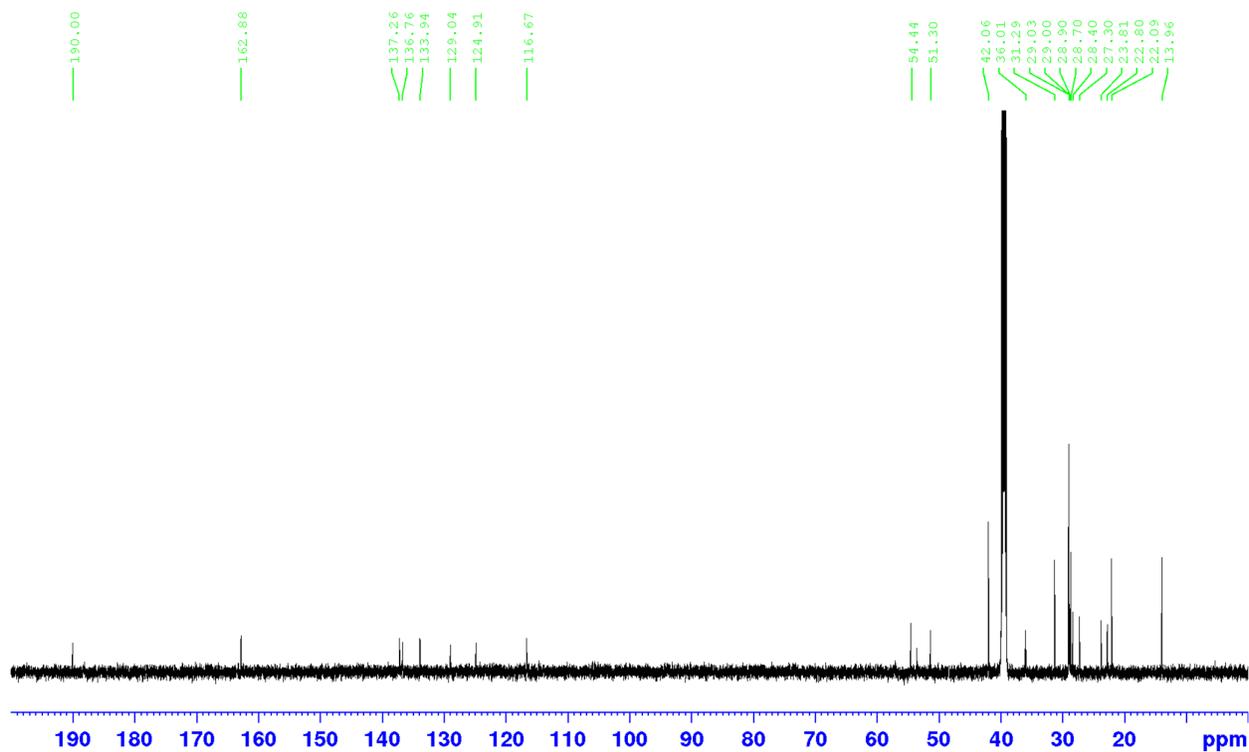


3-(2-(5-Bromo-2-(hexadecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride (**15b**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

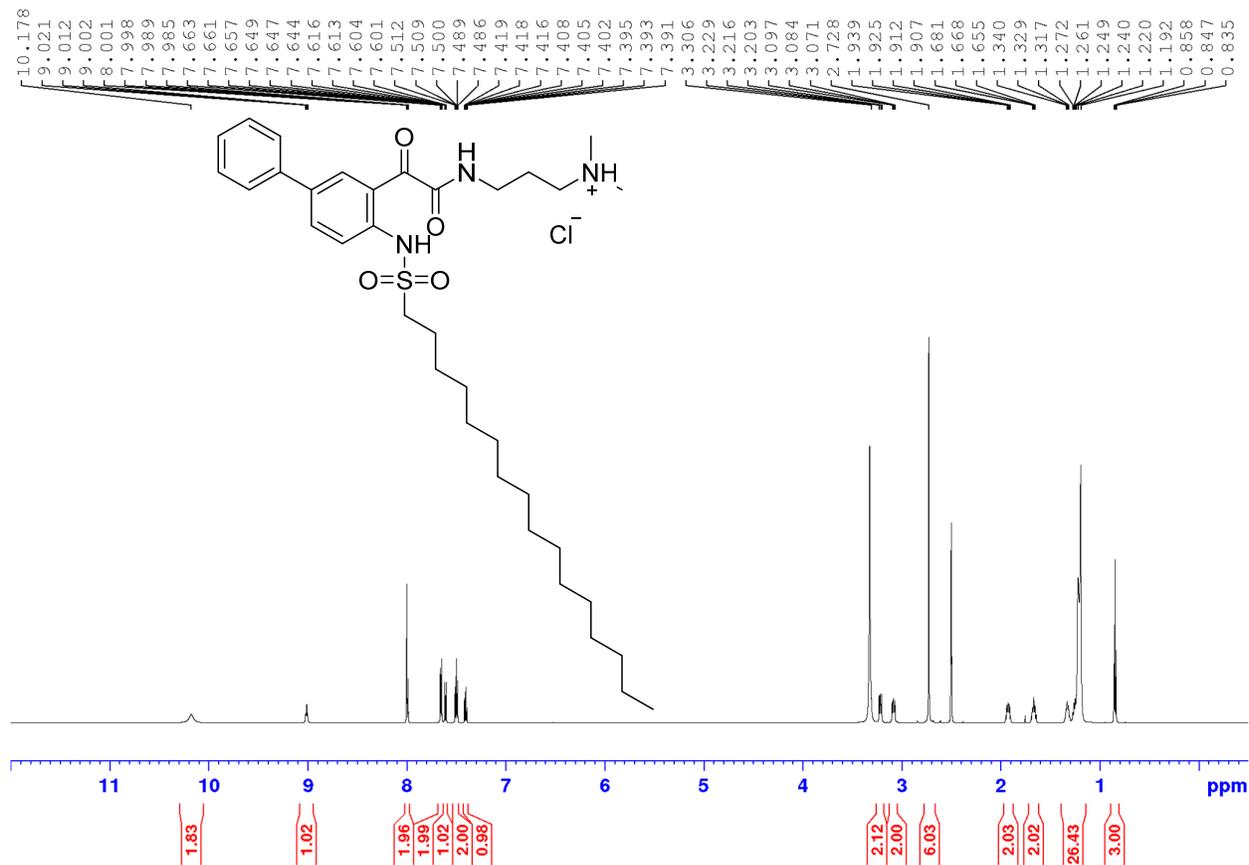


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

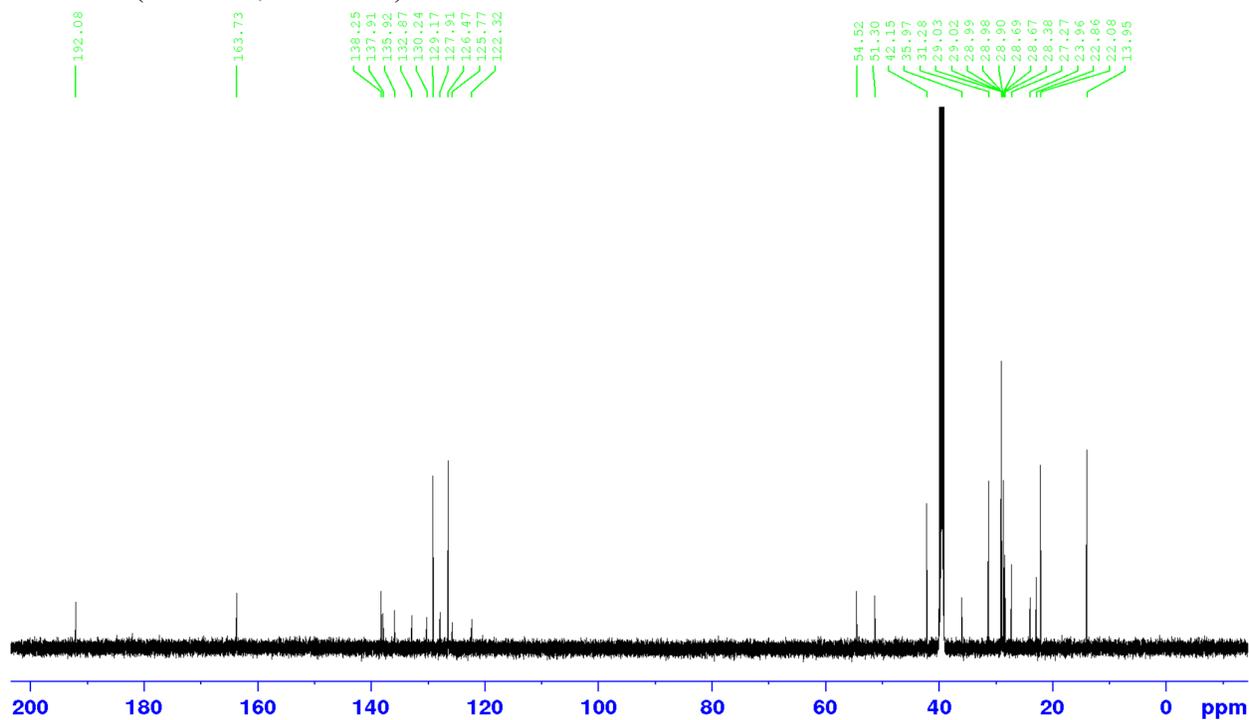


3-(2-(4-(Hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)-*N,N*-dimethylpropan-1-aminium chloride (**15c**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

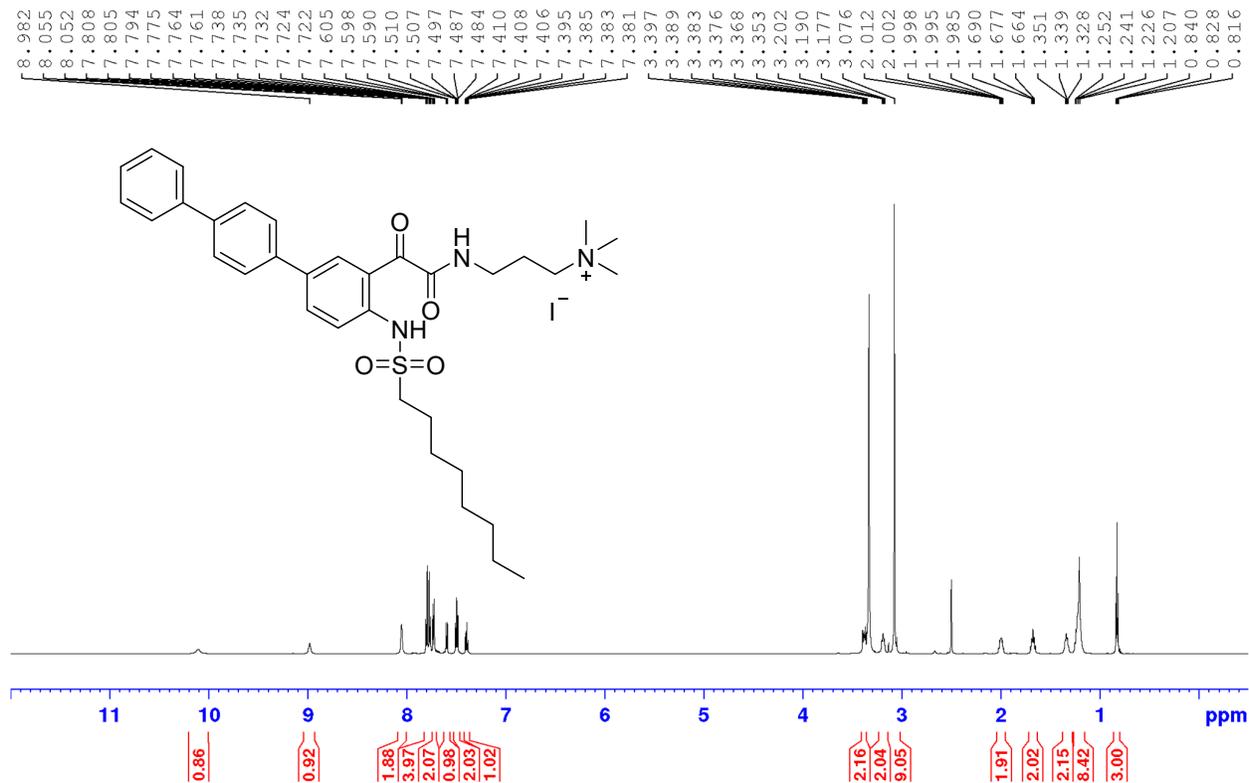


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

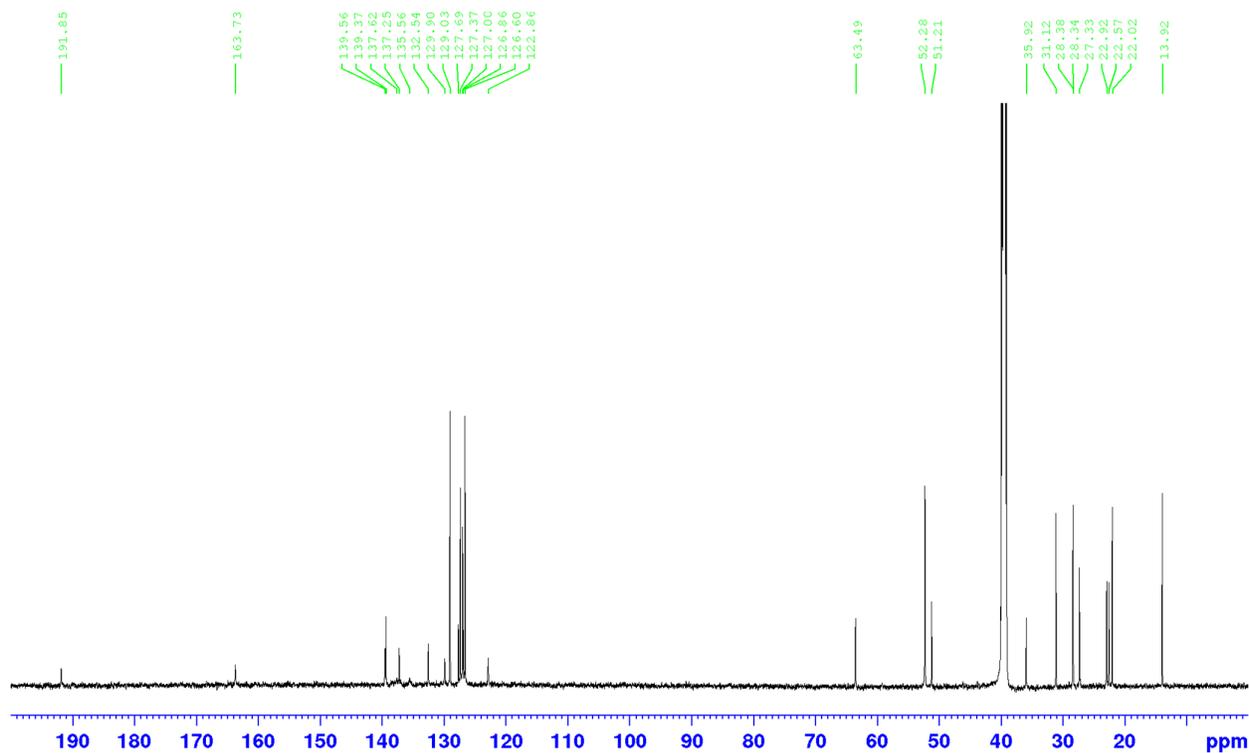


N,N,N-Trimethyl-3-(2-(4-(octylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamido)propan-1-aminium iodide (**16d**)

¹H NMR (600 MHz, DMSO-*d*₆):

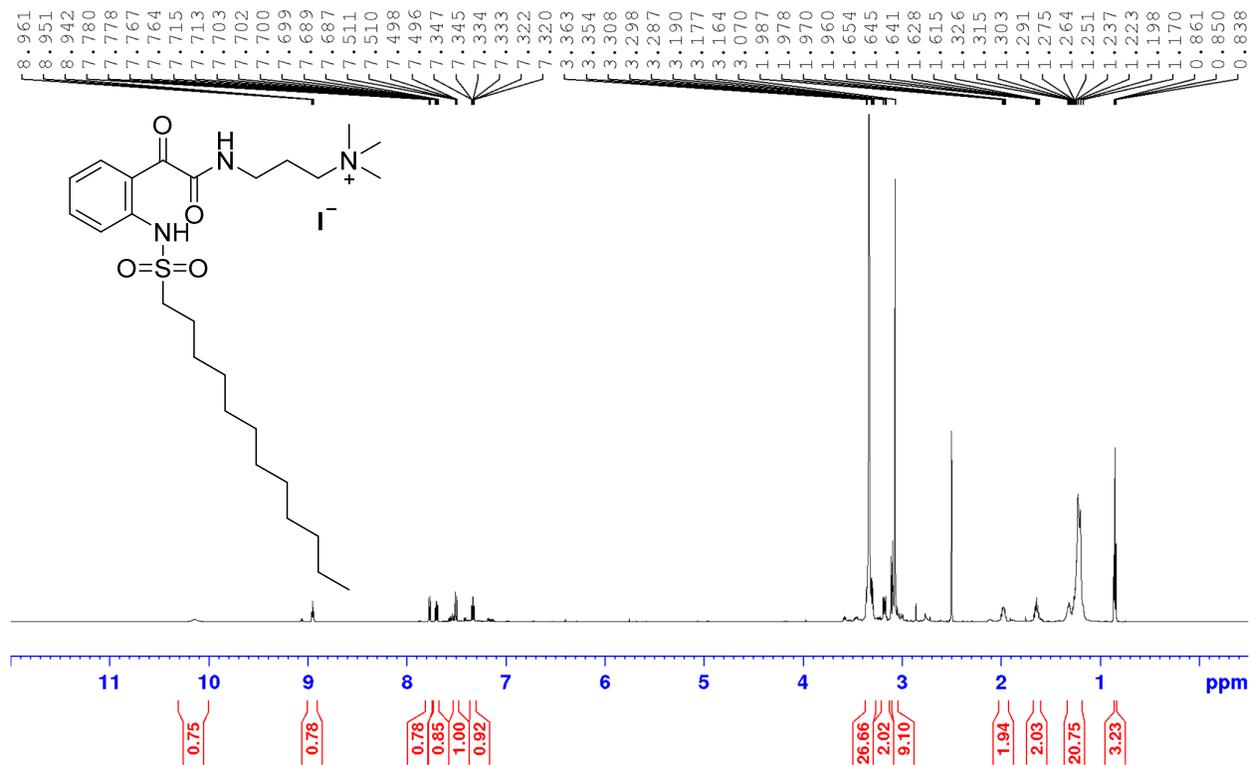


¹³C NMR (150 MHz, DMSO-*d*₆):

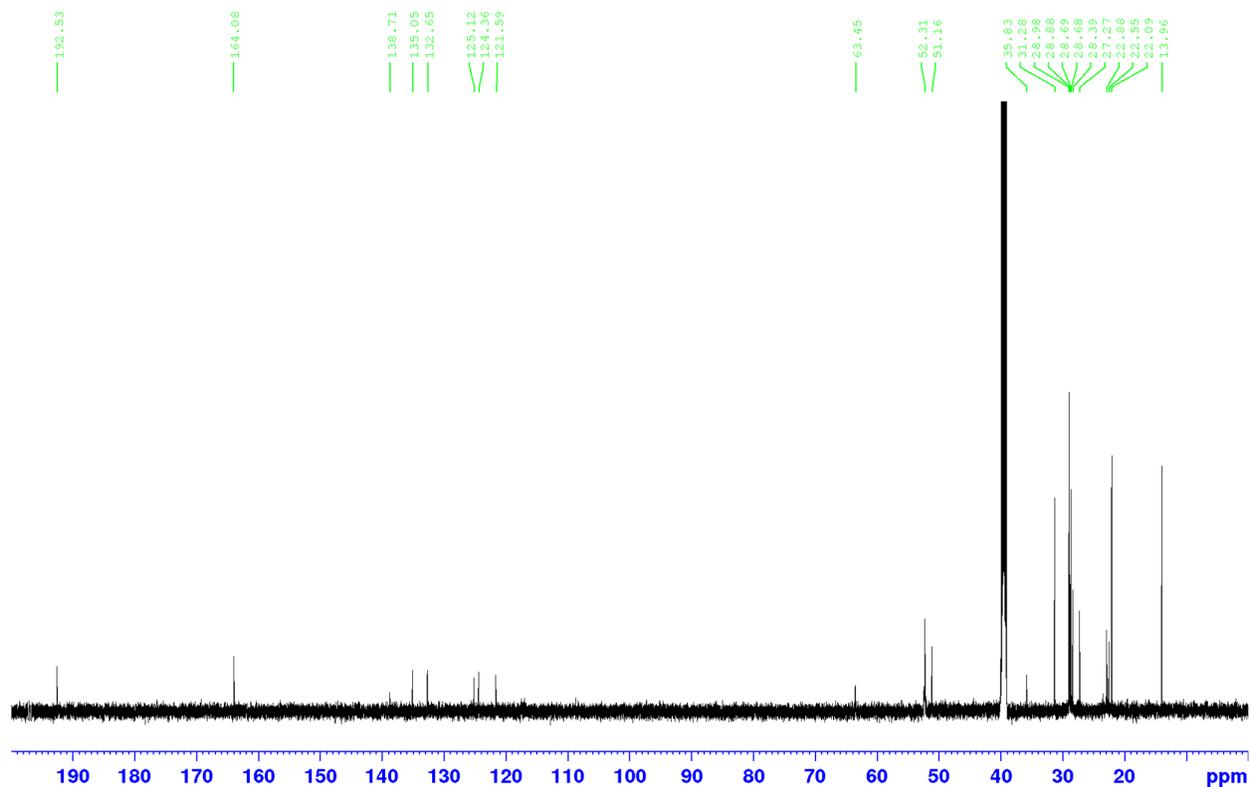


3-(2-(2-(Dodecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide
(17a)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

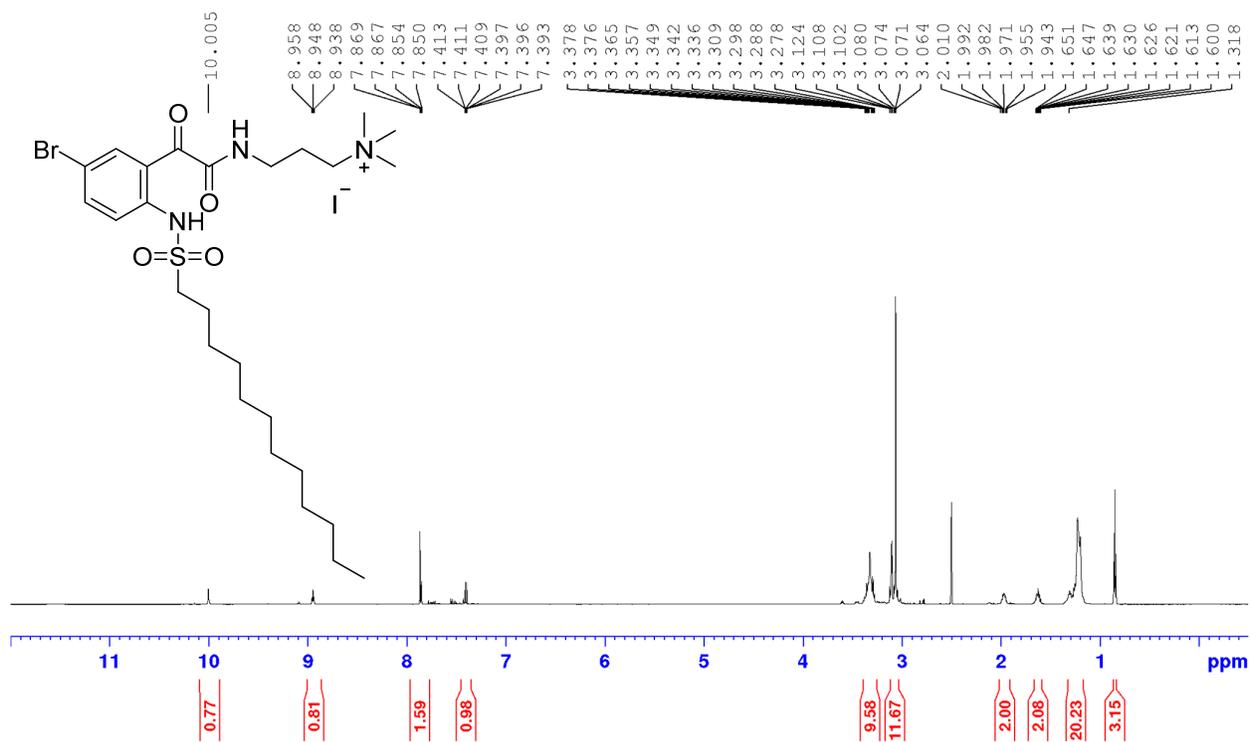


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

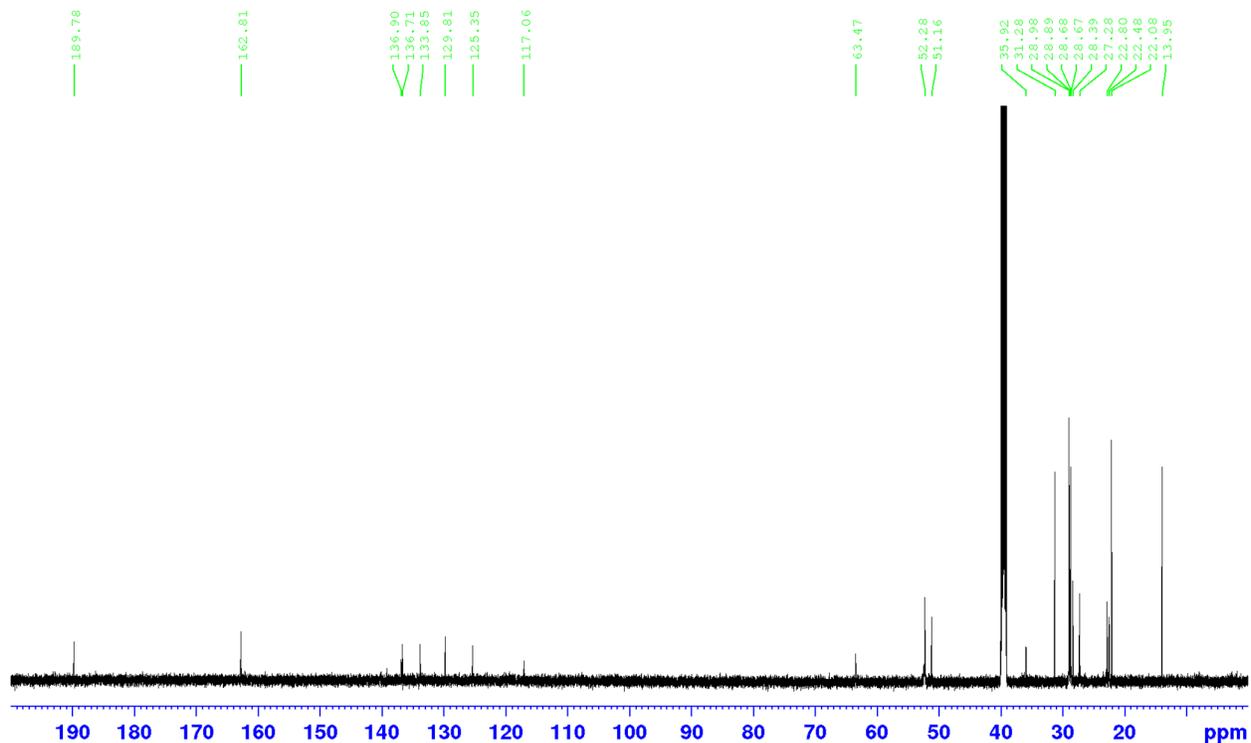


3-(2-(5-Bromo-2-(dodecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide (**17b**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

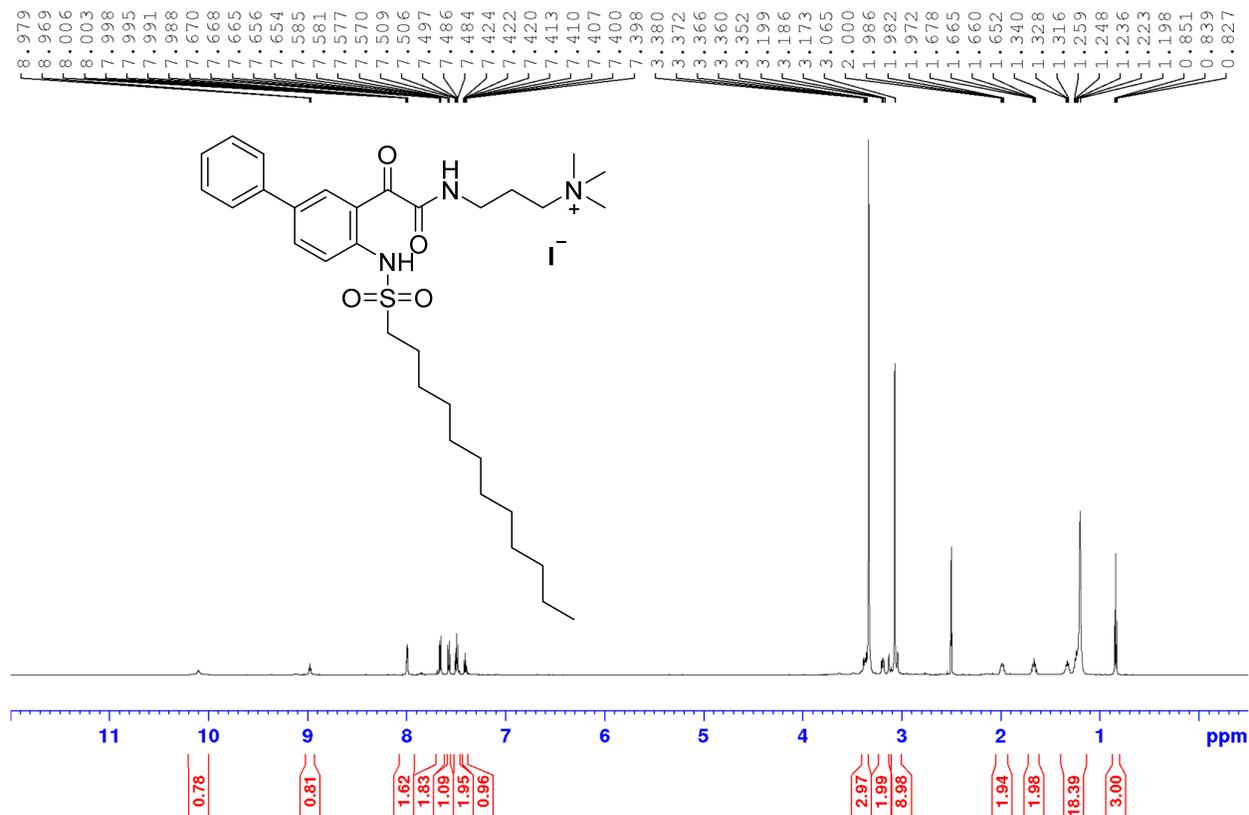


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

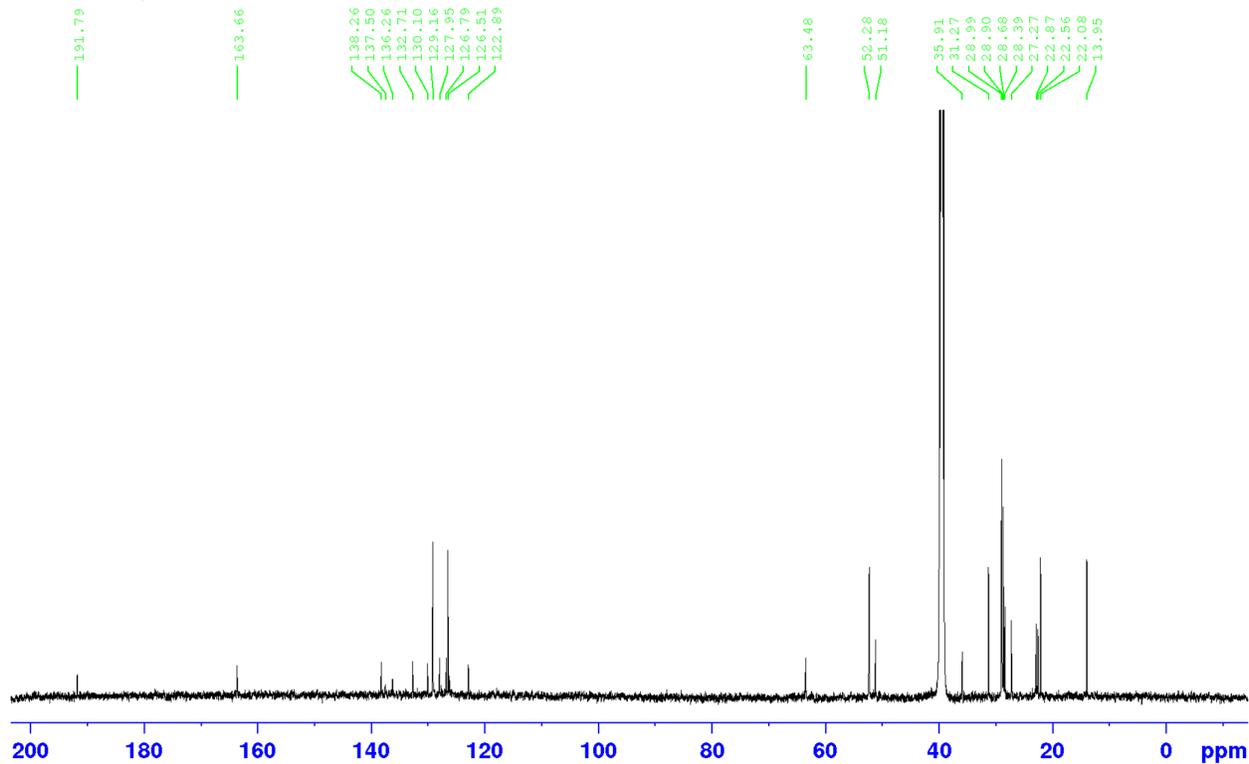


3-(2-(4-(Dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide (**17c**)

¹H NMR (600 MHz, DMSO-*d*₆):

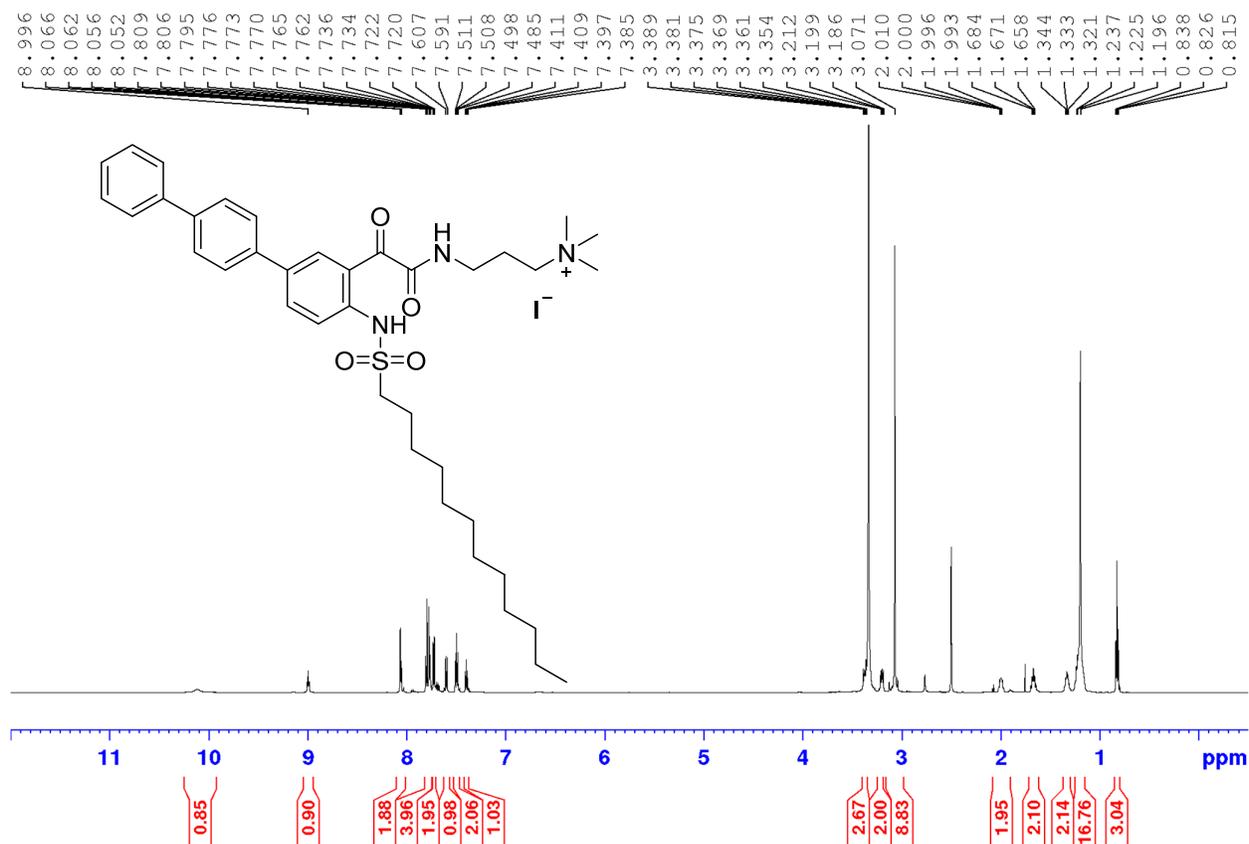


¹³C NMR (150 MHz, DMSO-*d*₆):

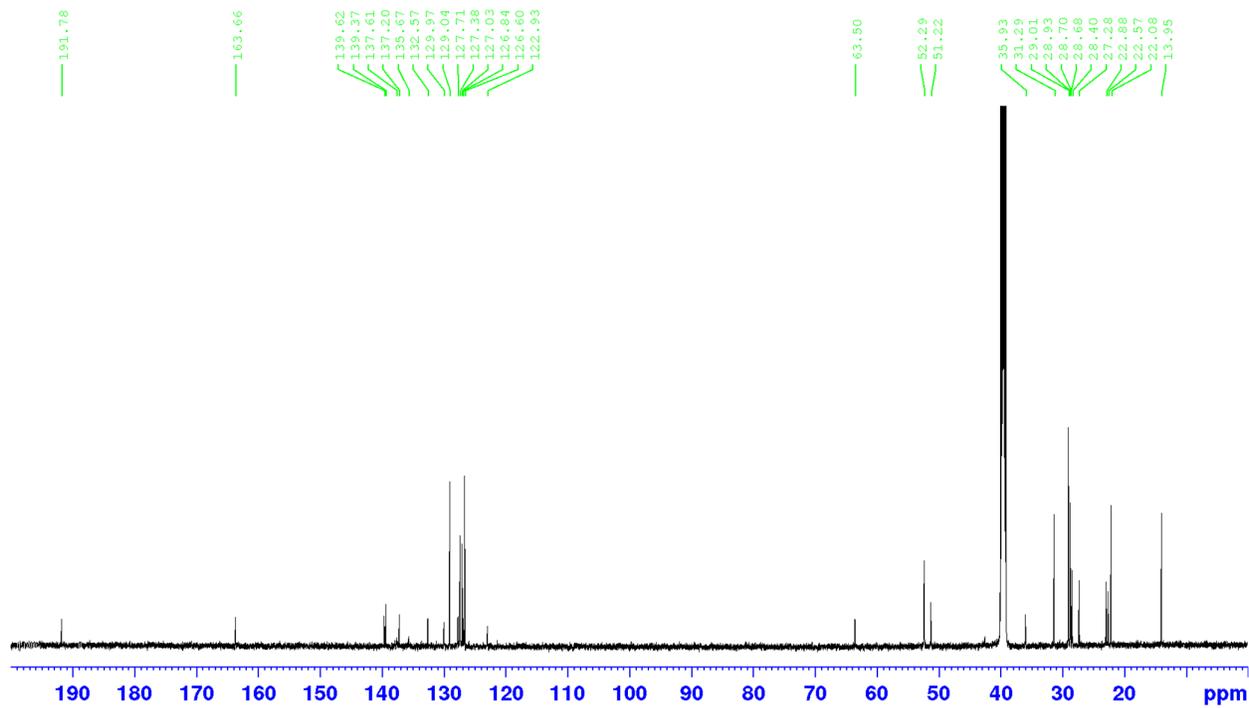


3-(2-(4-(Dodecylsulfonamido)-[1,1':4,1''-terphenyl]-3-yl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide (**17d**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

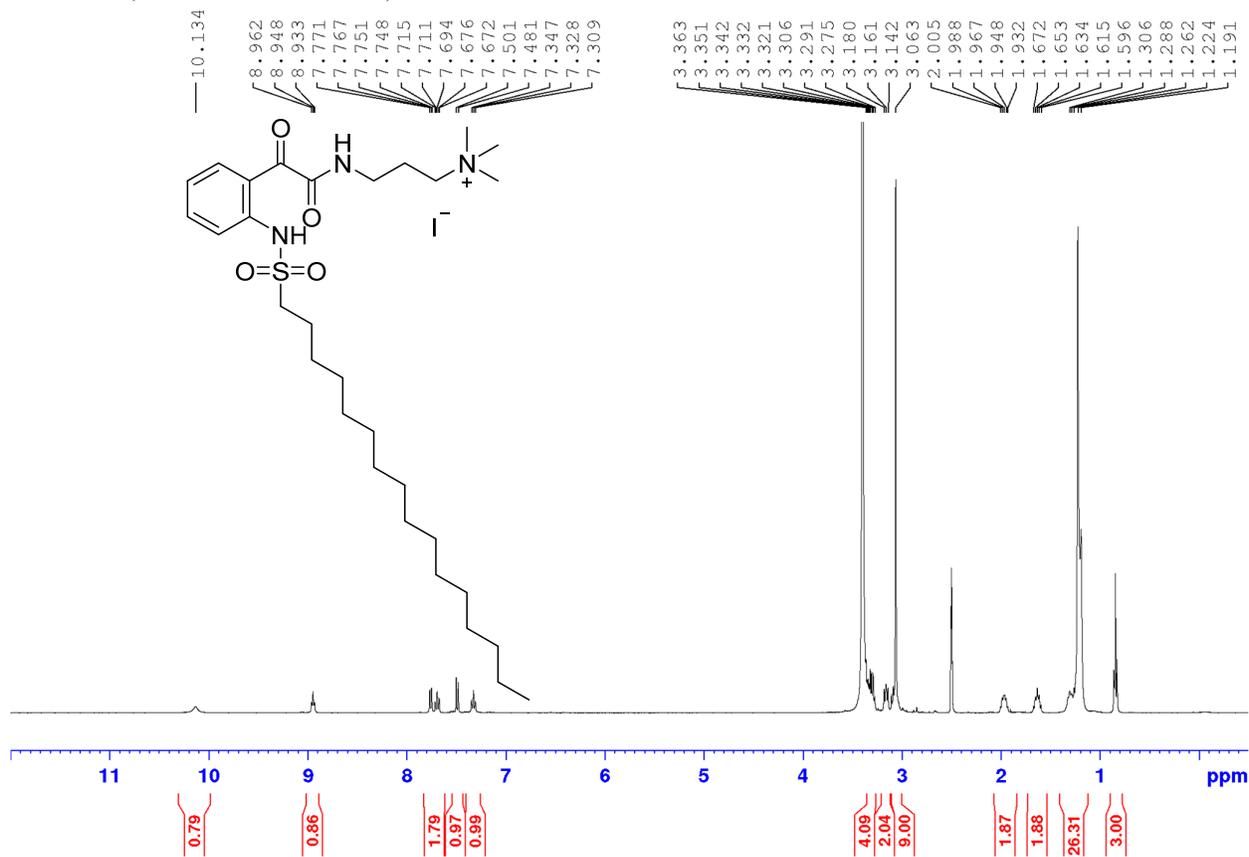


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

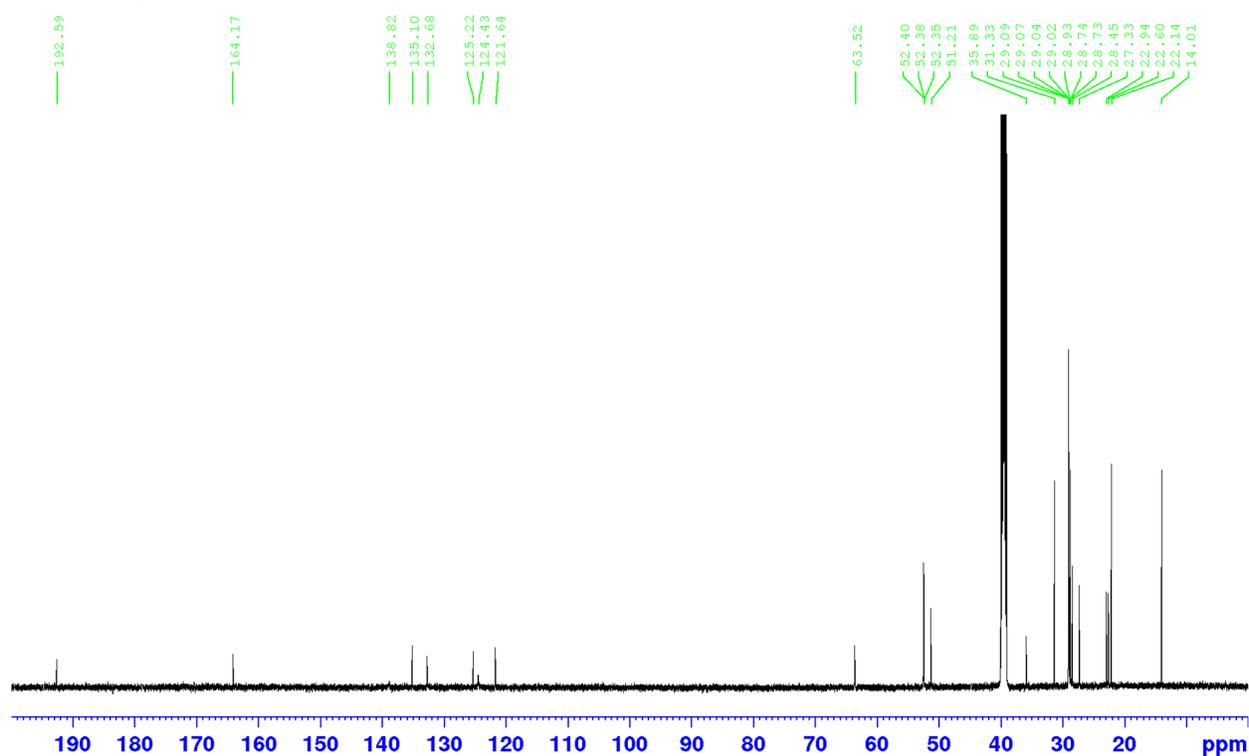


3-(2-(2-(Hexadecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide
(18a)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

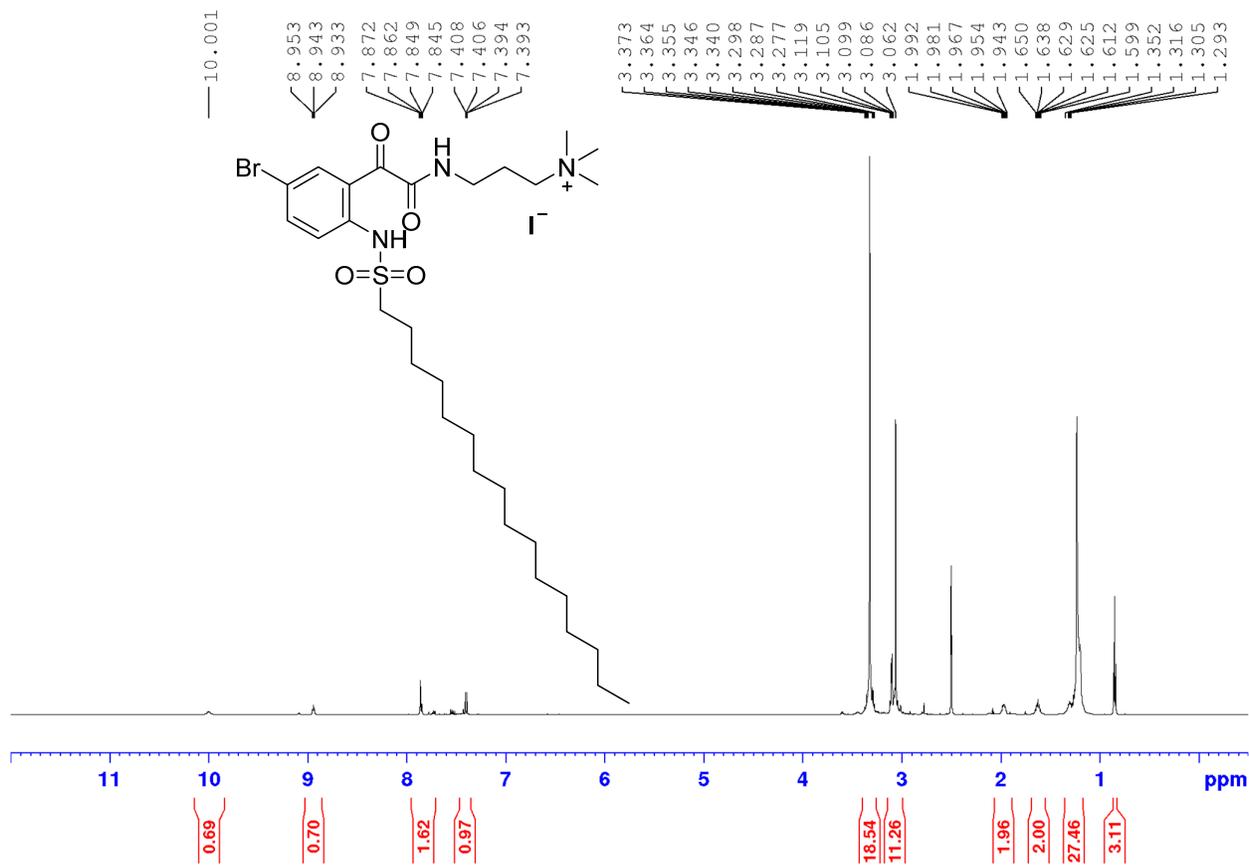


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

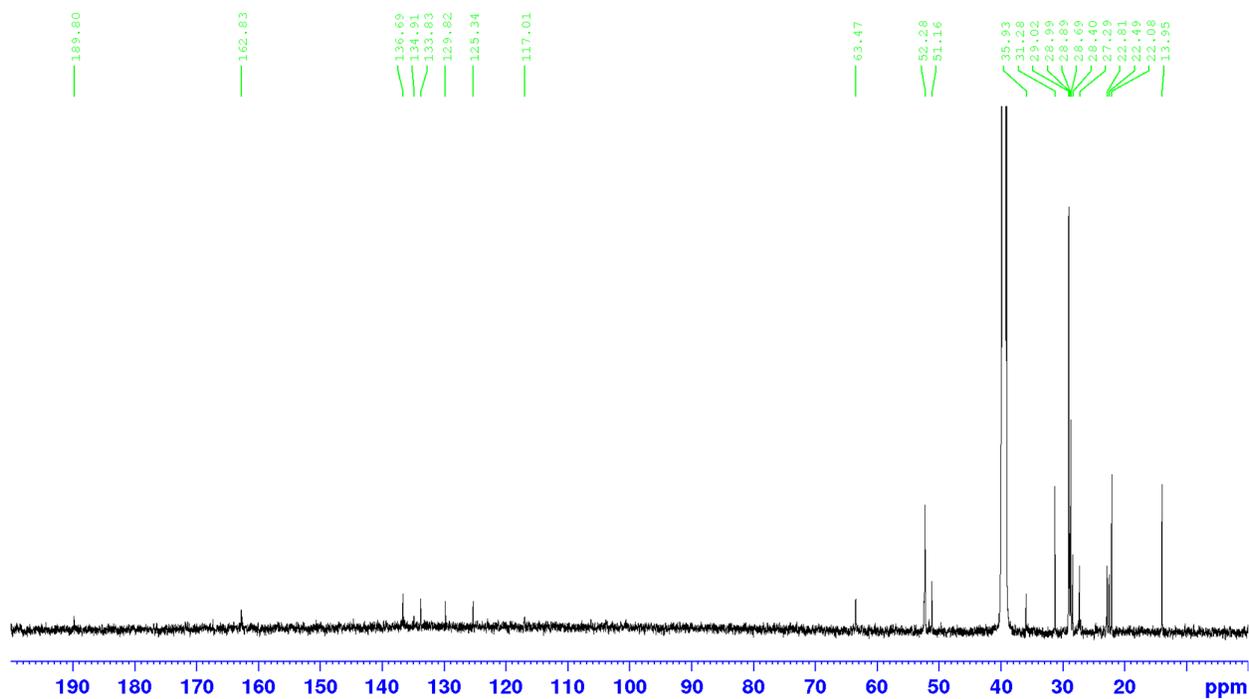


3-(2-(5-Bromo-2-(hexadecylsulfonamido)phenyl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide (**18b**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

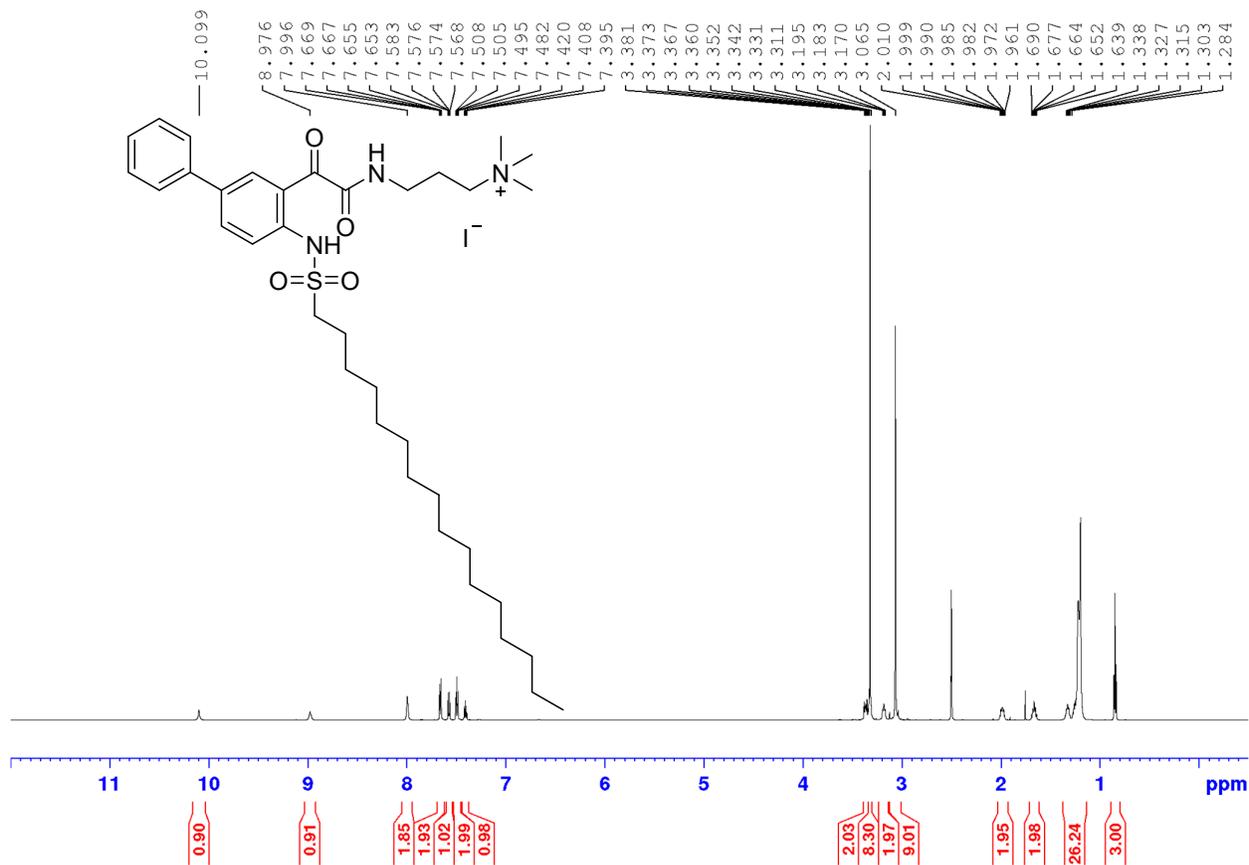


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

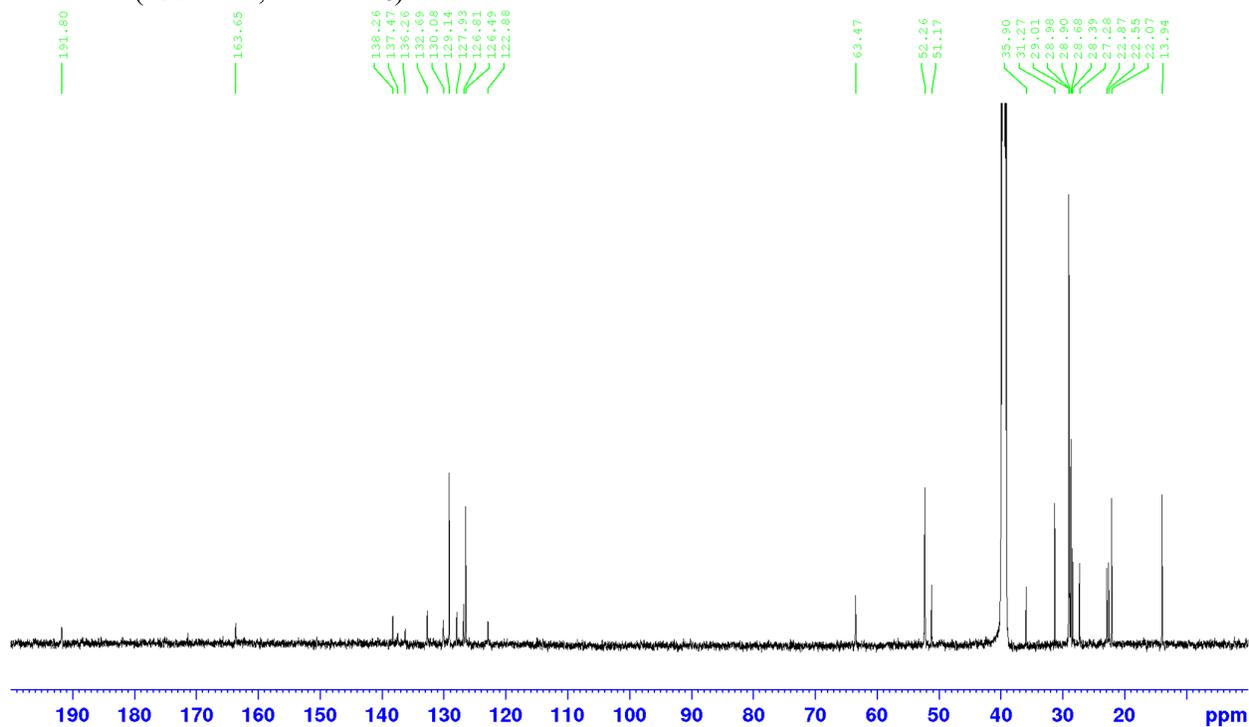


3-(2-(4-(Hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)-*N,N,N*-trimethylpropan-1-aminium iodide (**18c**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

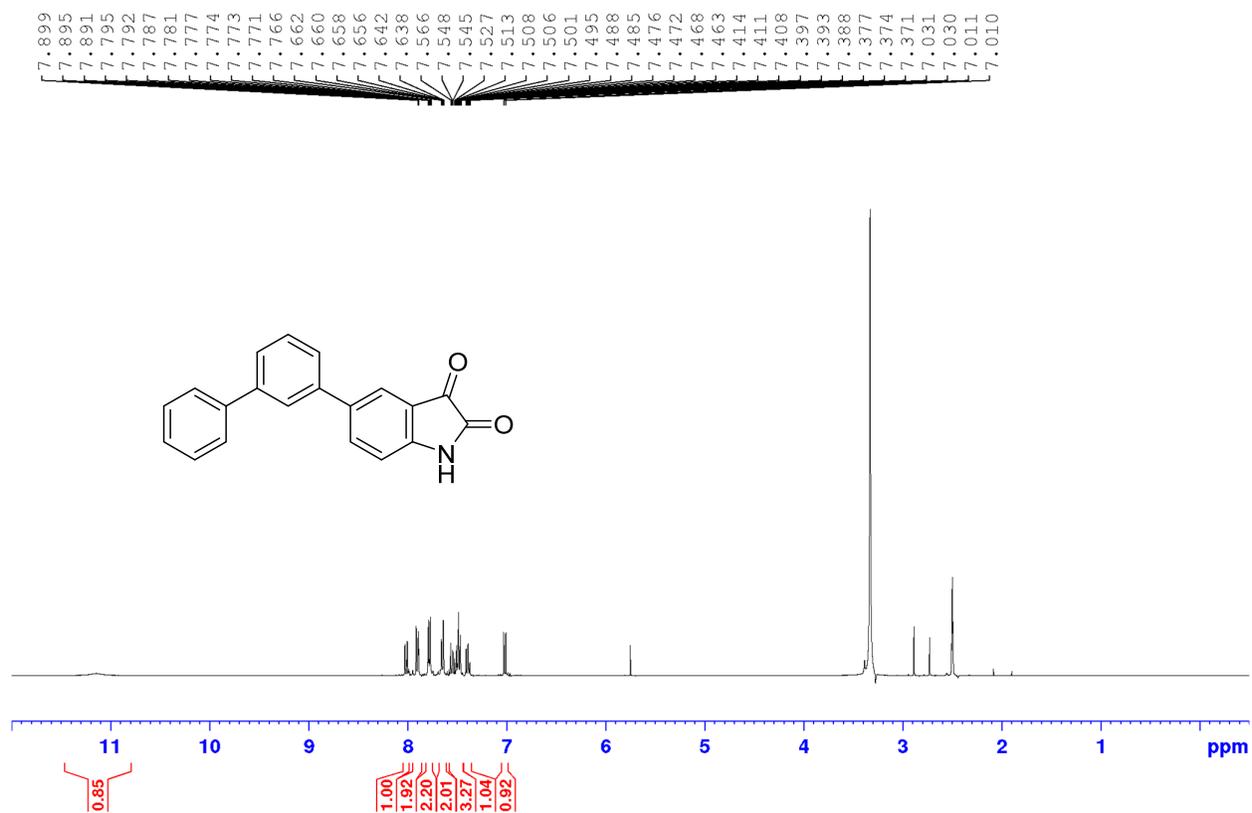


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):



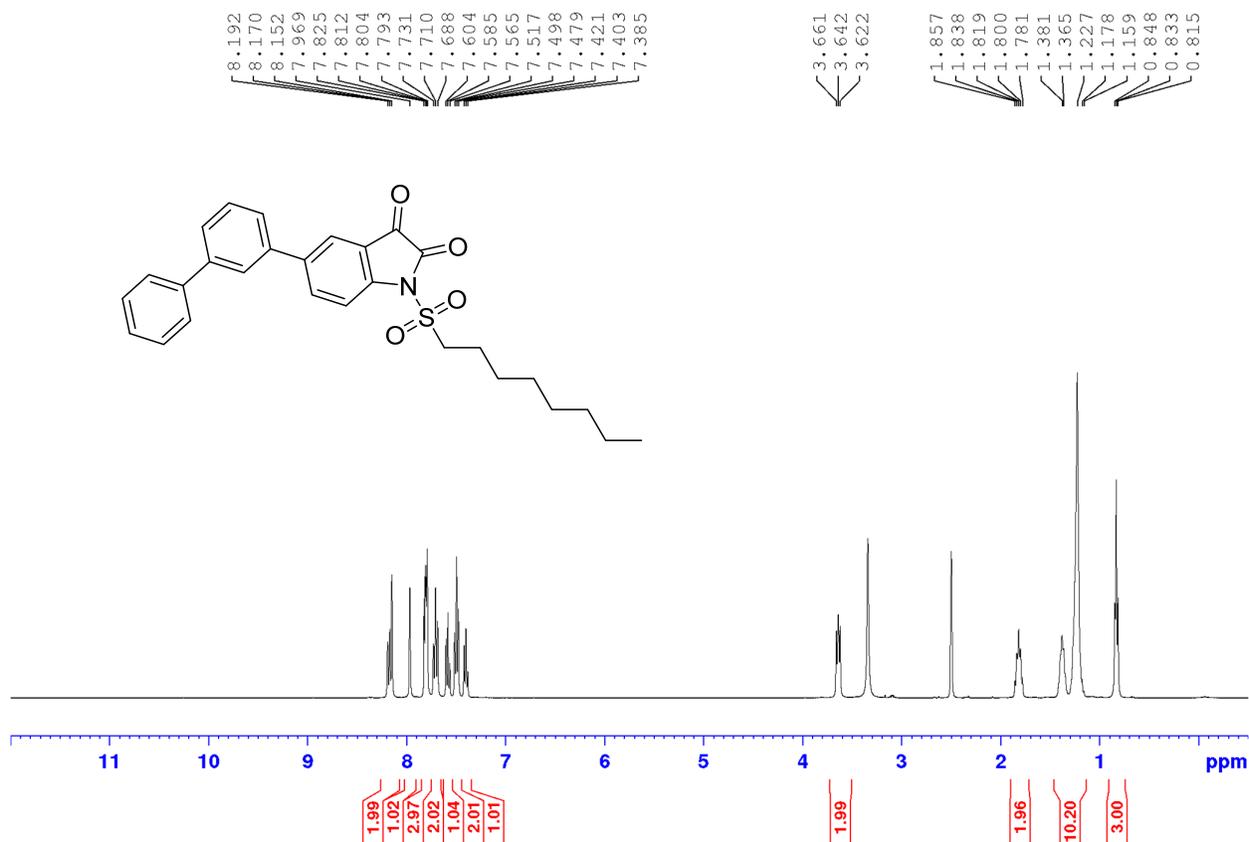
5-([1,1'-Biphenyl]-3-yl)indoline-2,3-dione (**19**)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

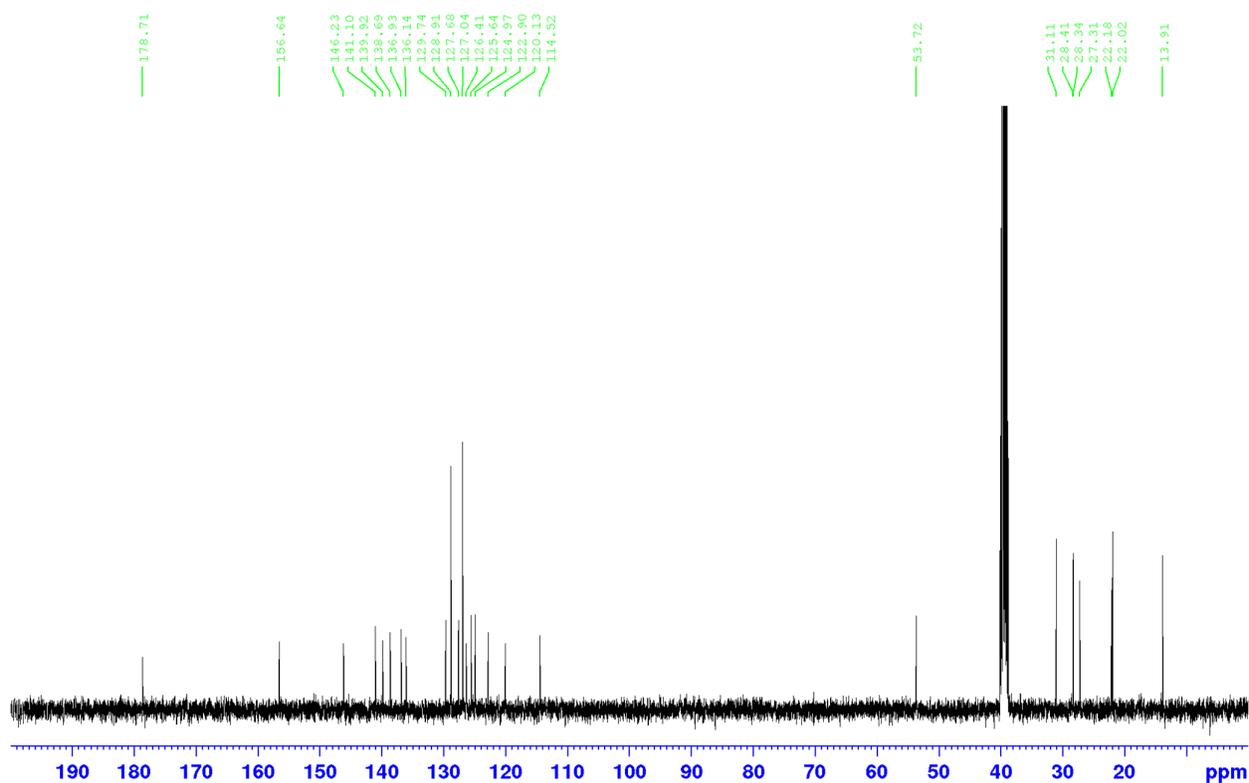


5-([1,1'-Biphenyl]-3-yl)-1-(octylsulfonyl)indoline-2,3-dione (**20**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):



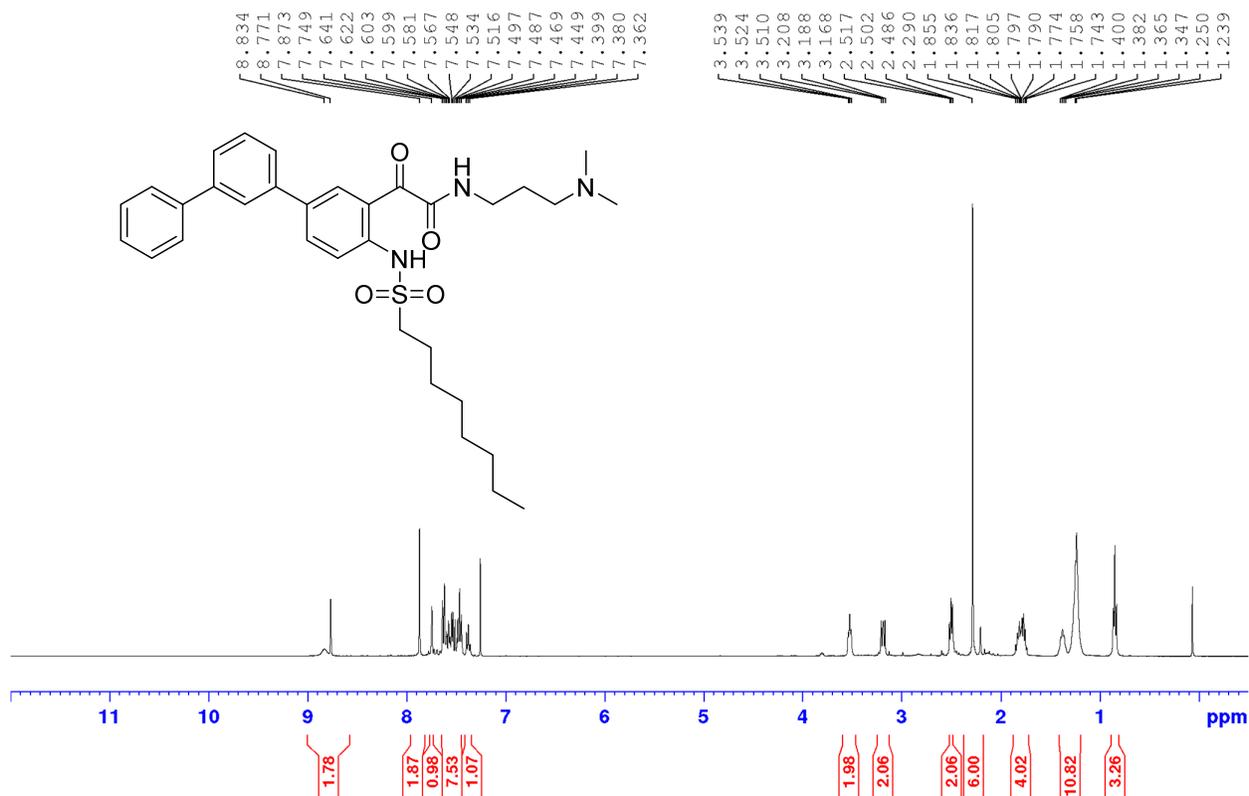
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):



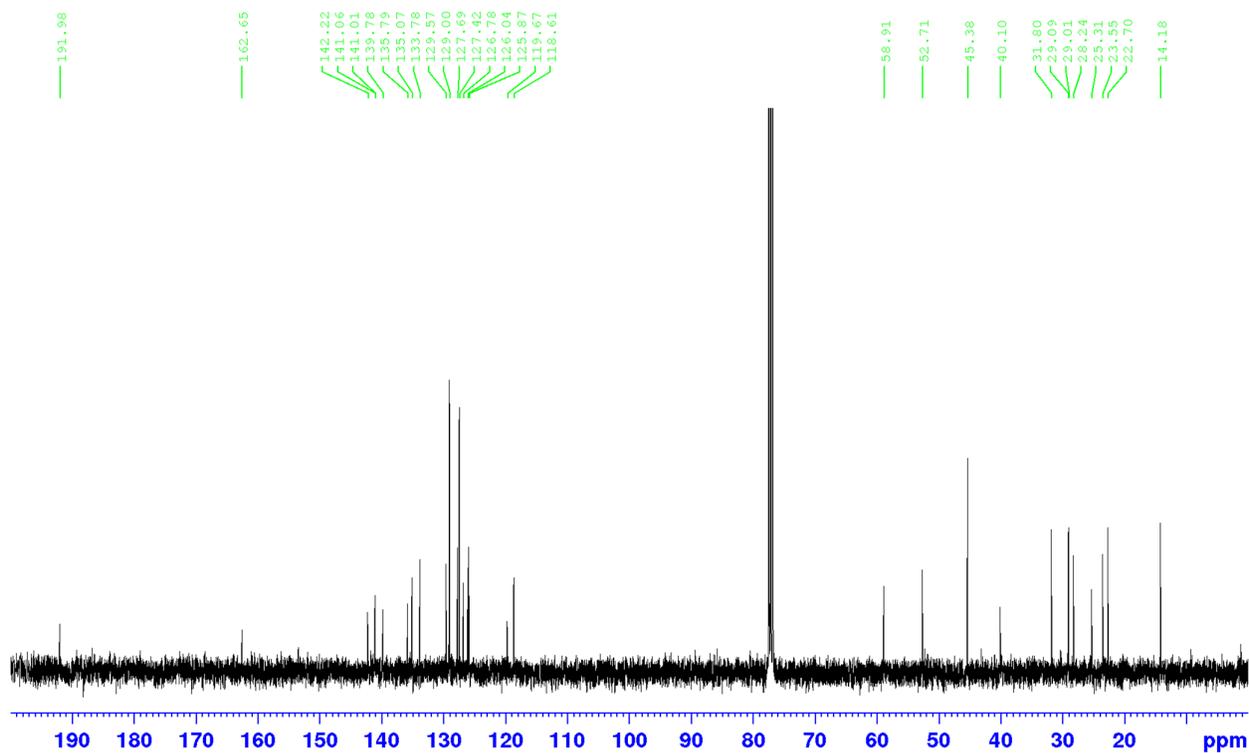
N-(3-(Dimethylamino)propyl)-2-(4-(octylsulfonamido)-[1,1':3',1''-terphenyl]-3-yl)-2-oxoacetamide

(21)

¹H NMR (400 MHz, CDCl₃):

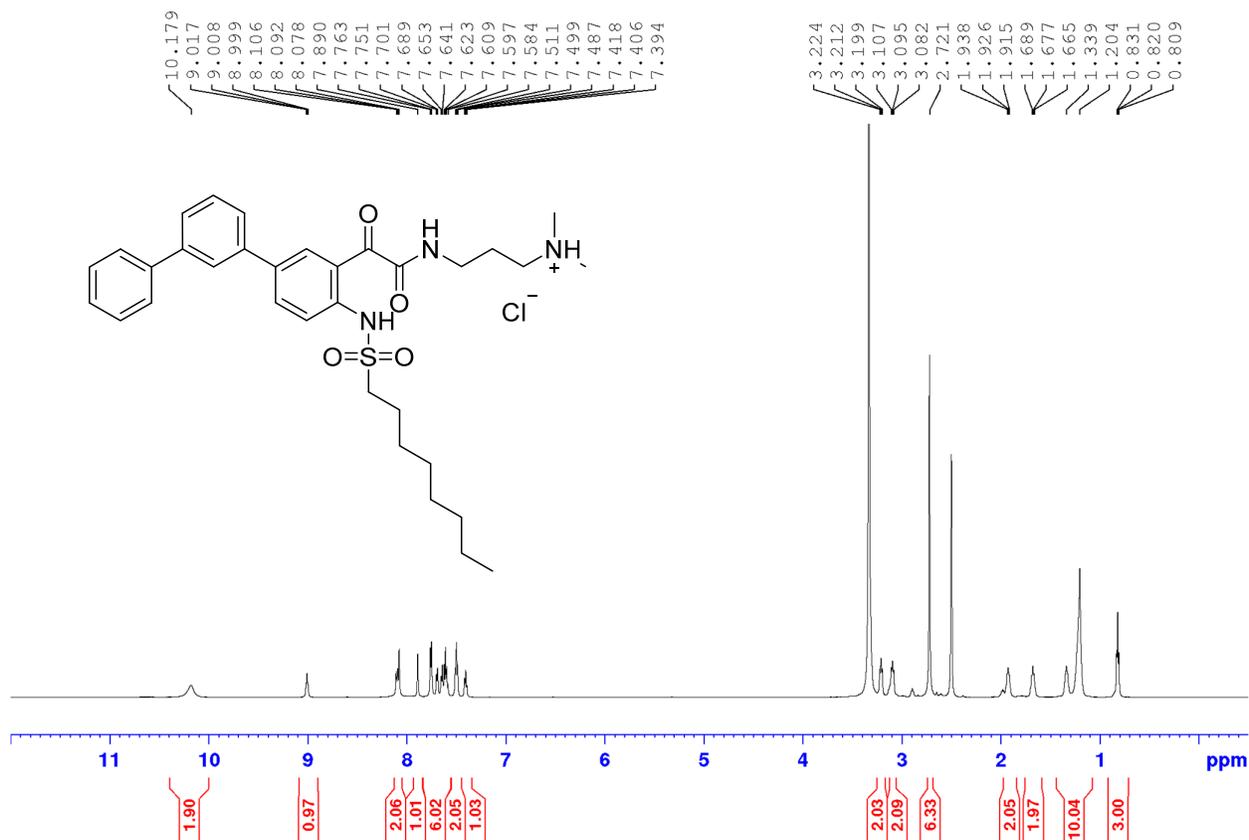


¹³C NMR (100 MHz, CDCl₃):

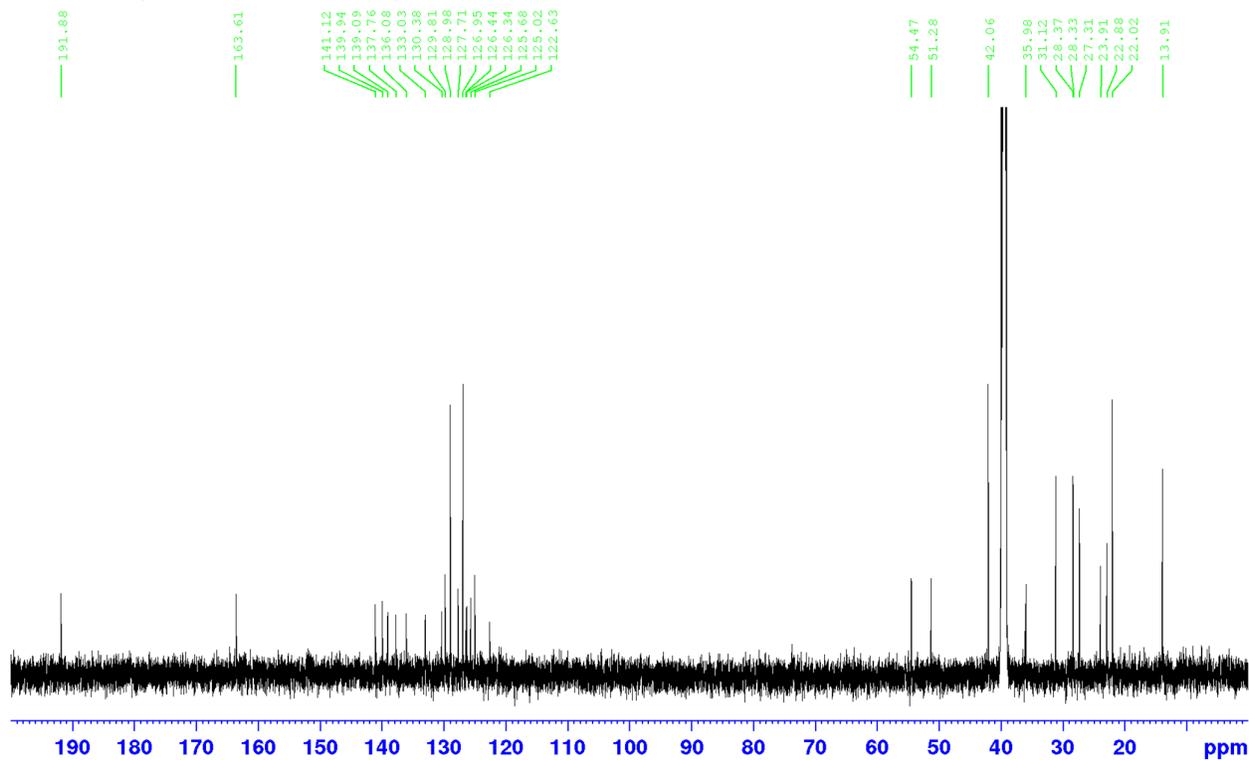


N,N-Dimethyl-3-(2-(4-(octylsulfonamido)-[1,1':3',1''-terphenyl]-3-yl)-2-oxoacetamido)propan-1-aminium chloride (**22**)

¹H NMR (600 MHz, DMSO-*d*₆):

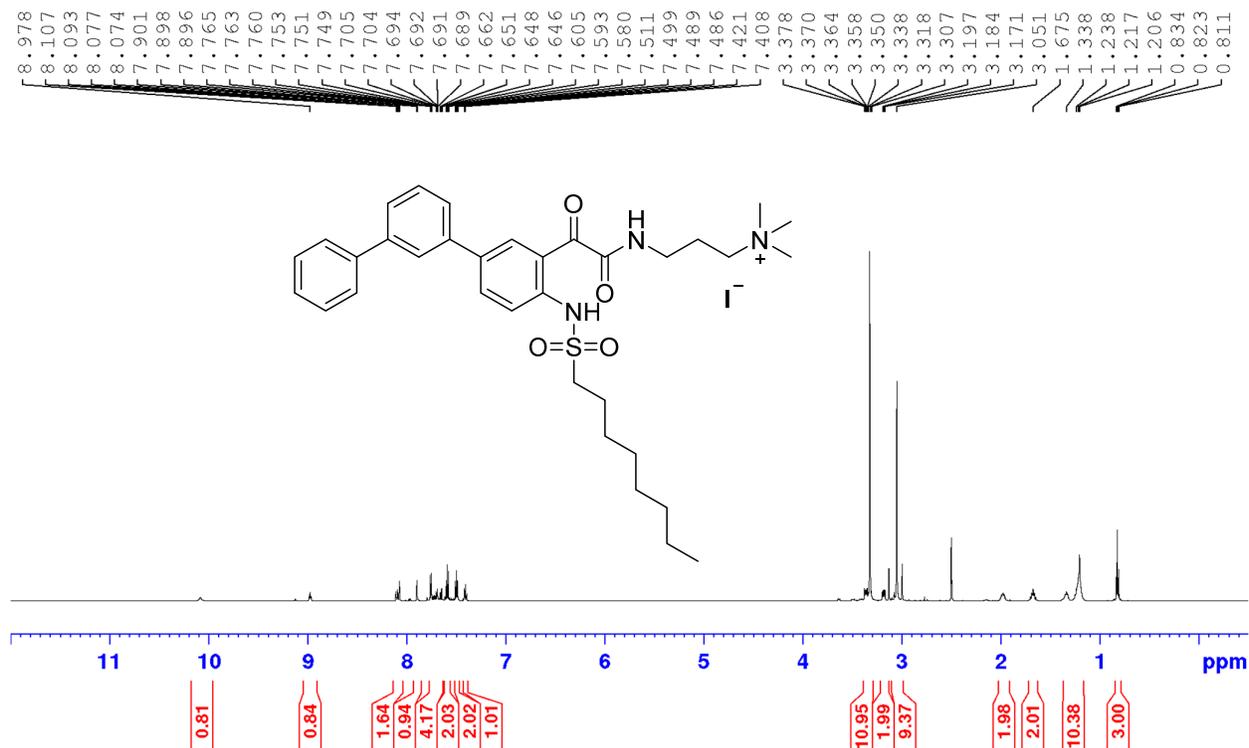


¹³C NMR (150 MHz, DMSO-*d*₆):

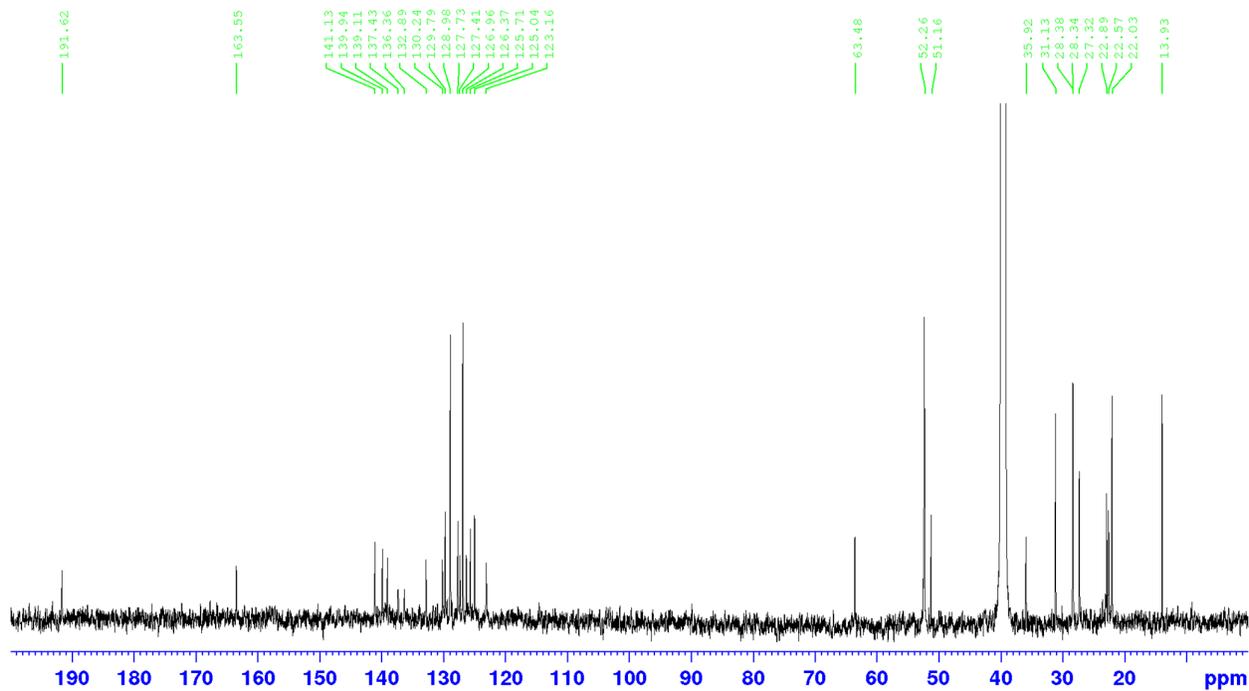


N,N,N-Trimethyl-3-(2-(4-(octylsulfonamido)-[1,1':3',1''-terphenyl]-3-yl)-2-oxoacetamido)propan-1-aminium iodide (**23**)

¹H NMR (600 MHz, DMSO-*d*₆):

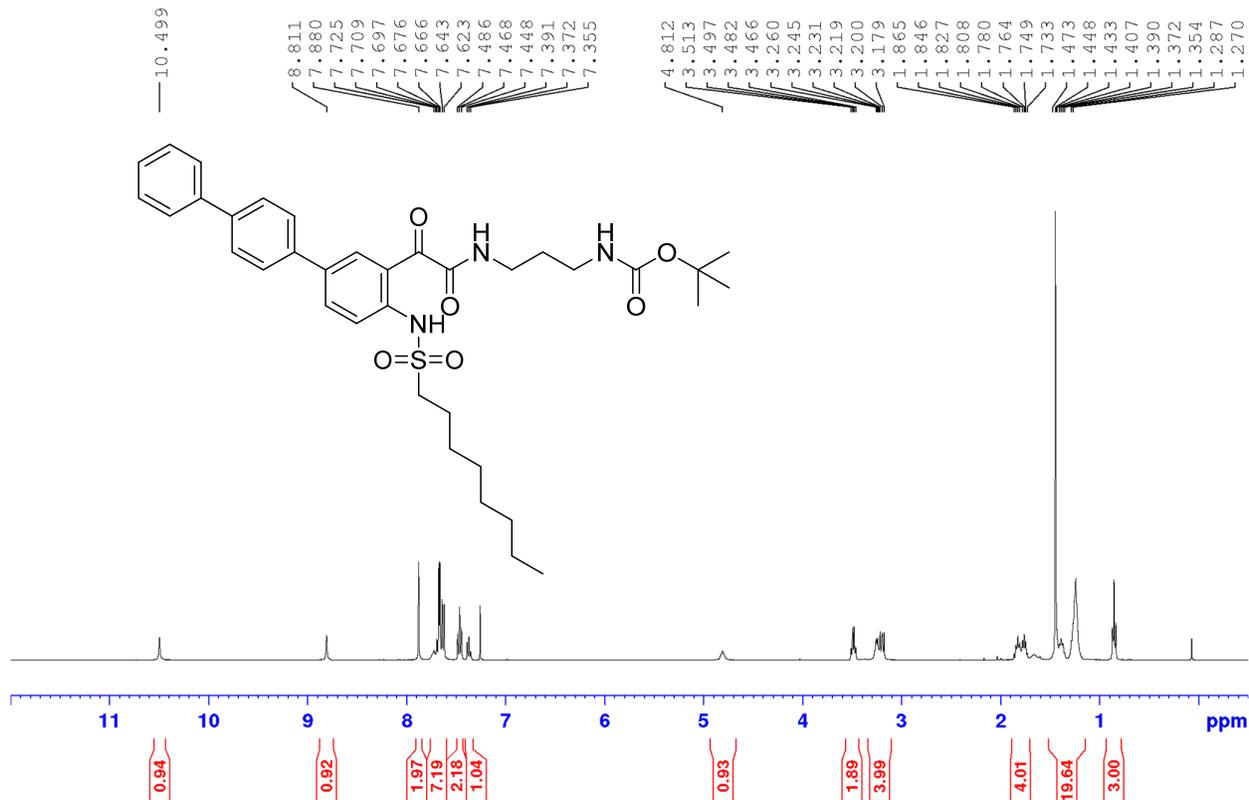


¹³C NMR (150 MHz, DMSO-*d*₆):

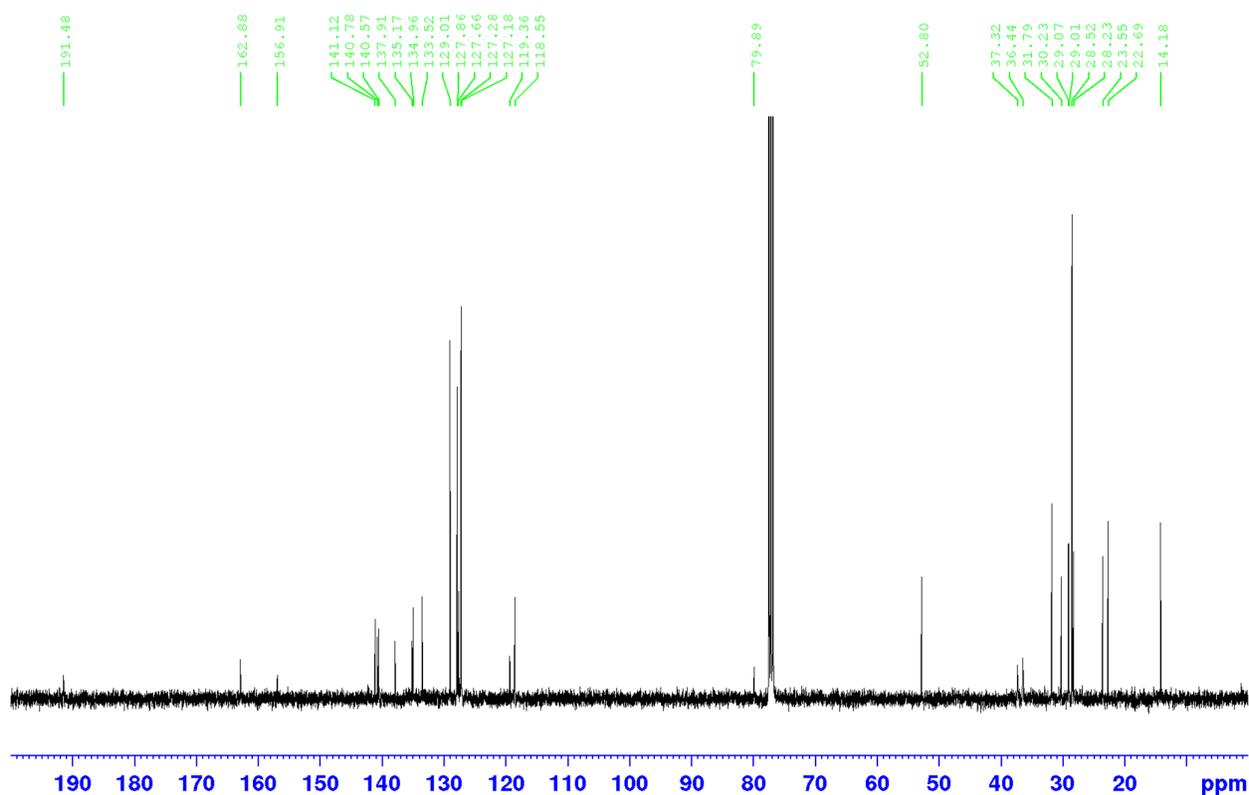


tert-Butyl (3-(2-(4-(octylsulfonamido)-[1,1':4,1''-terphenyl]-3-yl)-2-oxoacetamido)propyl)carbamate
(24d)

¹H NMR (400 MHz, CDCl₃):

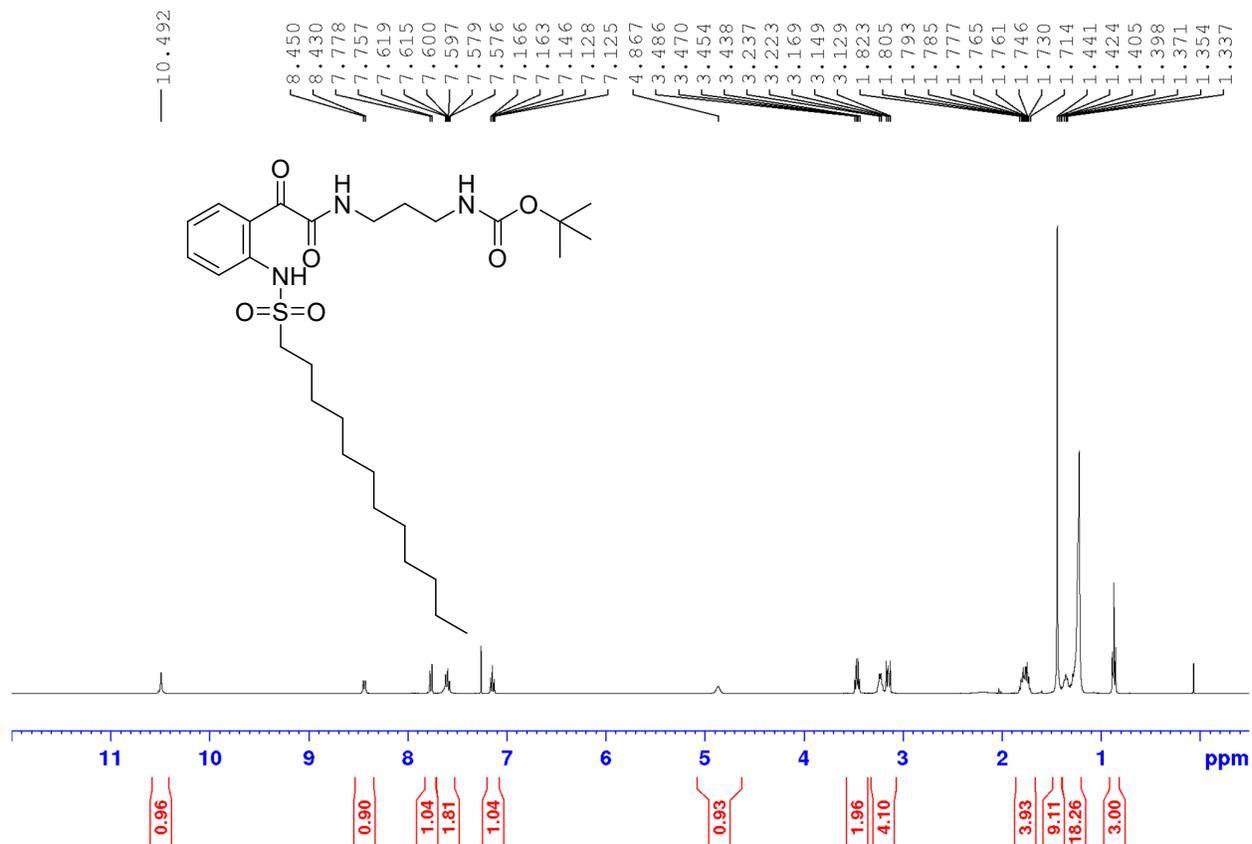


¹³C NMR (100 MHz, CDCl₃):

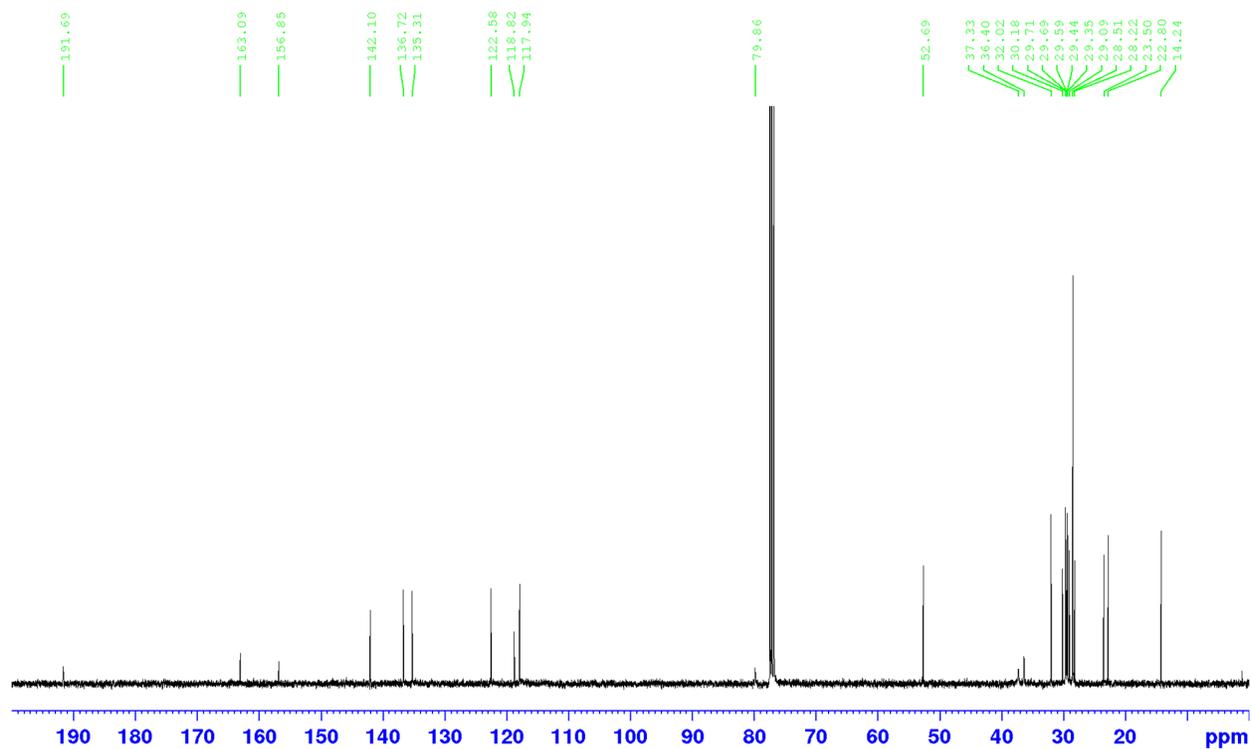


tert-Butyl (3-(2-(2-(dodecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamate (**25a**)

^1H NMR (400 MHz, CDCl_3):

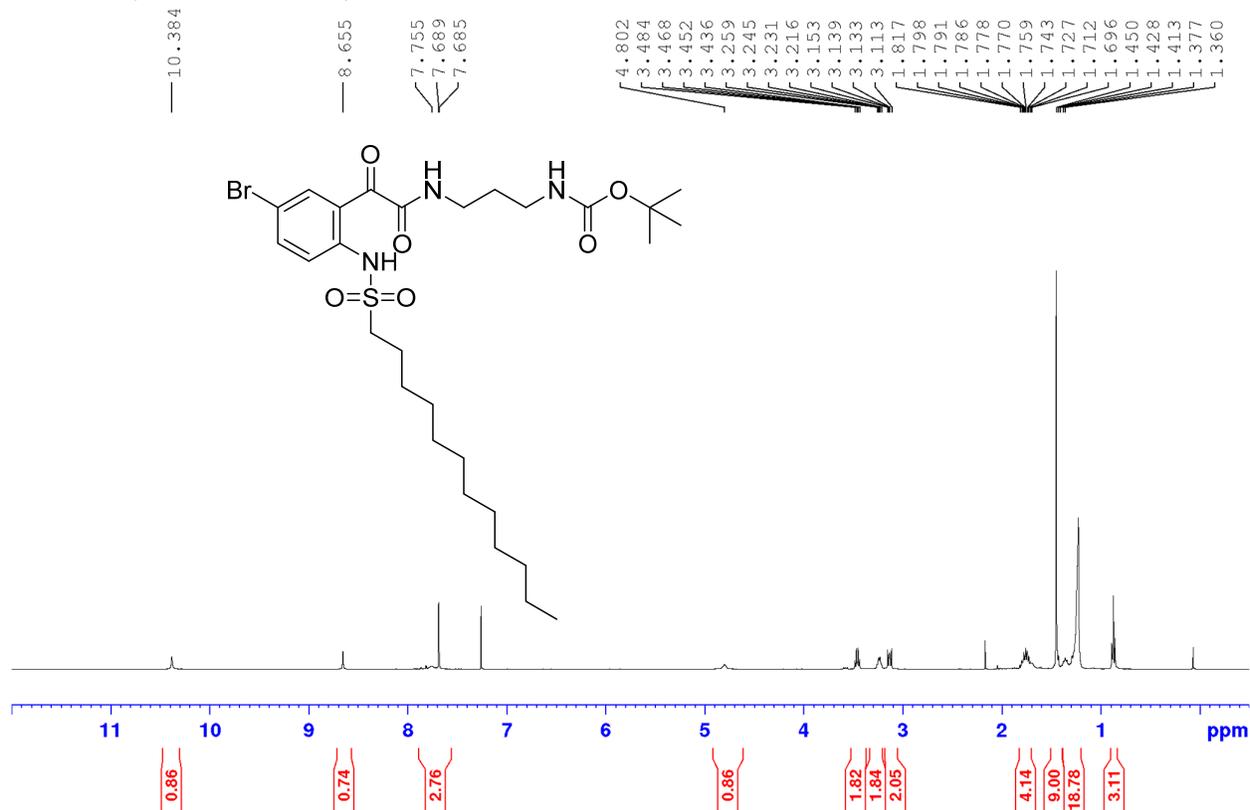


^{13}C NMR (100 MHz, CDCl_3):

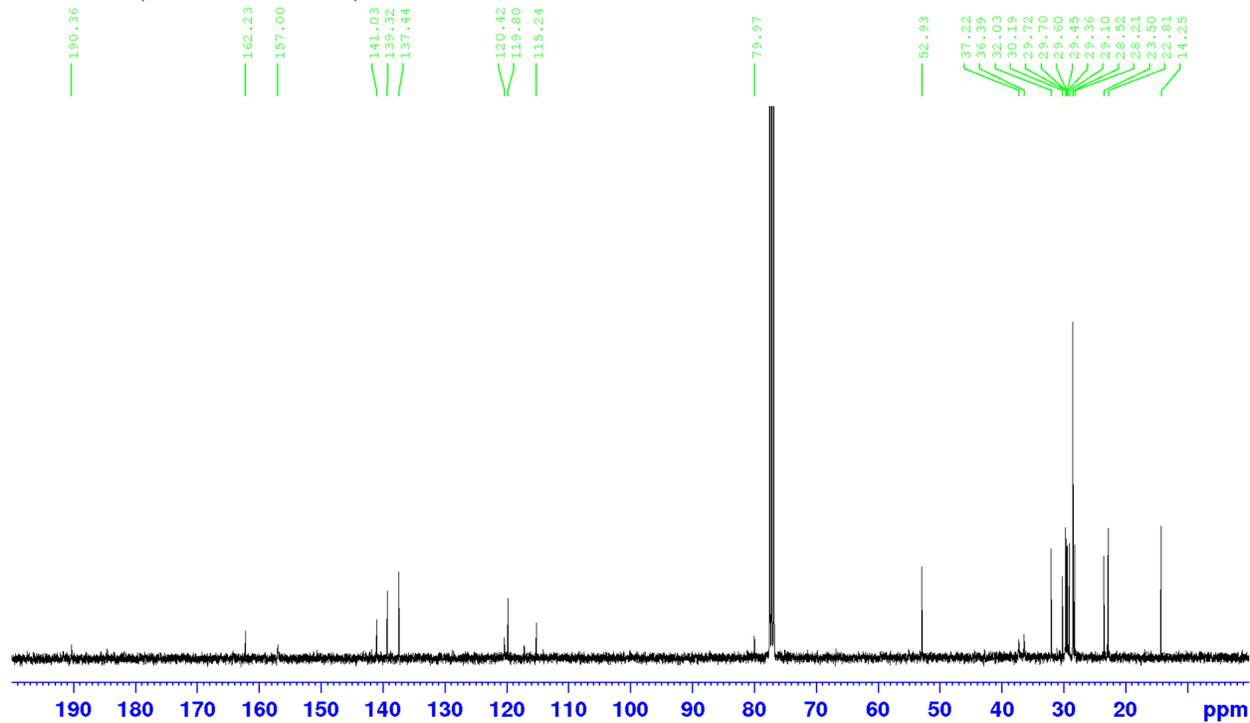


tert-Butyl (3-(2-(5-bromo-2-(dodecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamate (**25b**)

^1H NMR (400 MHz, CDCl_3):

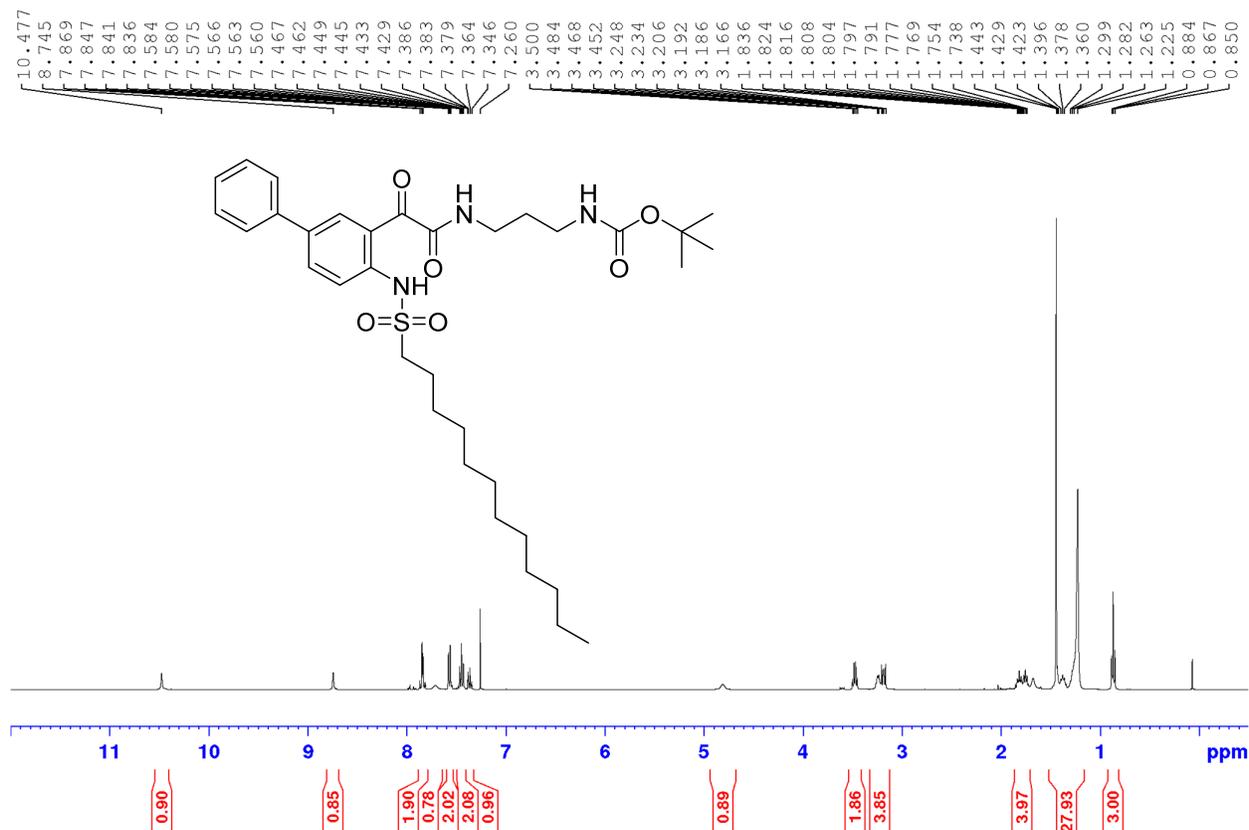


^{13}C NMR (100 MHz, CDCl_3):

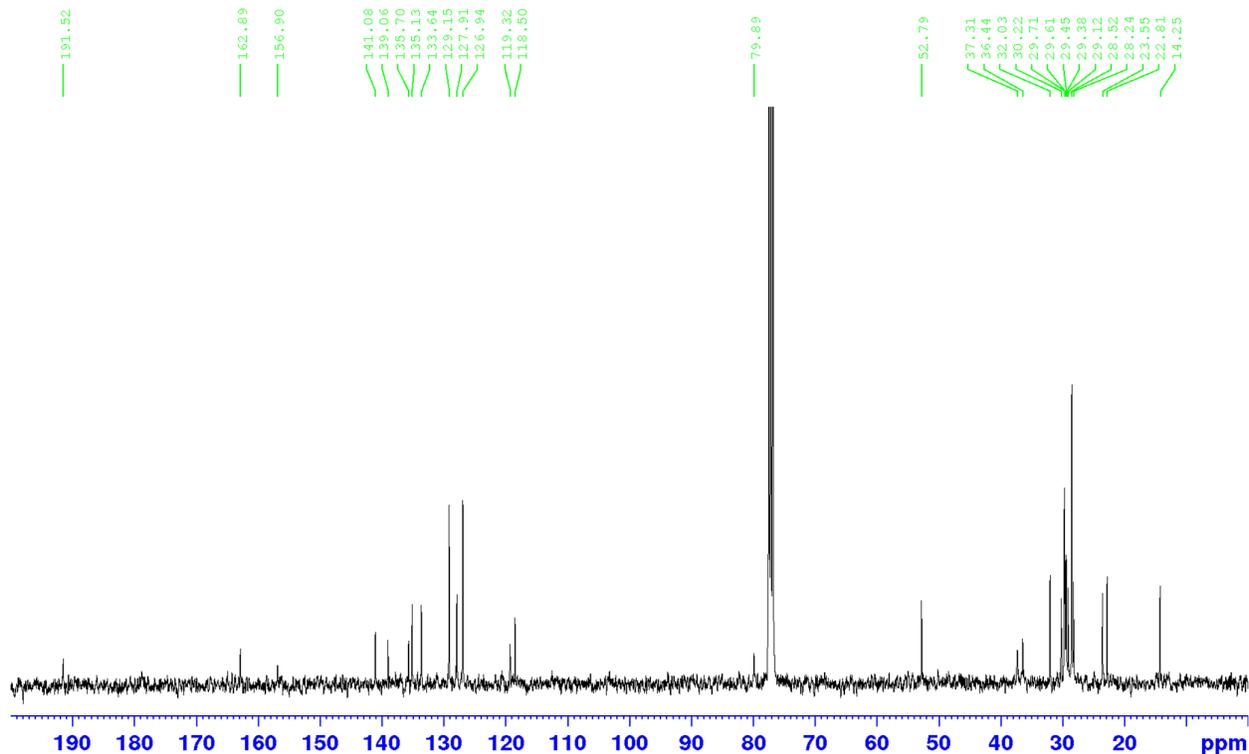


tert-Butyl (3-(2-(4-(dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)propyl)carbamate (25c)

¹H NMR (400 MHz, CDCl₃):

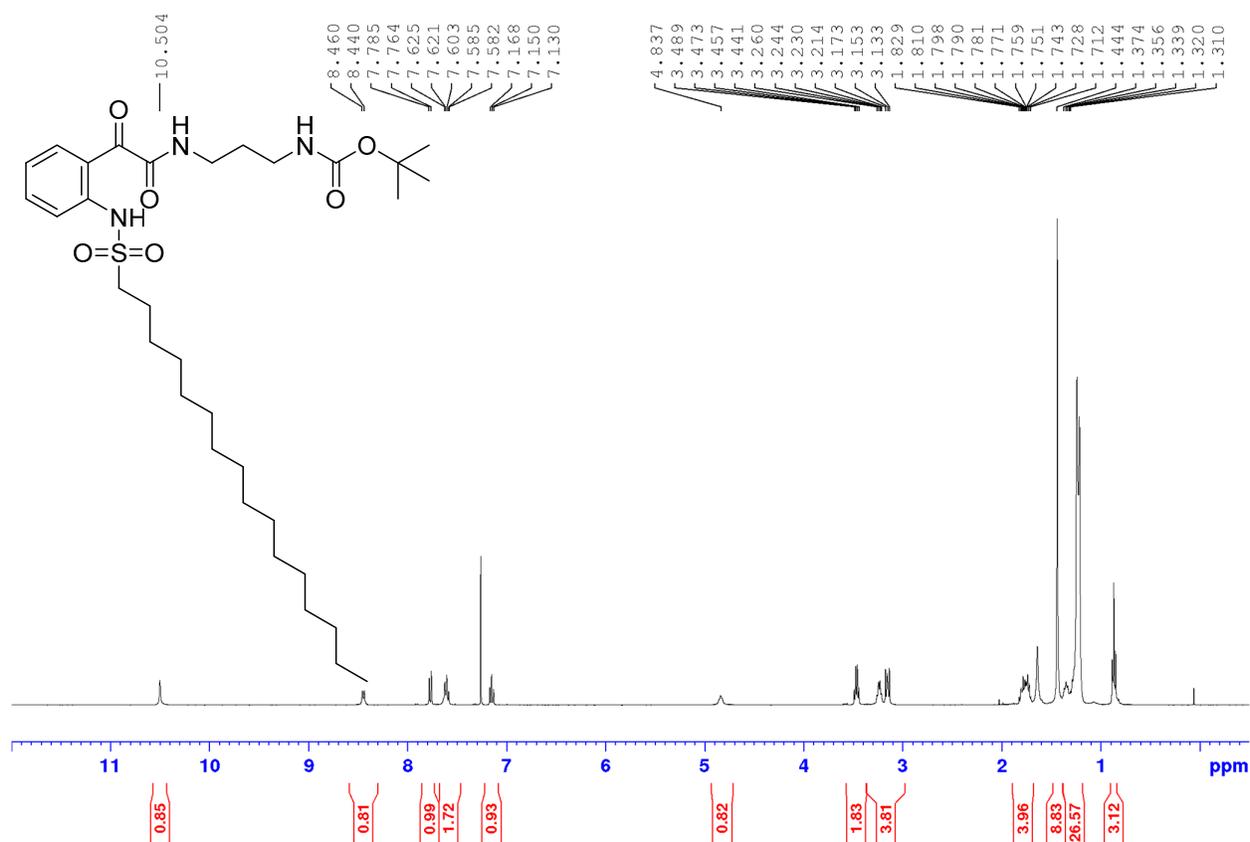


¹³C NMR (100 MHz, CDCl₃):

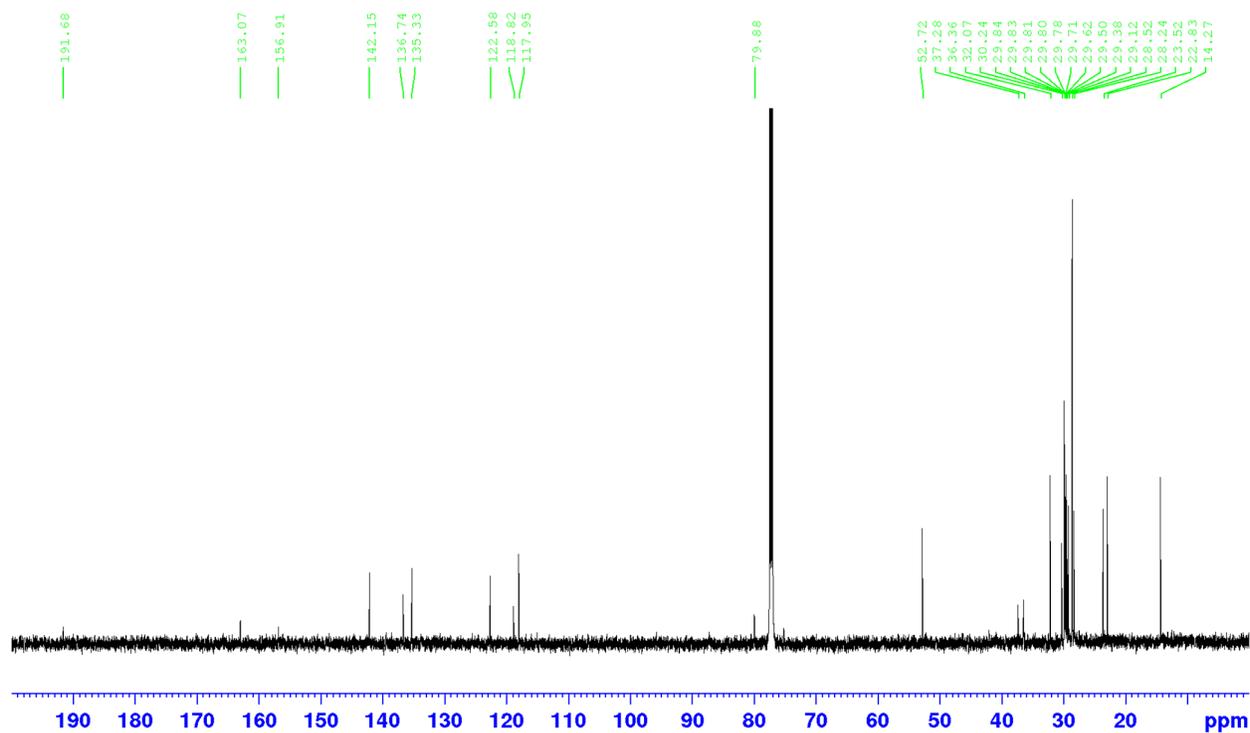


tert-Butyl (3-(2-(2-(hexadecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamate (**26a**)

^1H NMR (400 MHz, CDCl_3):

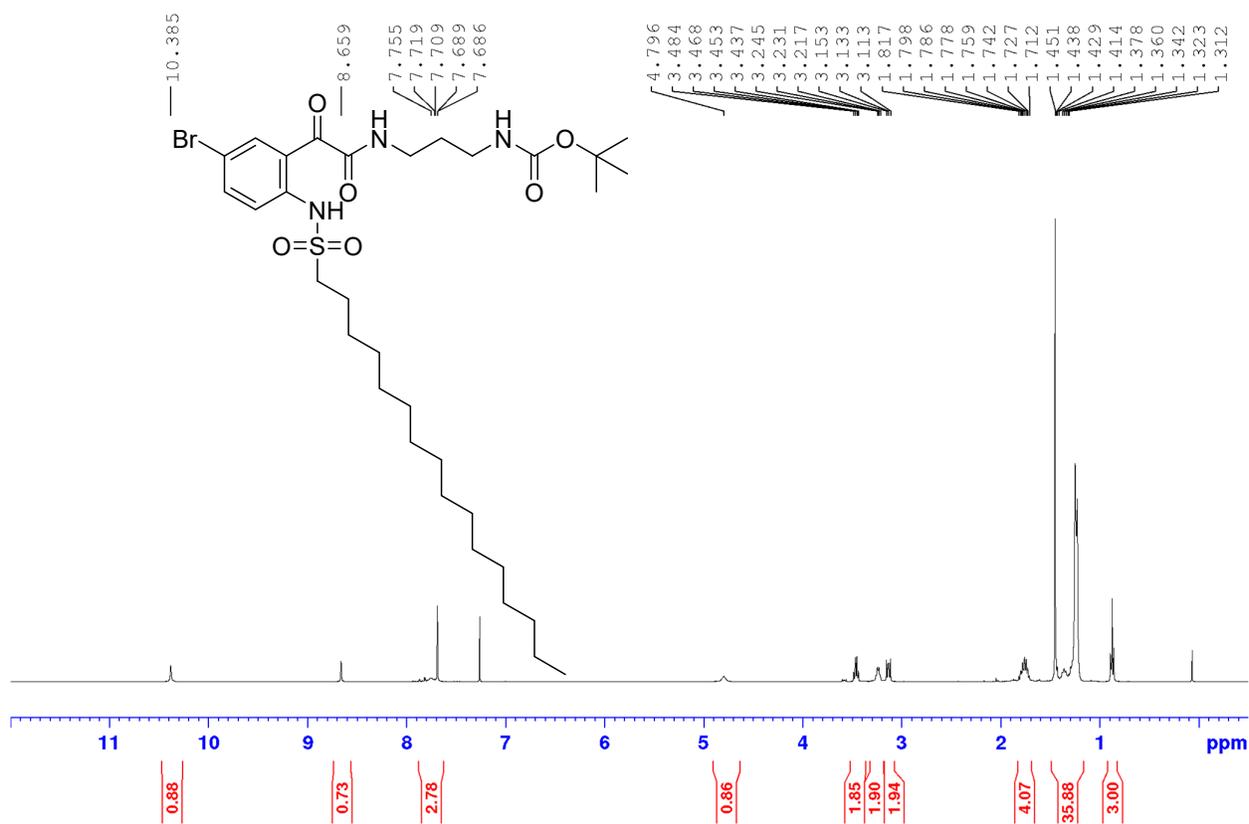


^{13}C NMR (150 MHz, CDCl_3):

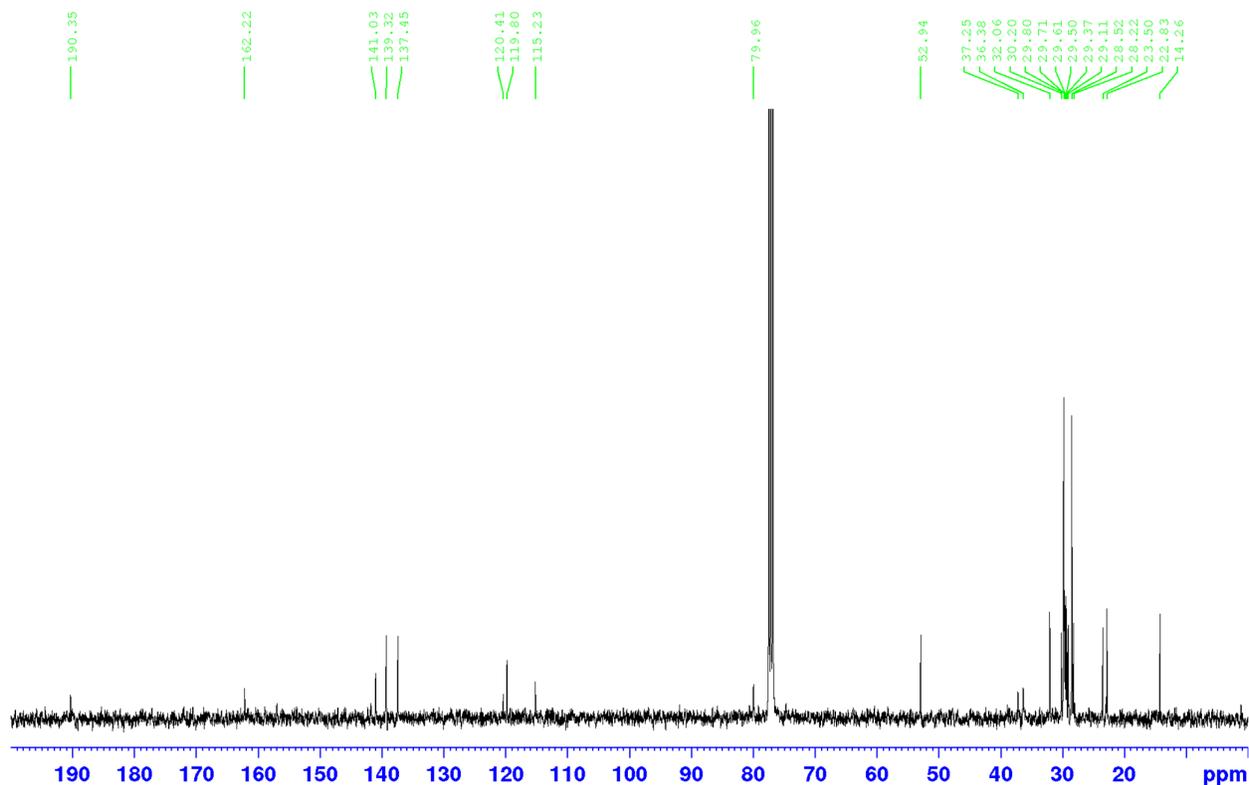


tert-Butyl (3-(2-(5-bromo-2-(hexadecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamate (**26b**)

^1H NMR (400 MHz, CDCl_3):

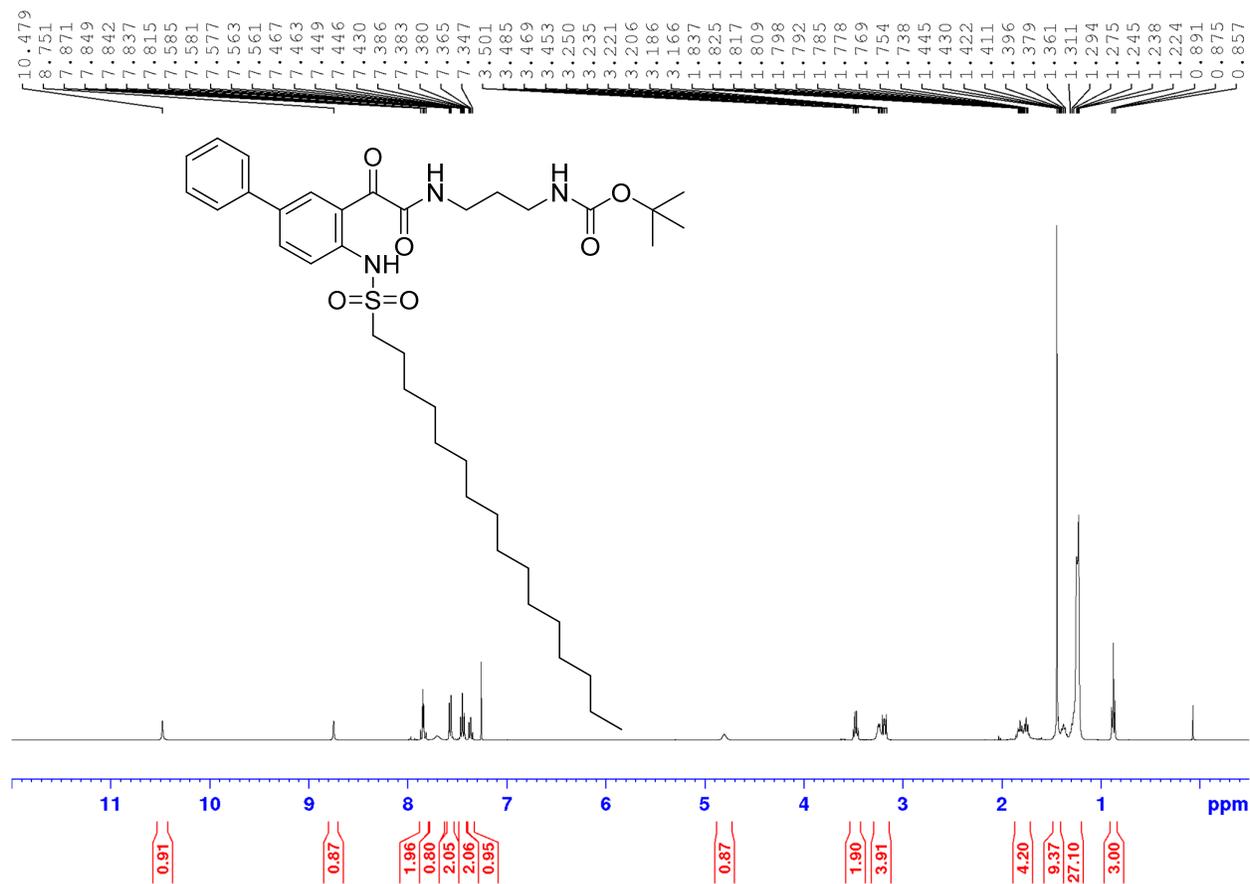


^{13}C NMR (100 MHz, CDCl_3):

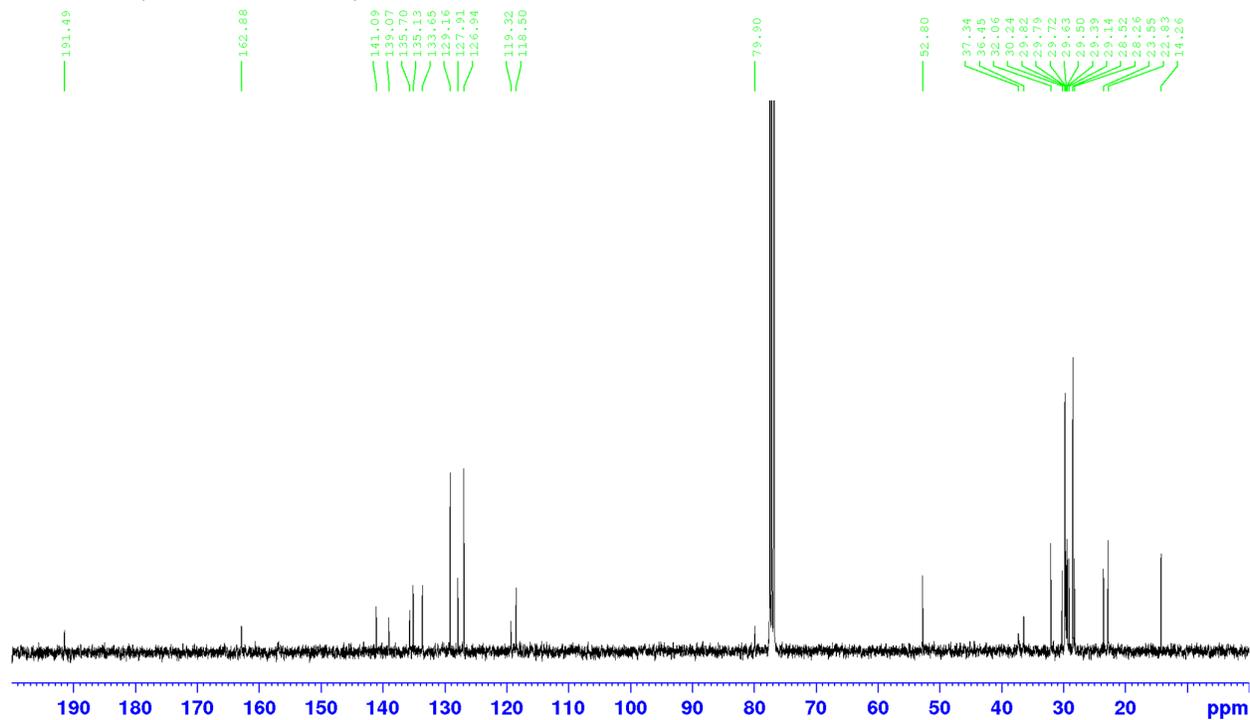


tert-Butyl (3-(2-(4-(hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)propyl)carbamate (26c)

¹H NMR (400 MHz, CDCl₃):

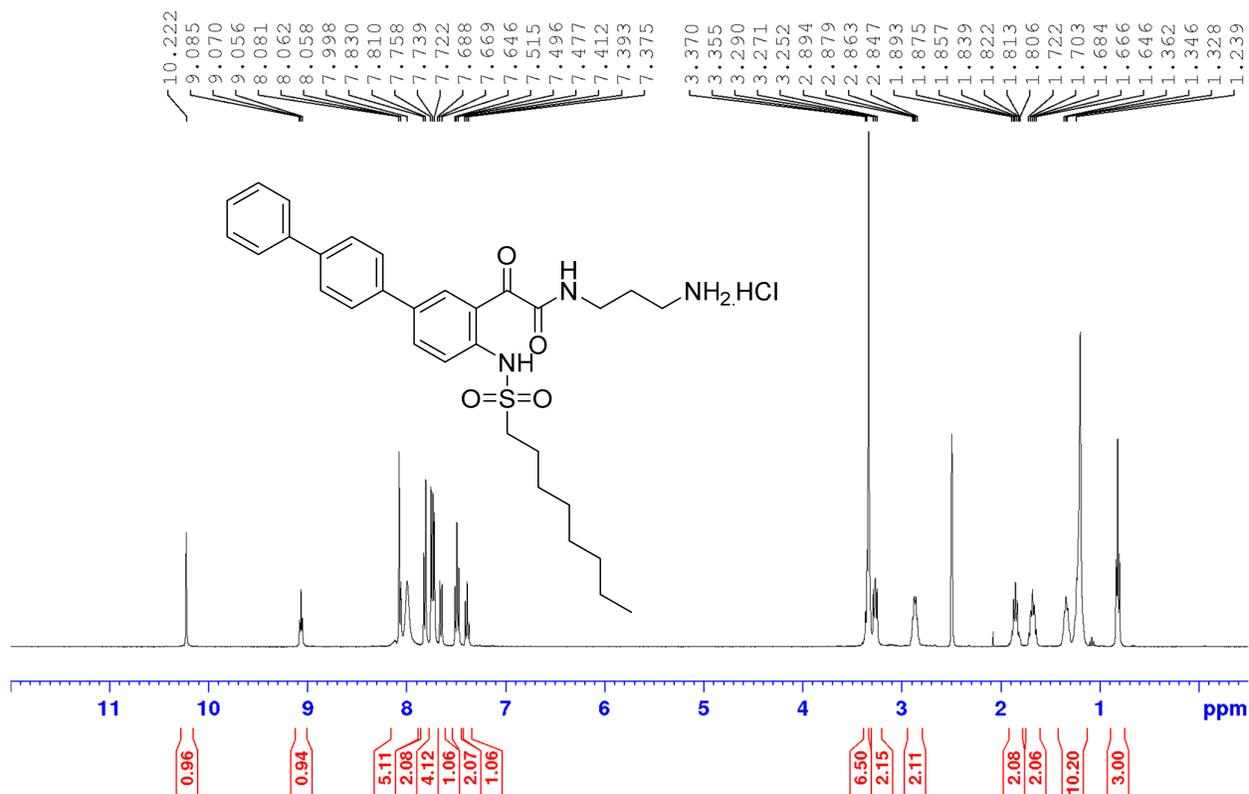


¹³C NMR (100 MHz, CDCl₃):

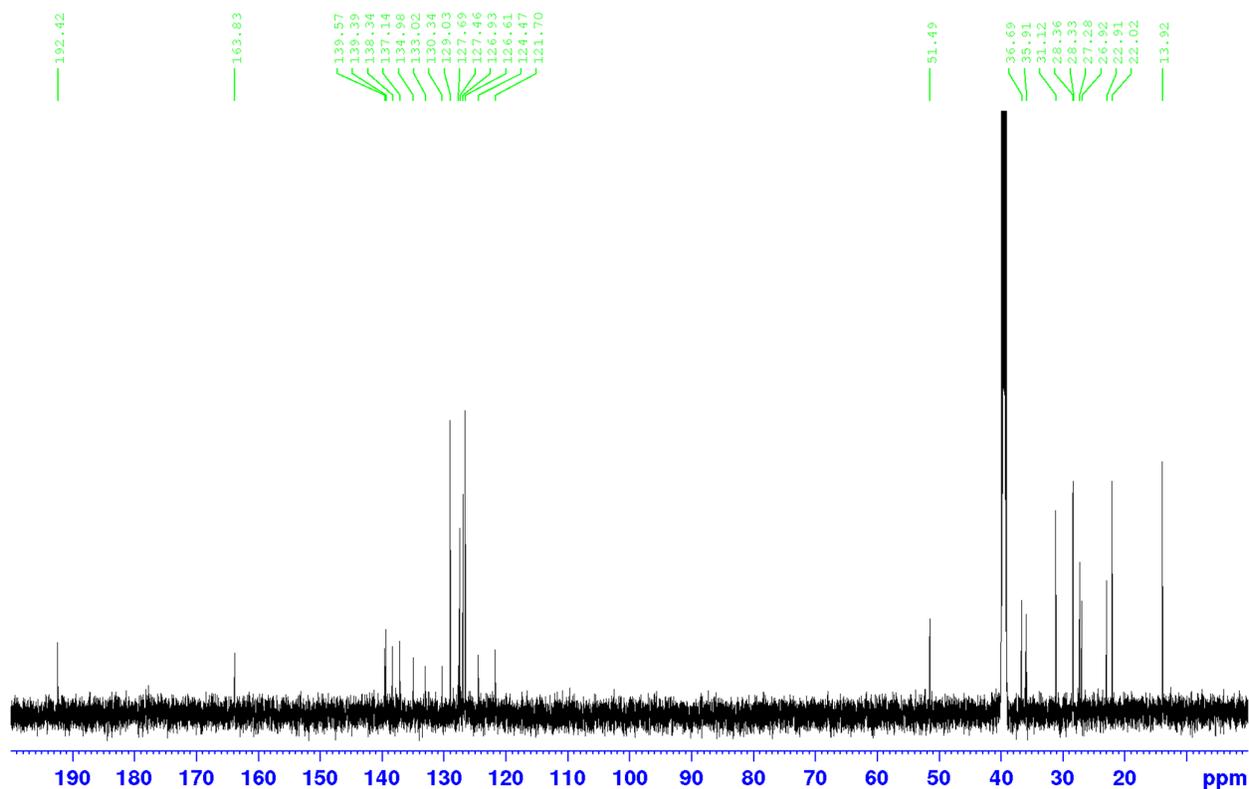


N-(3-aminopropyl)-2-(4-(octylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamide hydrochloride (**27d**)

¹H NMR (400 MHz, DMSO-*d*₆):

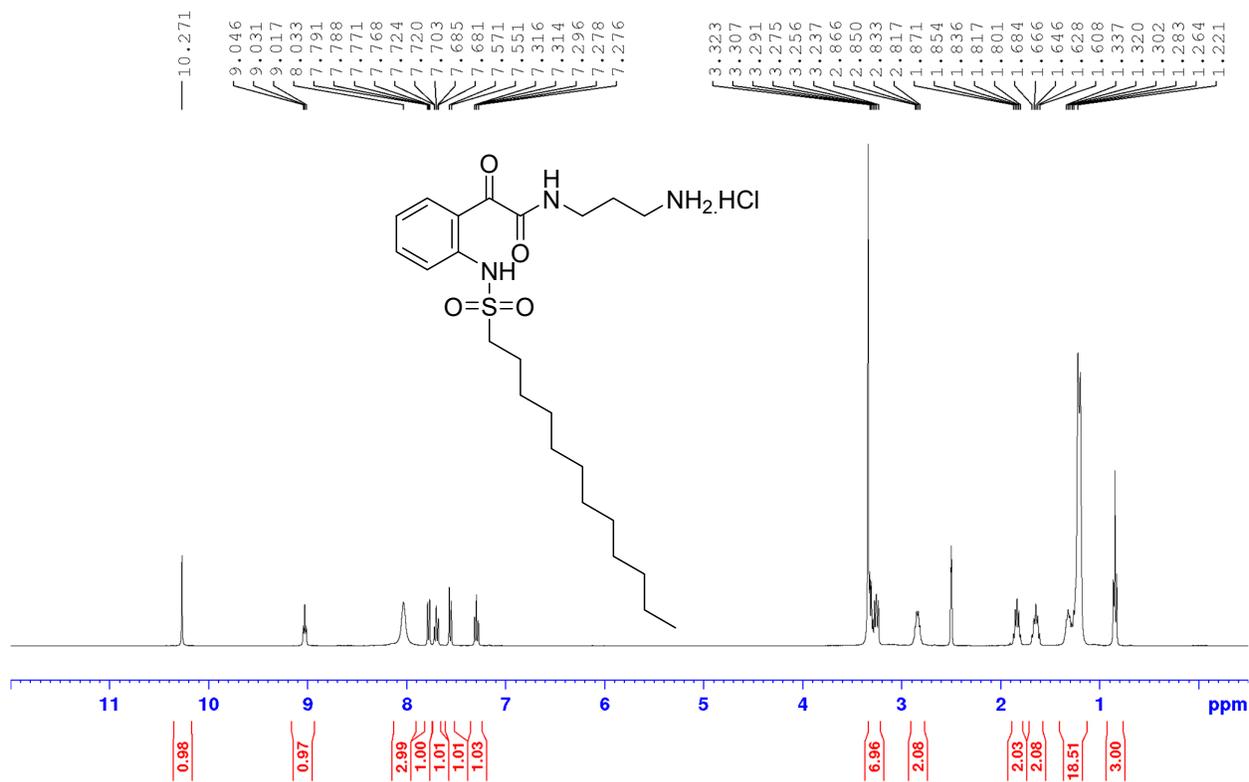


¹³C NMR (150 MHz, DMSO-*d*₆):

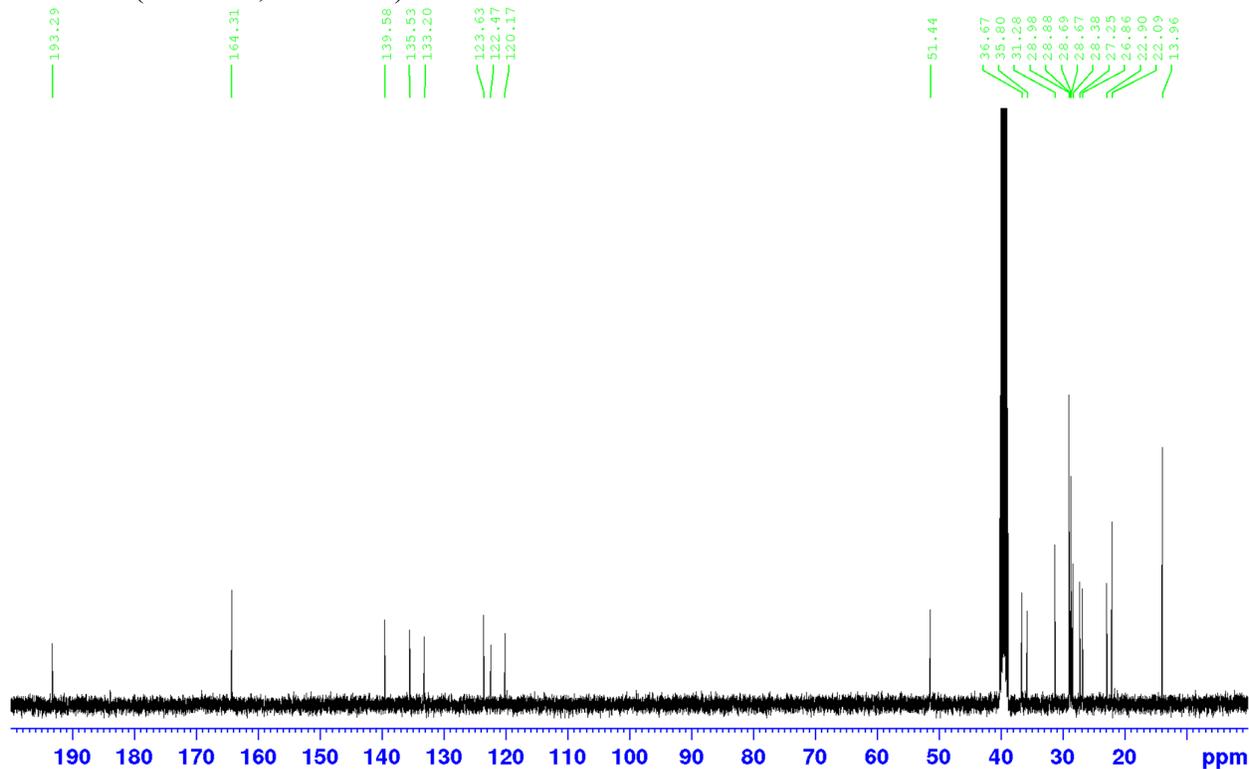


N-(3-Aminopropyl)-2-(2-(dodecylsulfonamido)phenyl)-2-oxoacetamide hydrochloride (**28a**)

¹H NMR (400 MHz, DMSO-*d*₆):

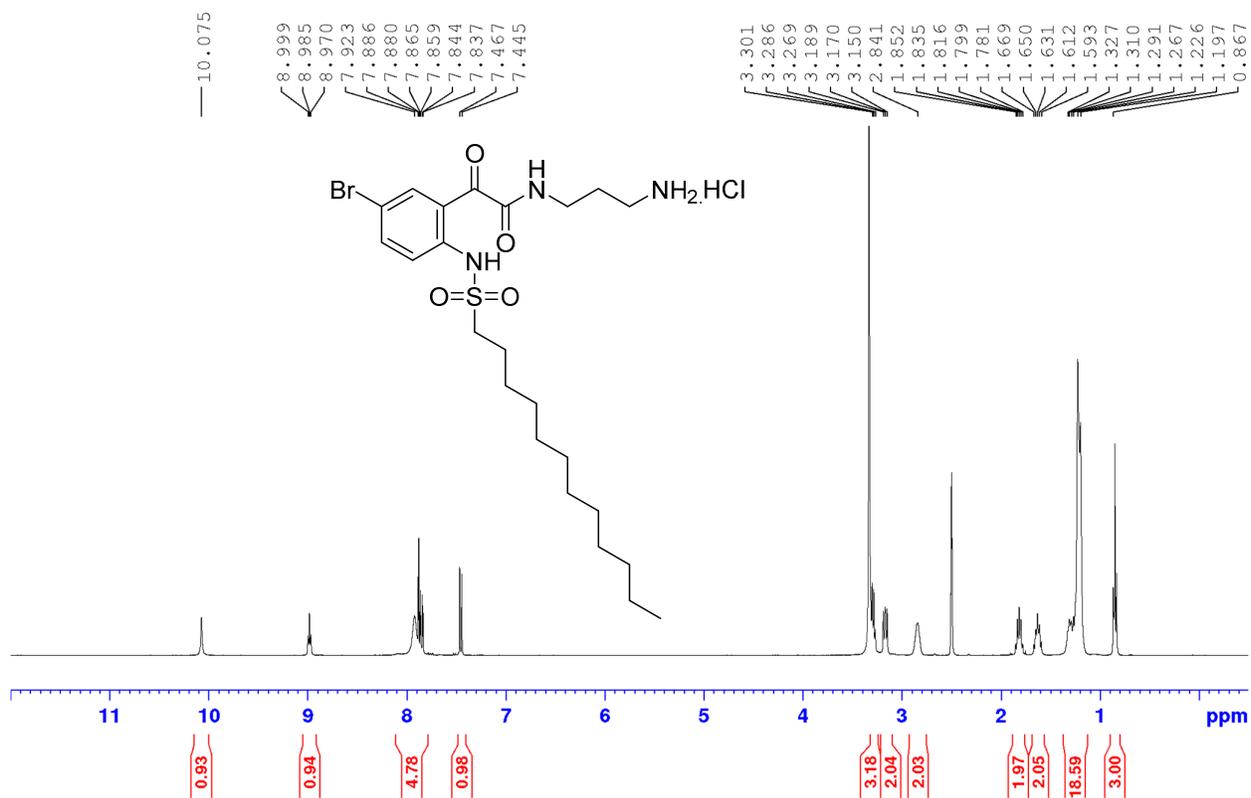


¹³C NMR (100 MHz, DMSO-*d*₆):

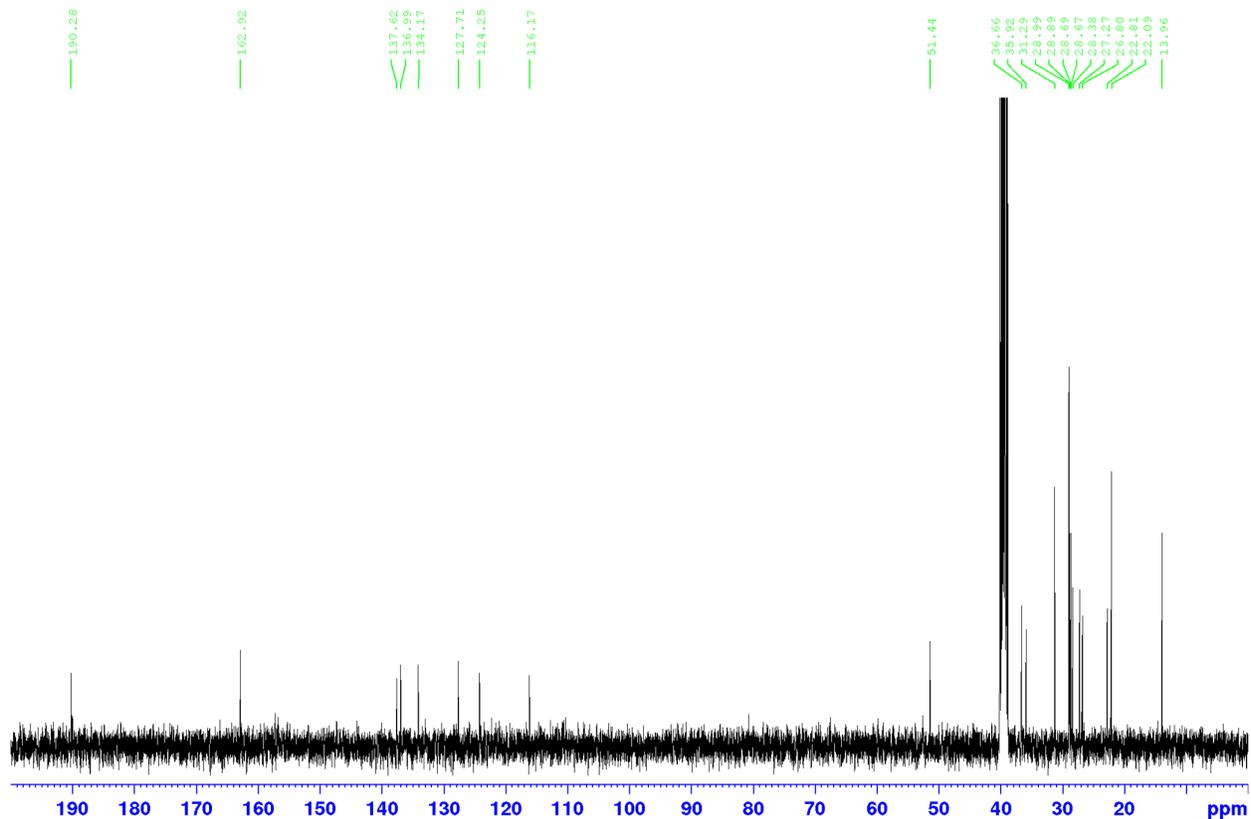


N-(3-Aminopropyl)-2-(5-bromo-2-(dodecylsulfonamido)phenyl)-2-oxoacetamide hydrochloride (**28b**)

¹H NMR (400 MHz, DMSO-*d*₆):

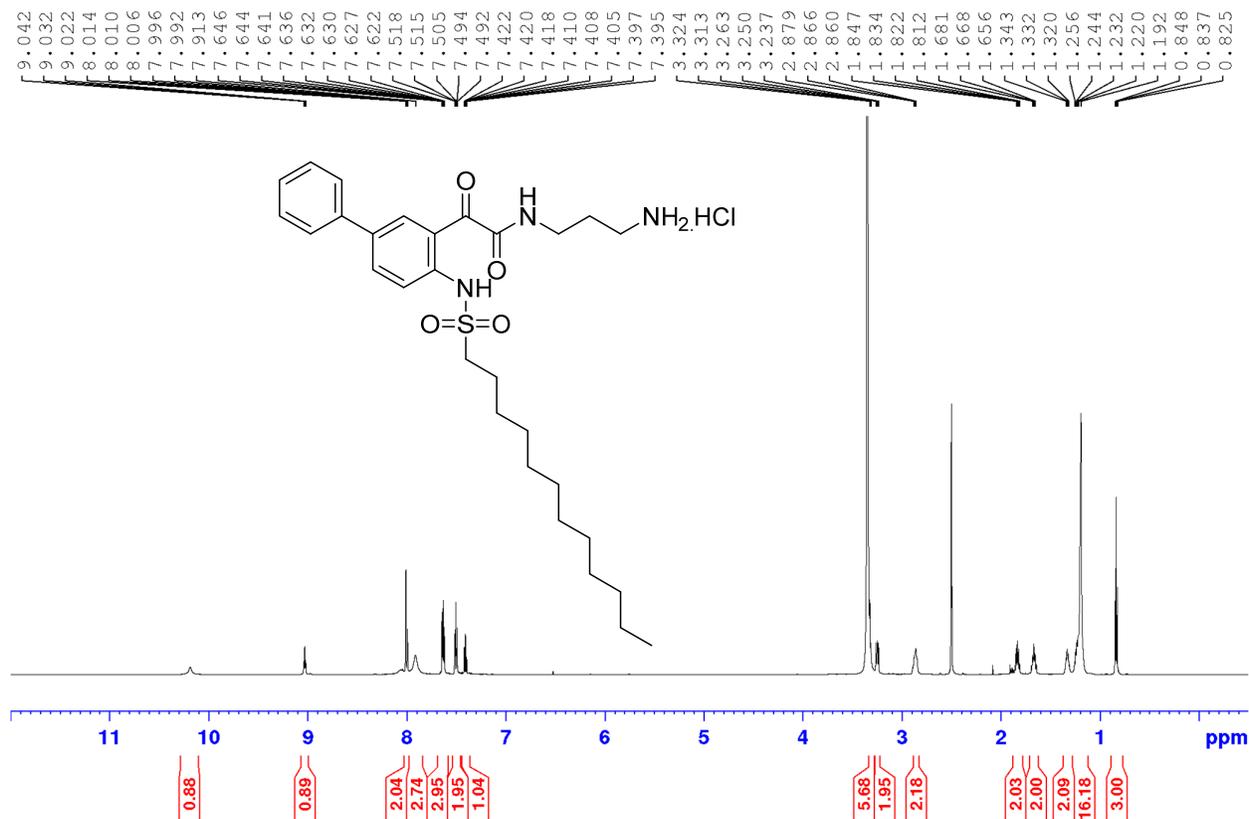


¹³C NMR (100 MHz, DMSO-*d*₆):

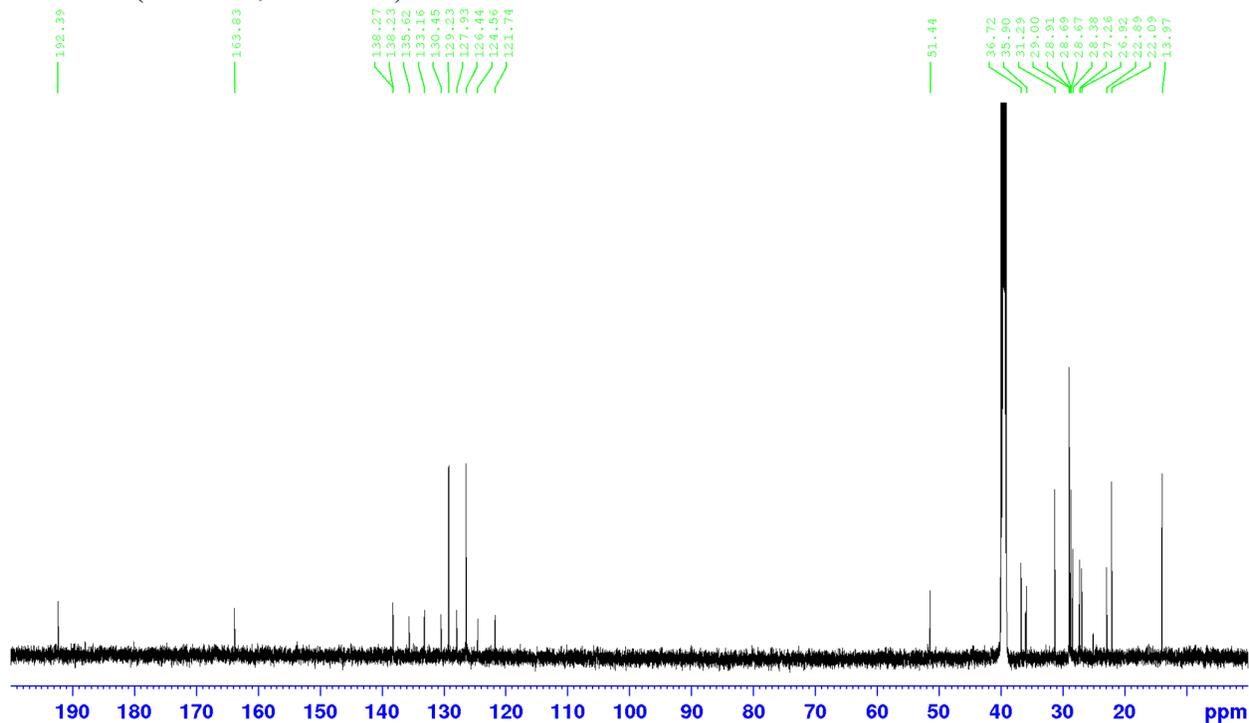


N-(3-aminopropyl)-2-(4-(dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamide hydrochloride
(28c)

¹H NMR (600 MHz, DMSO-*d*₆):

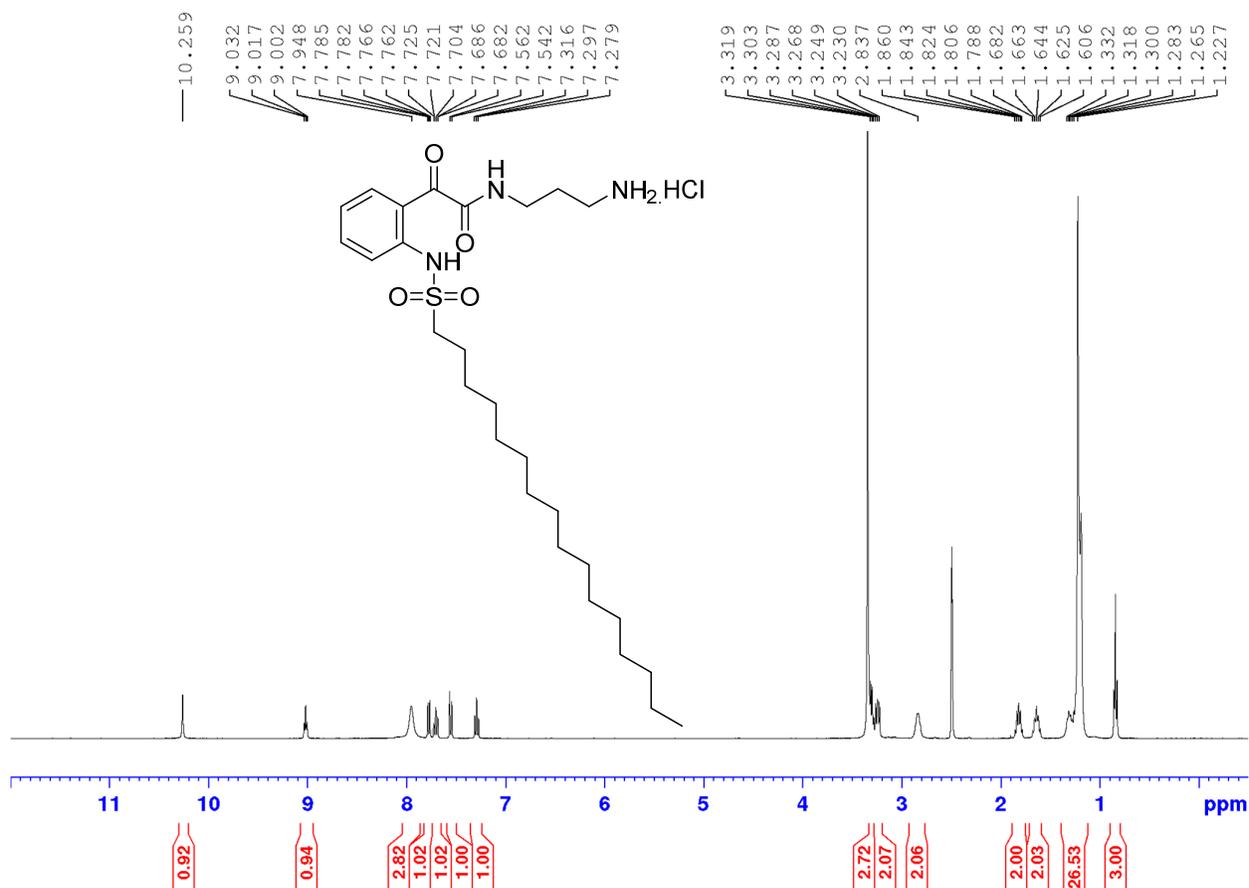


¹³C NMR (150 MHz, DMSO-*d*₆):

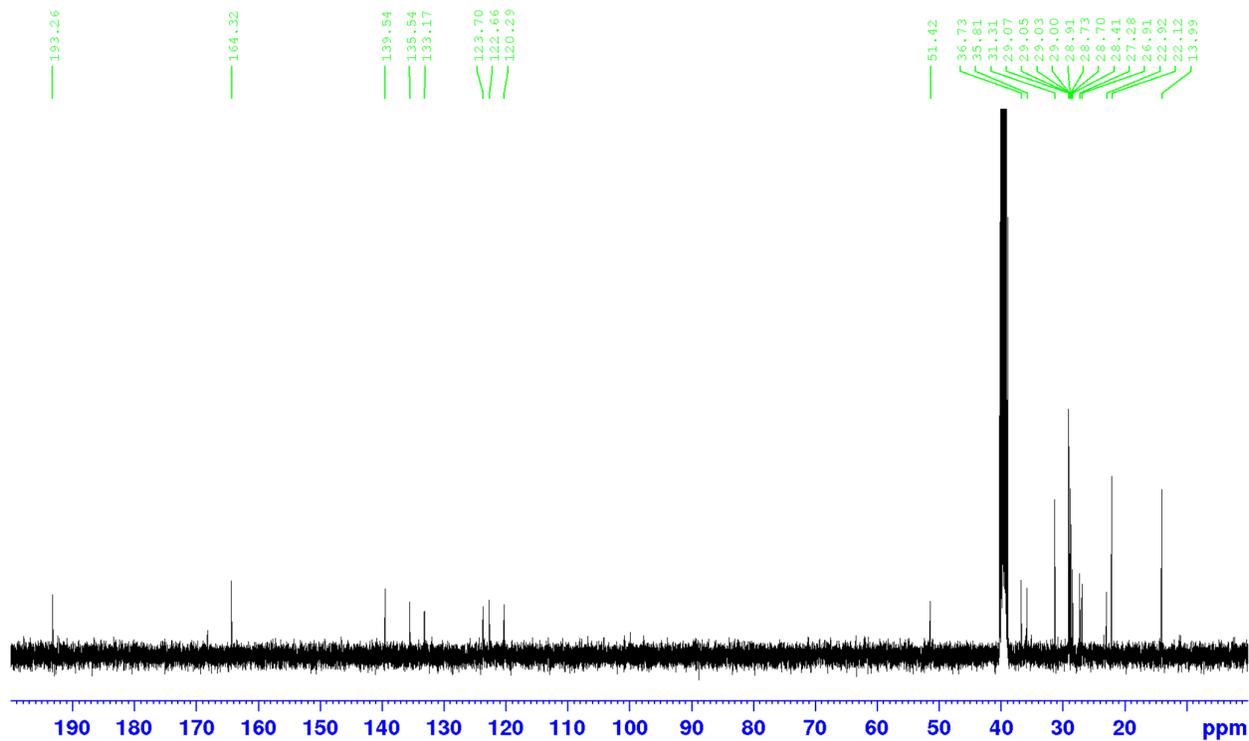


N-(3-Aminopropyl)-2-(2-(hexadecylsulfonamido)phenyl)-2-oxoacetamide hydrochloride (**29a**)

¹H NMR (400 MHz, DMSO-*d*₆):

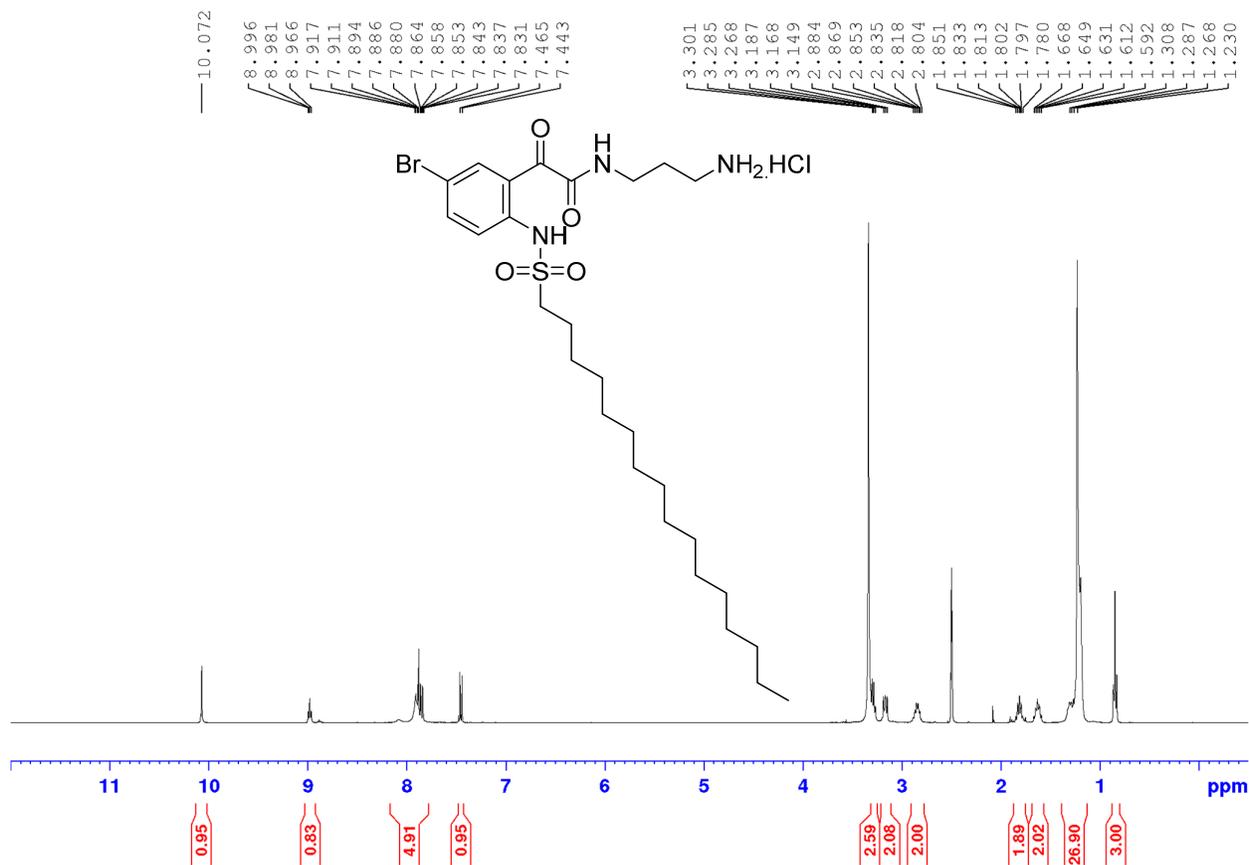


¹³C NMR (100 MHz, DMSO-*d*₆):

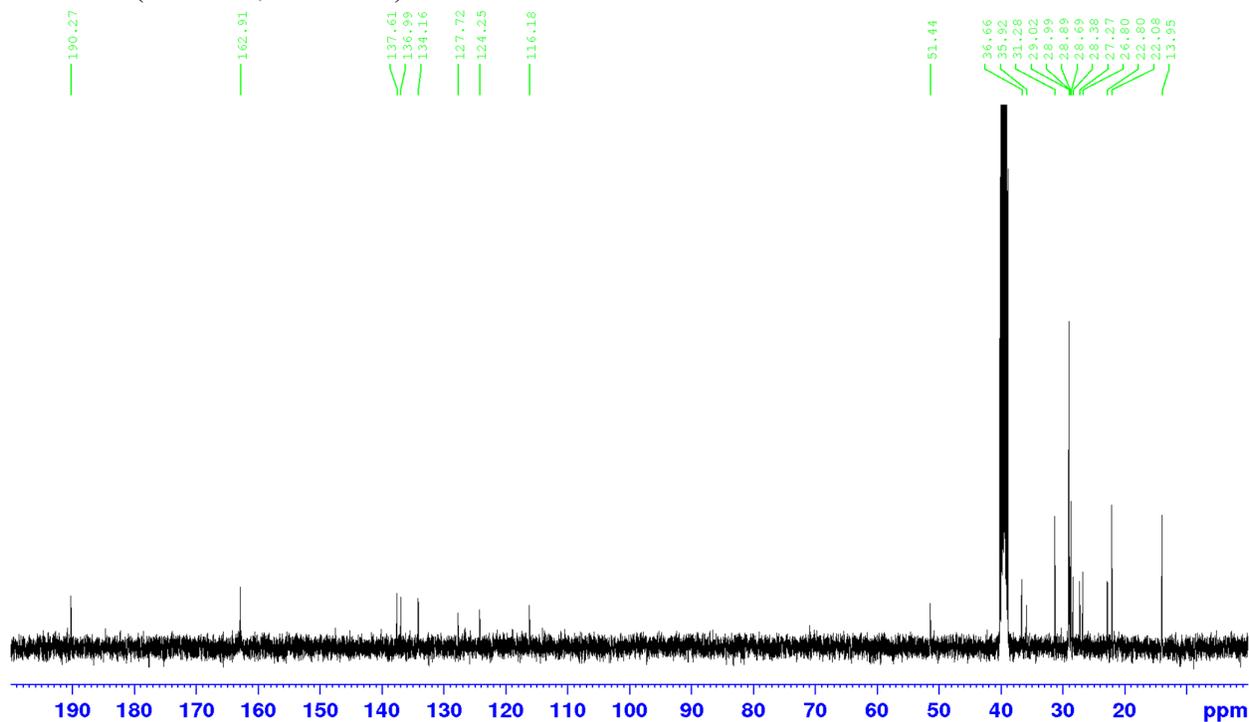


N-(3-Aminopropyl)-2-(5-bromo-2-(hexadecylsulfonamido)phenyl)-2-oxoacetamide hydrochloride
(29b)

¹H NMR (400 MHz, DMSO-*d*₆):

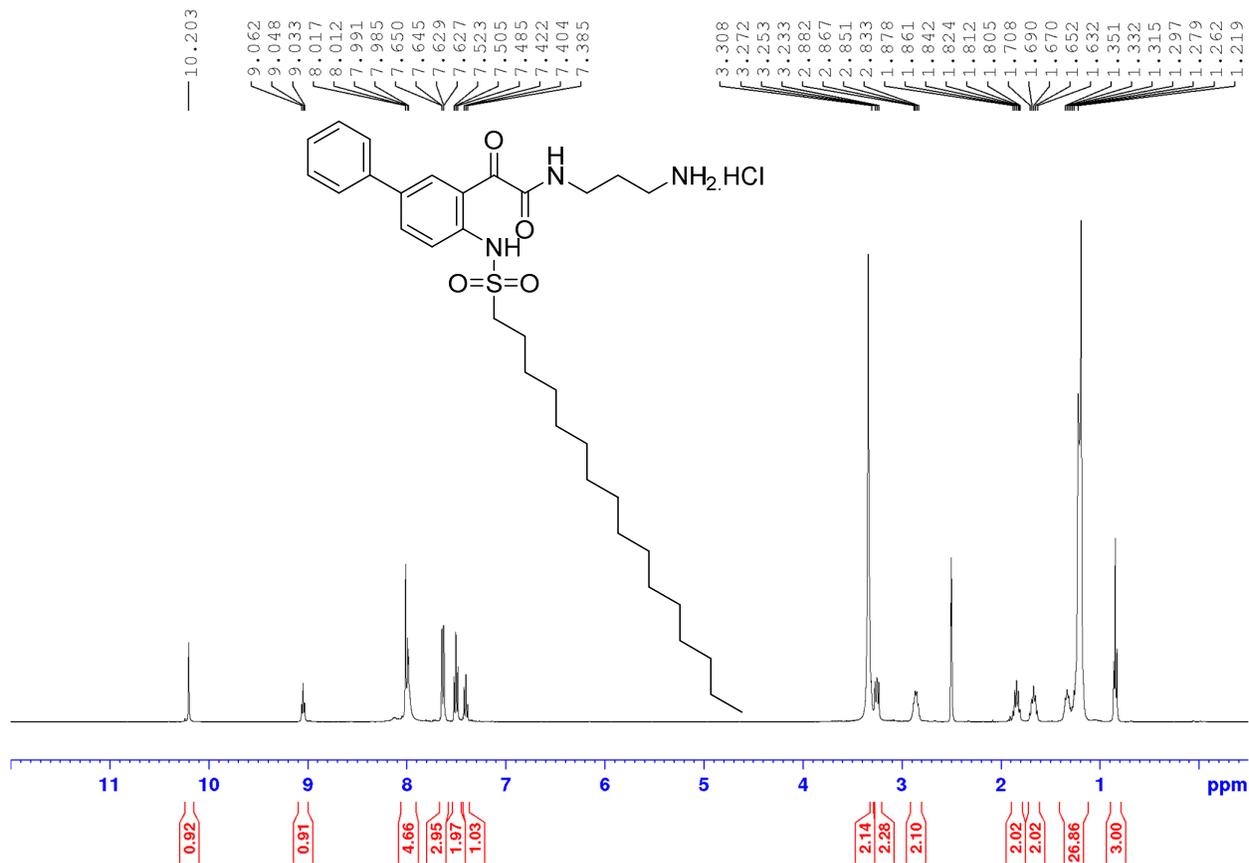


¹³C NMR (100 MHz, DMSO-*d*₆):

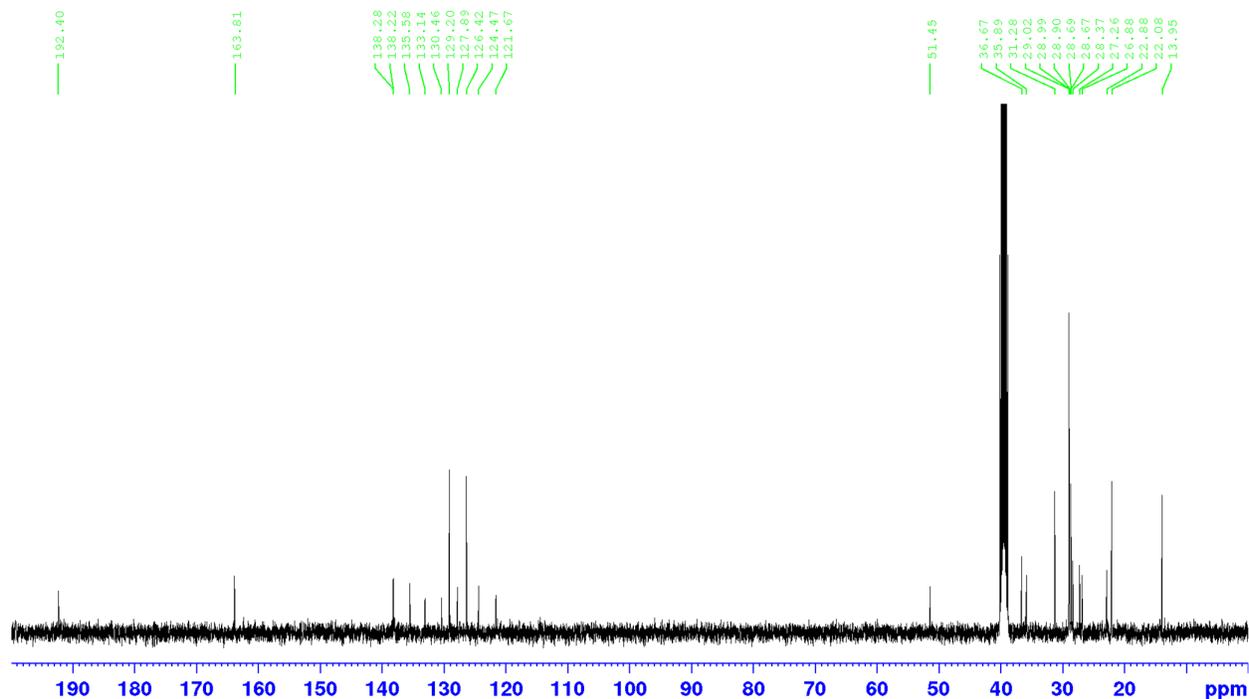


N-(3-Aminopropyl)-2-(4-(hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamide hydrochloride (**29c**)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

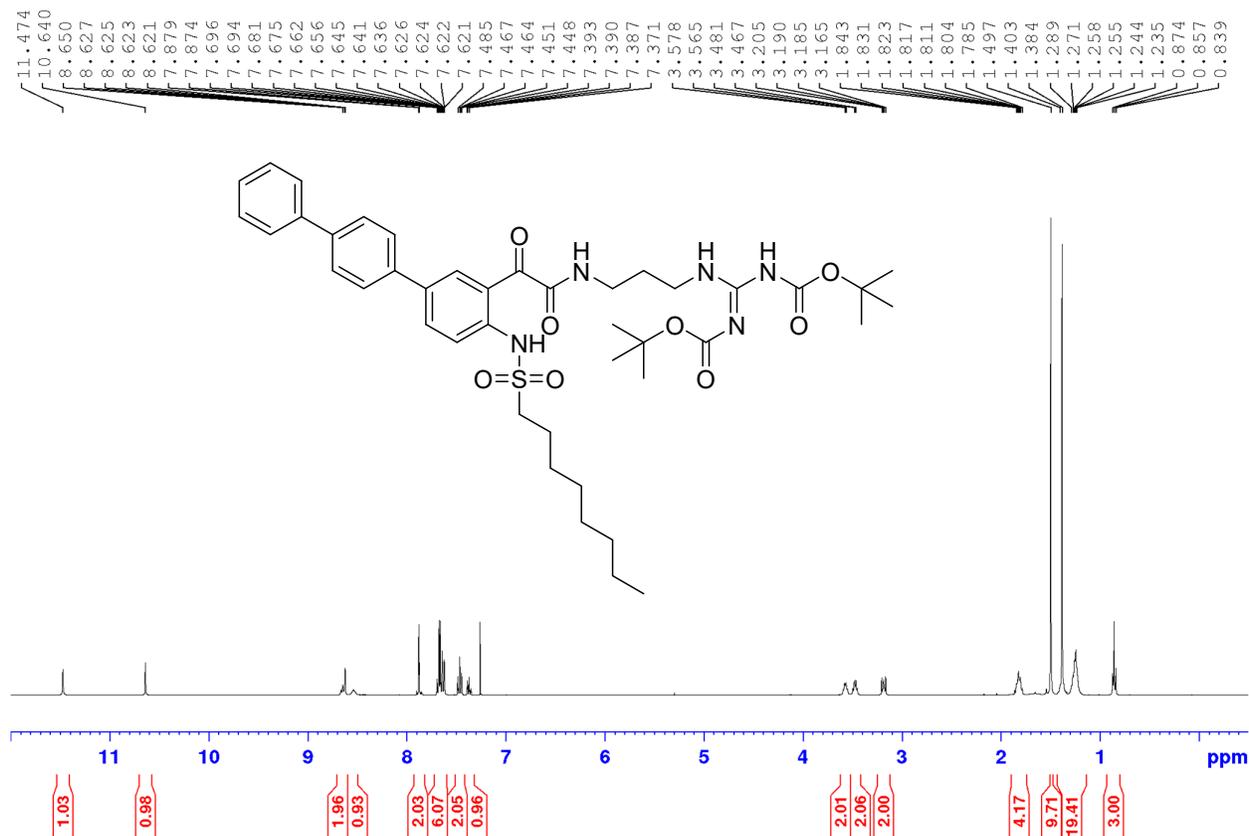


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):

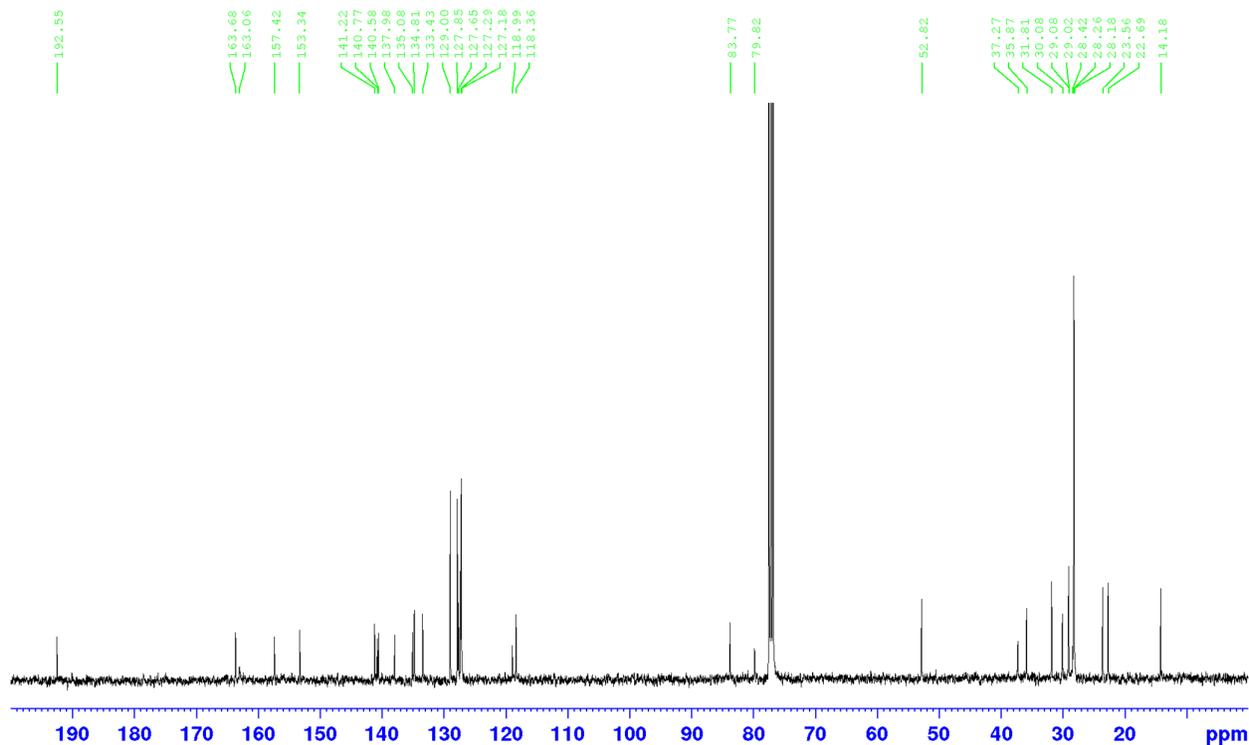


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(4-(octylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamido)propyl)carbamimidoyl)-1-oxidanecarboxamide (**30d**)

^1H NMR (400 MHz, CDCl_3):

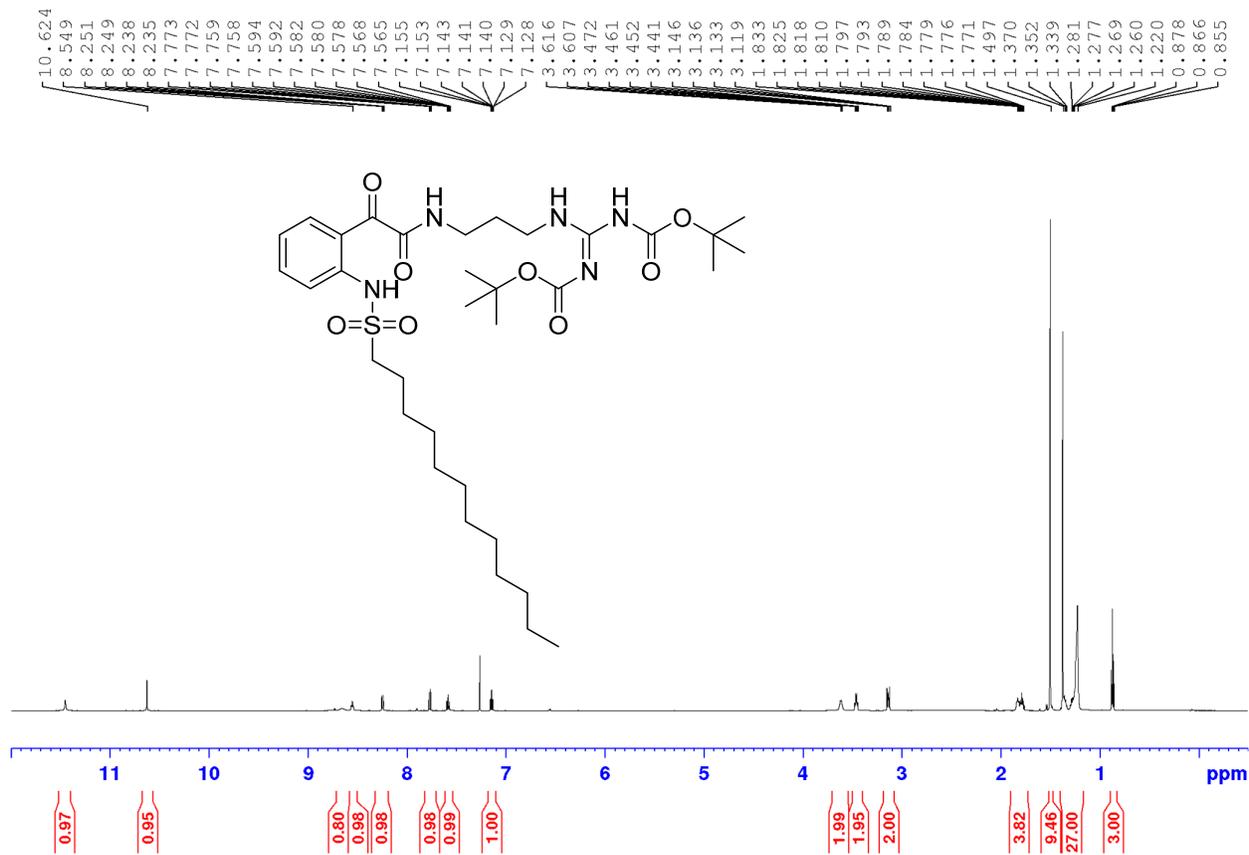


^{13}C NMR (100 MHz, CDCl_3):

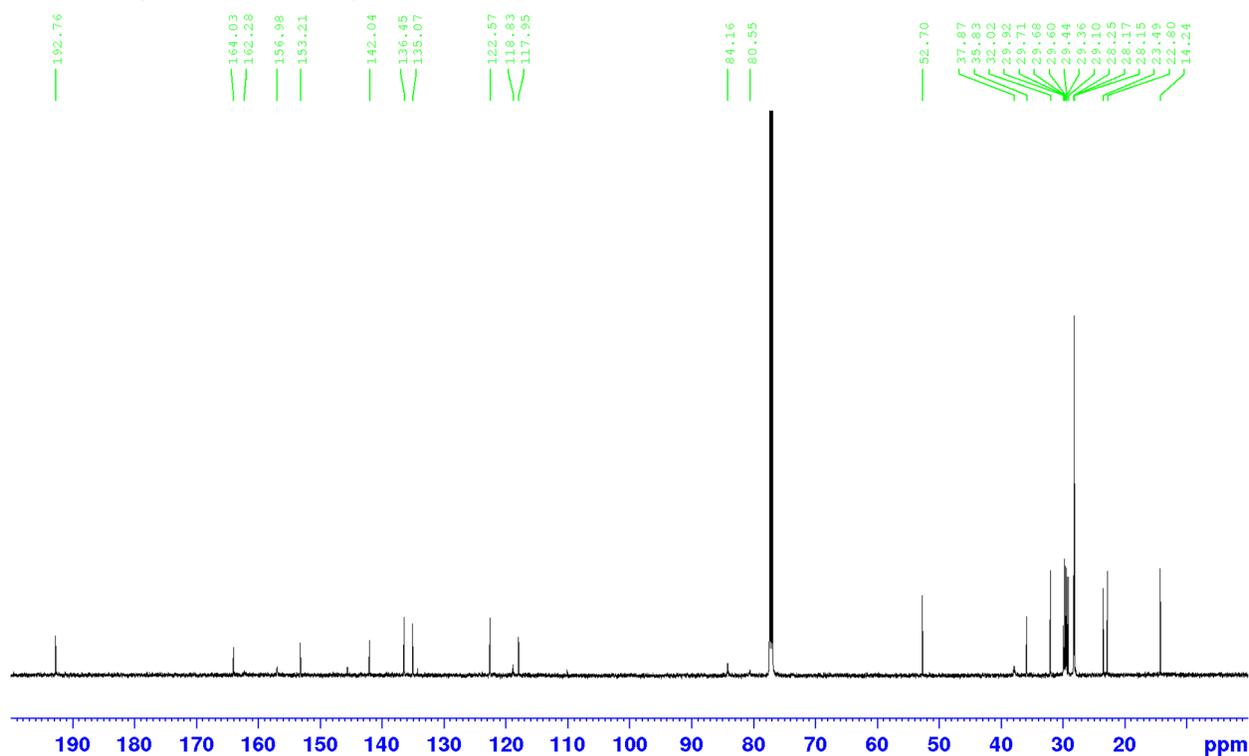


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(2-(dodecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamimidoyl)-1-oxidanecarboxamide (**31a**)

^1H NMR (600 MHz, CDCl_3):

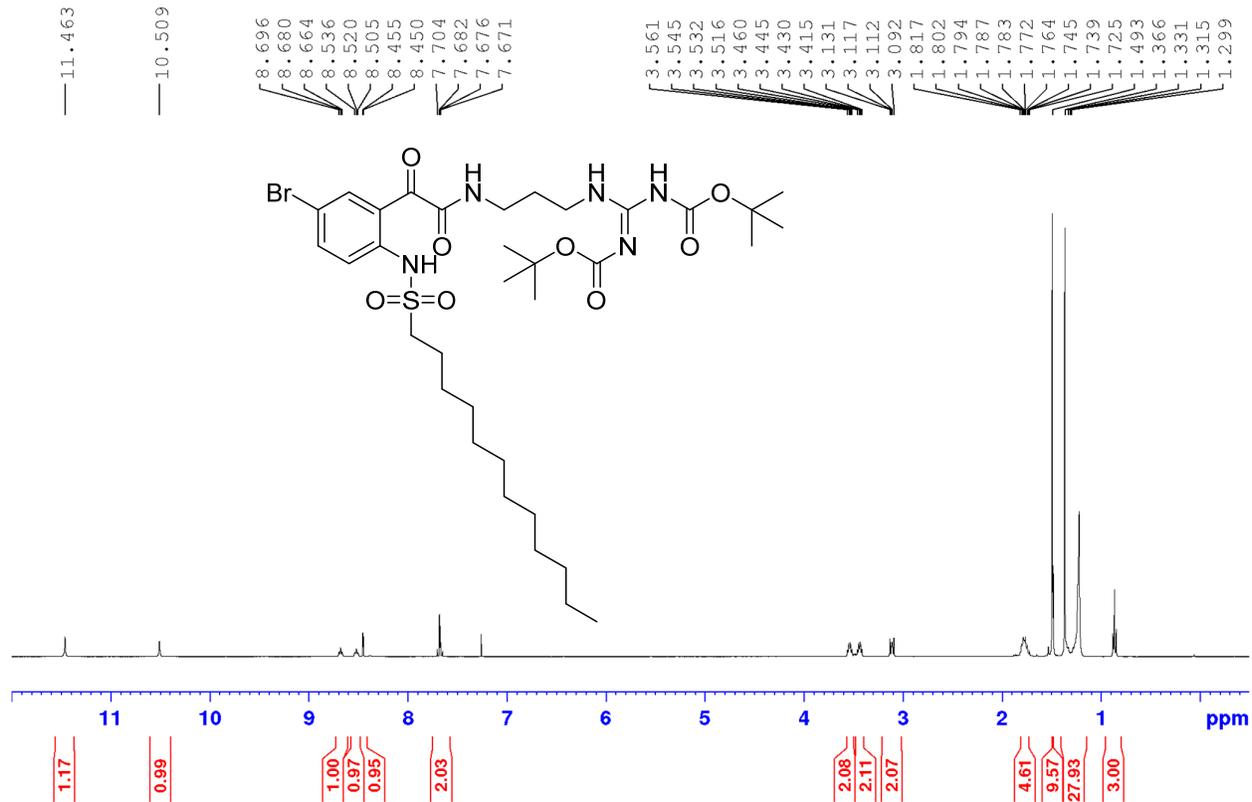


^{13}C NMR (150 MHz, CDCl_3):

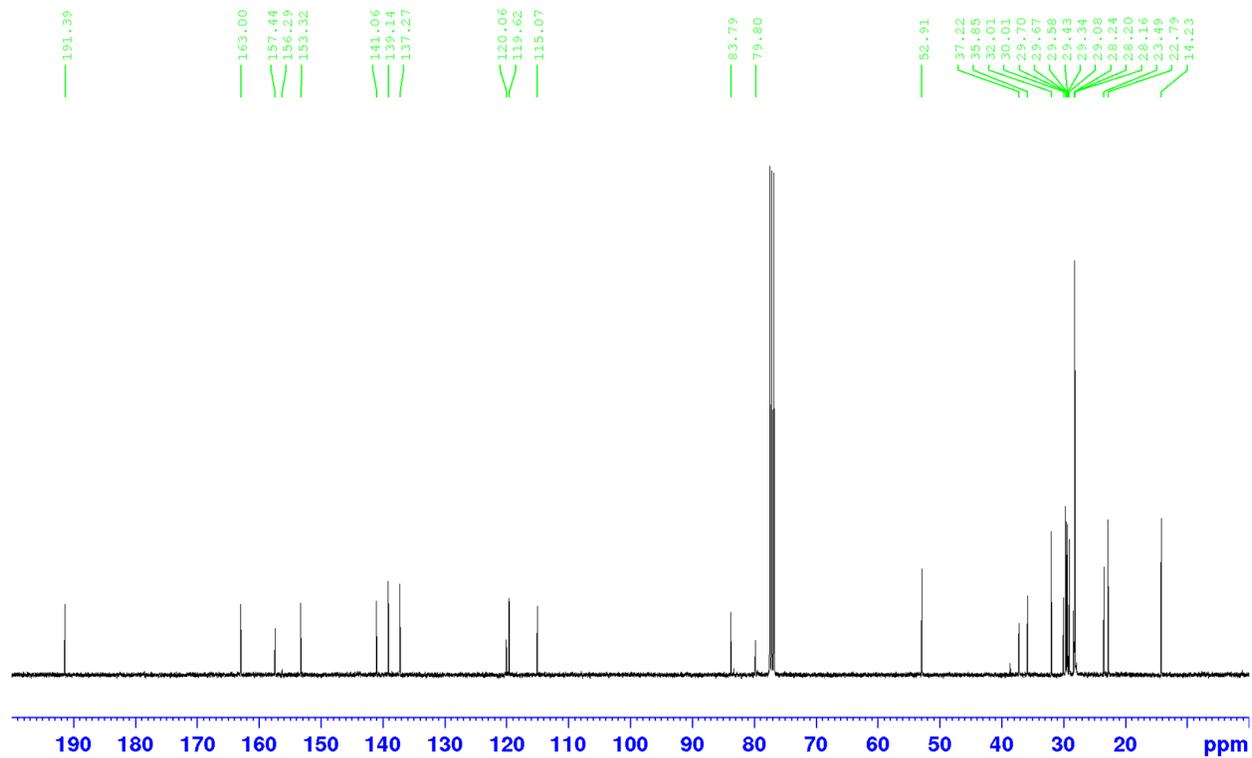


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(5-bromo-2-(dodecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamimidoyl)-1-oxidanecarboxamide (**31b**)

^1H NMR (400 MHz, CDCl_3):

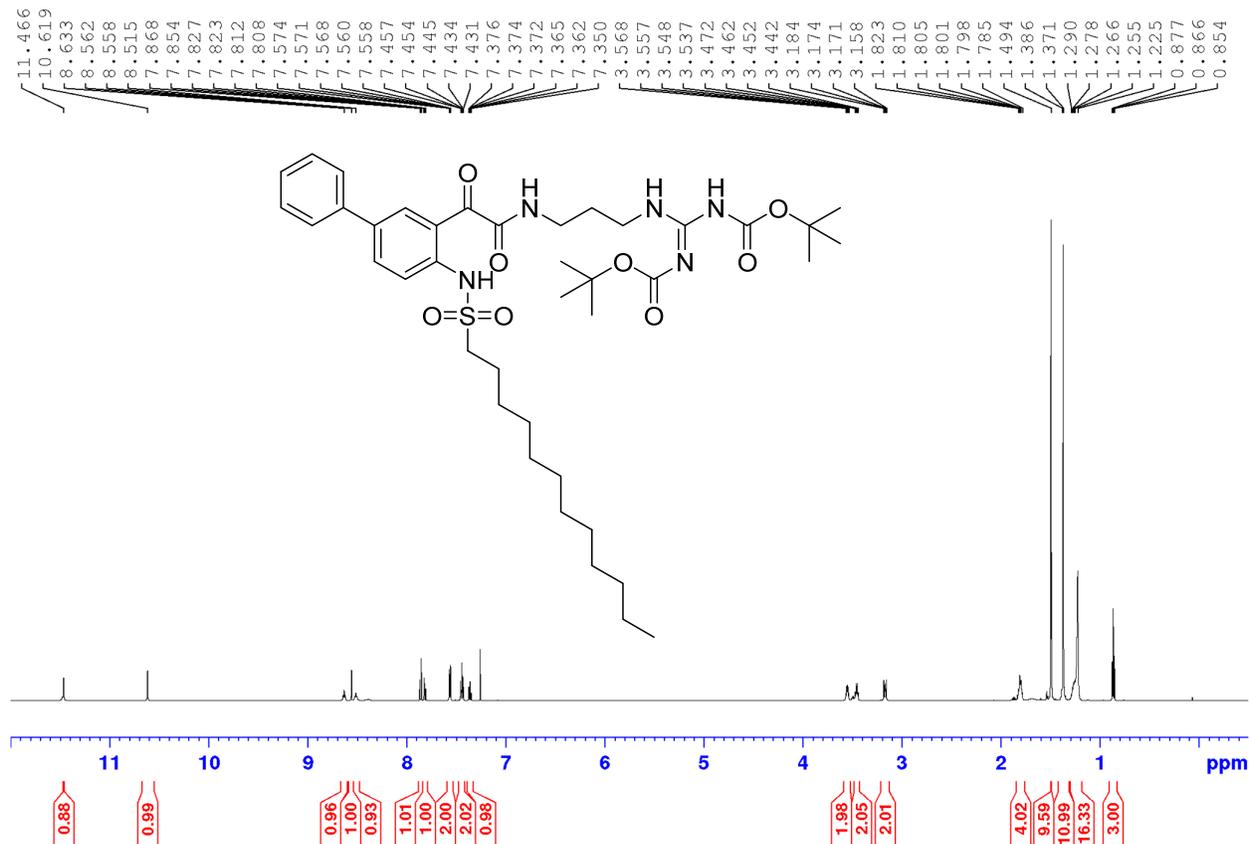


^{13}C NMR (100 MHz, CDCl_3):

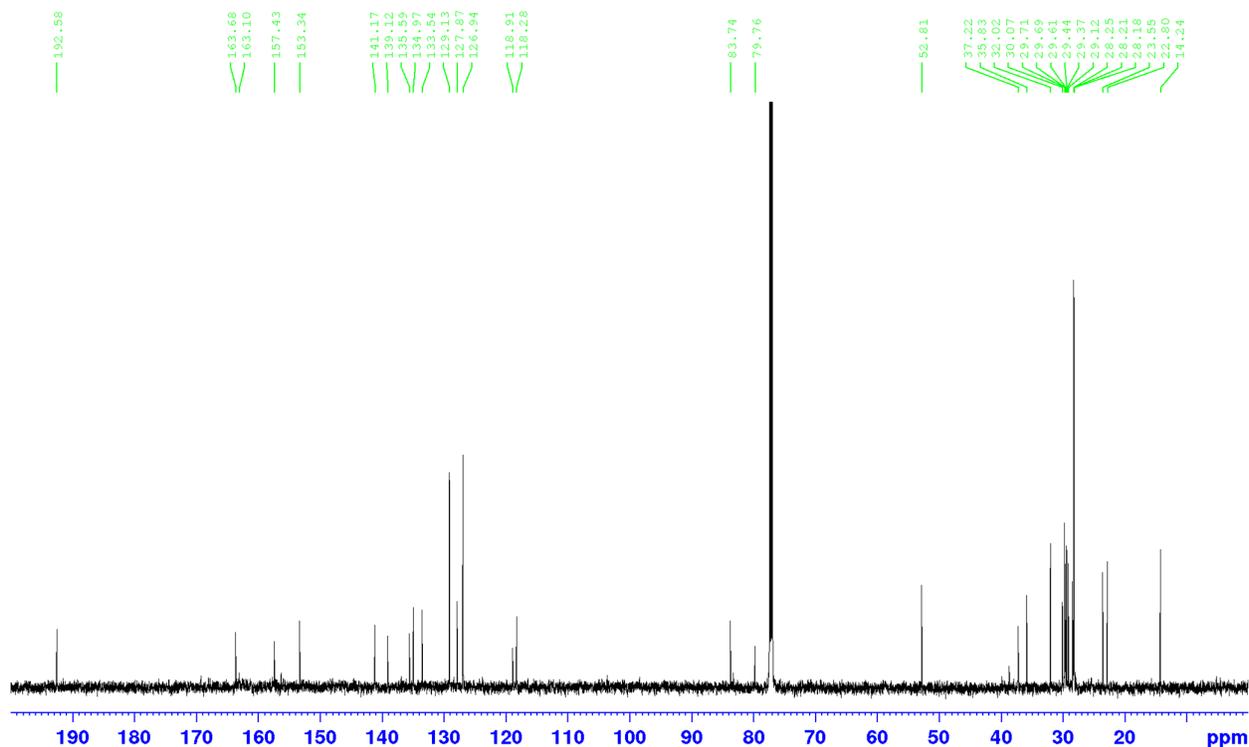


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(4-(dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)propyl)carbamimidoyl)-1-oxidanecarboxamide (**31c**)

^1H NMR (400 MHz, CDCl_3):

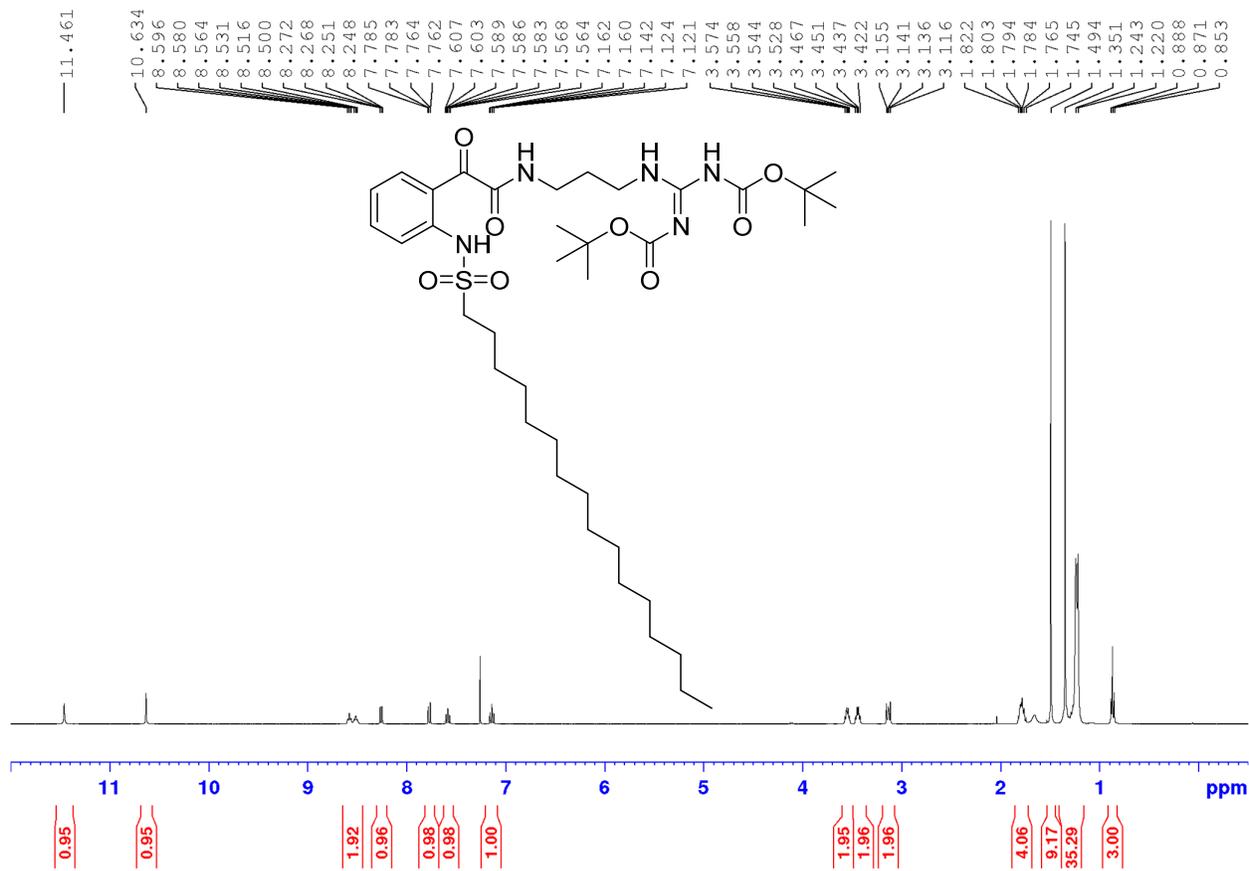


^{13}C NMR (100 MHz, CDCl_3):

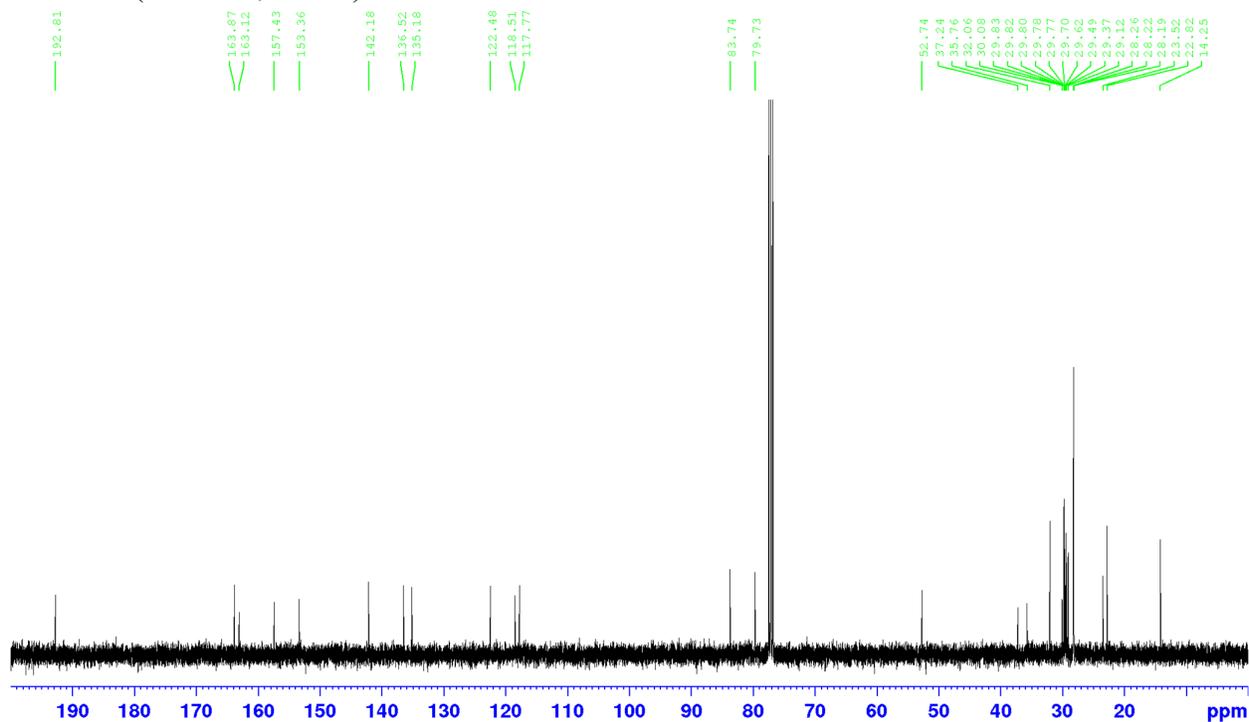


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(2-(hexadecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamimidoyl)-1-oxidanecarboxamide (**32a**)

^1H NMR (400 MHz, CDCl_3):

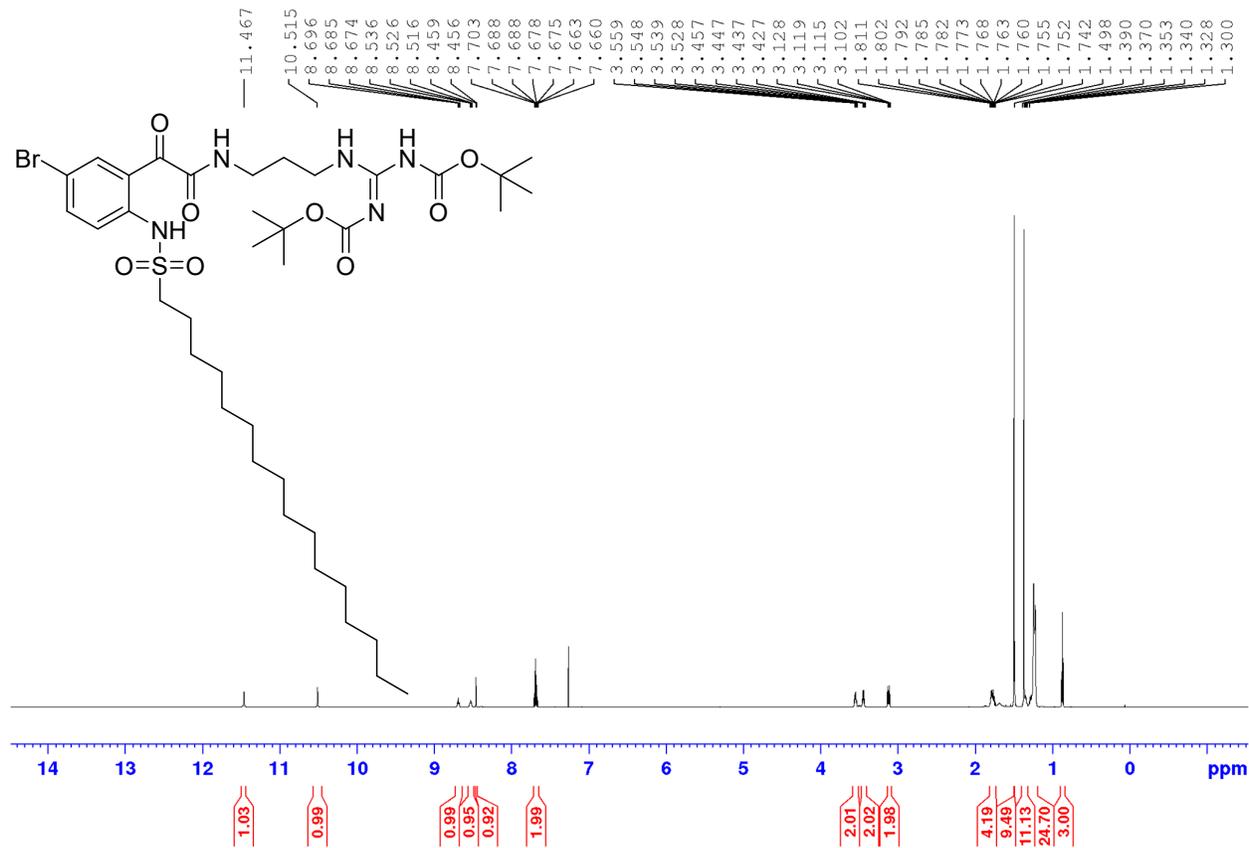


^{13}C NMR (100 MHz, CDCl_3):

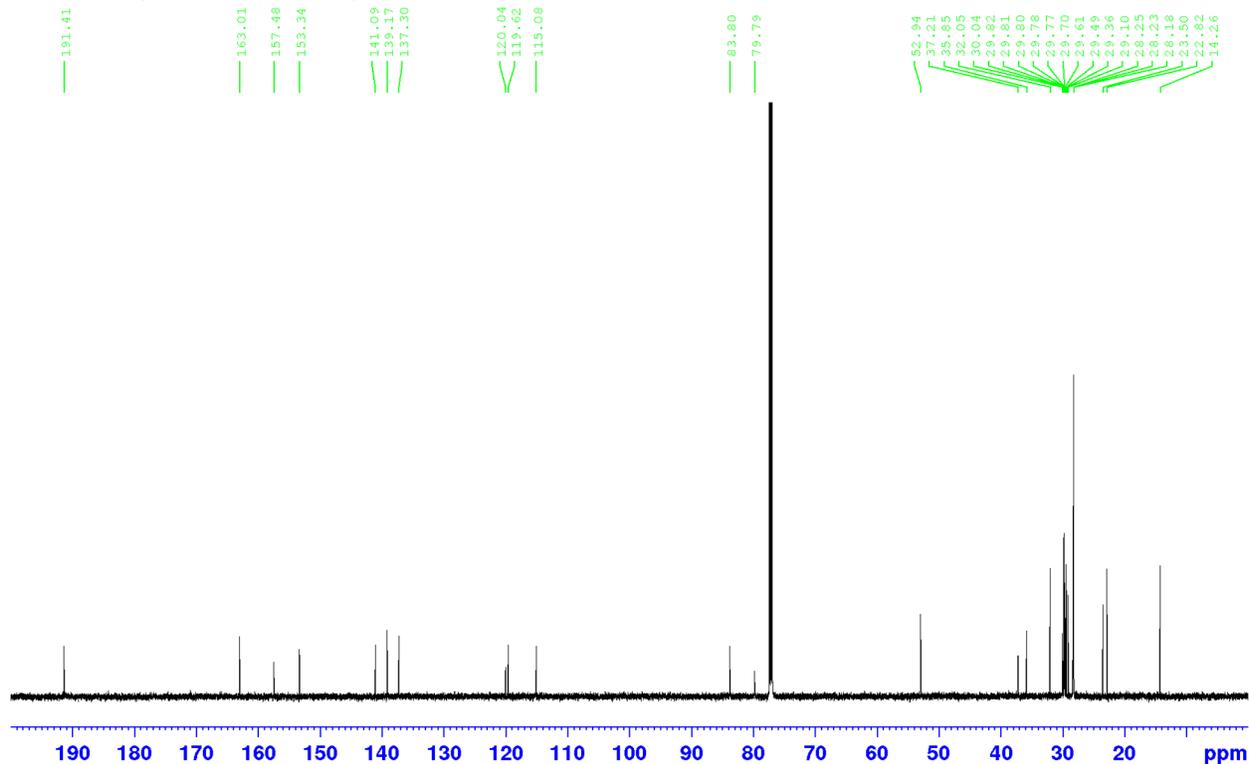


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(5-bromo-2-(hexadecylsulfonamido)phenyl)-2-oxoacetamido)propyl)carbamimidoyl)-1-oxidanecarboxamide (**32b**)

^1H NMR (600 MHz, CDCl_3):

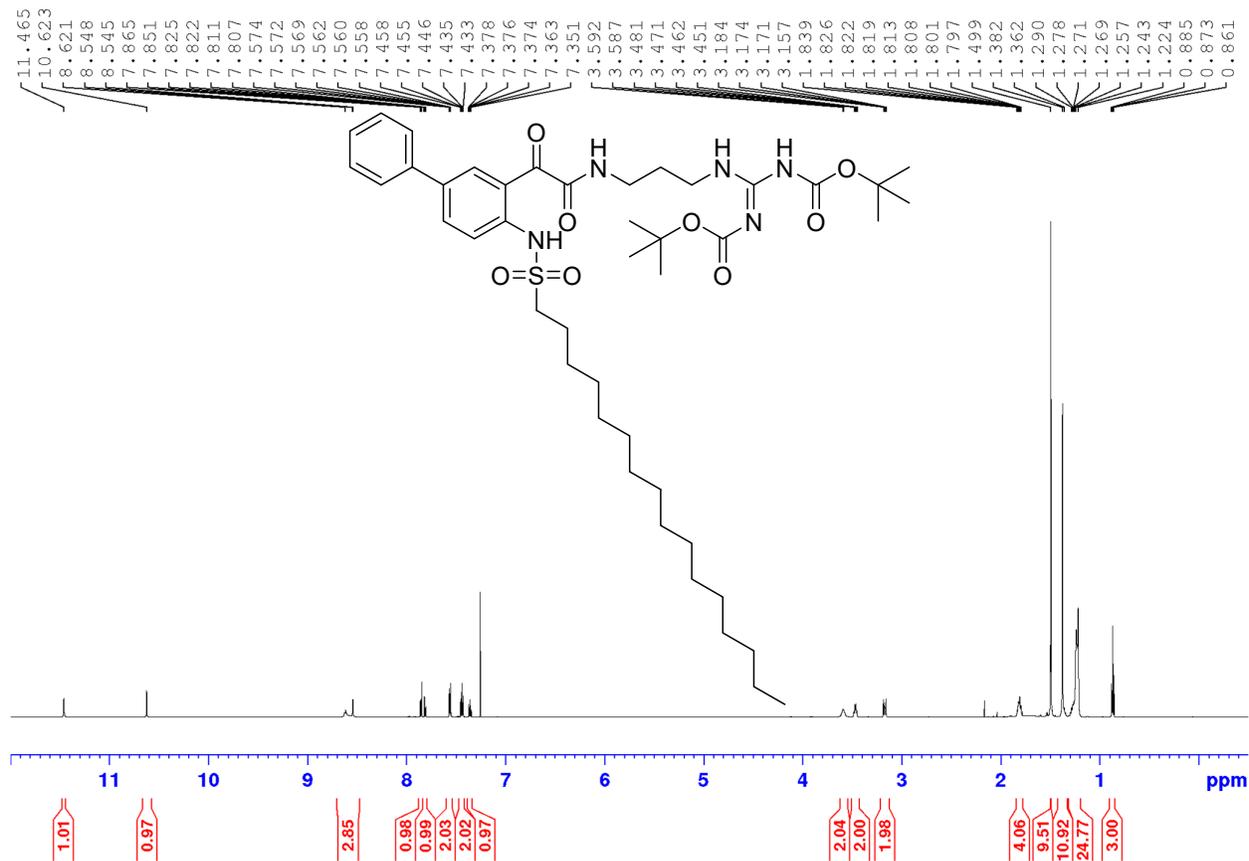


^{13}C NMR (150 MHz, CDCl_3):

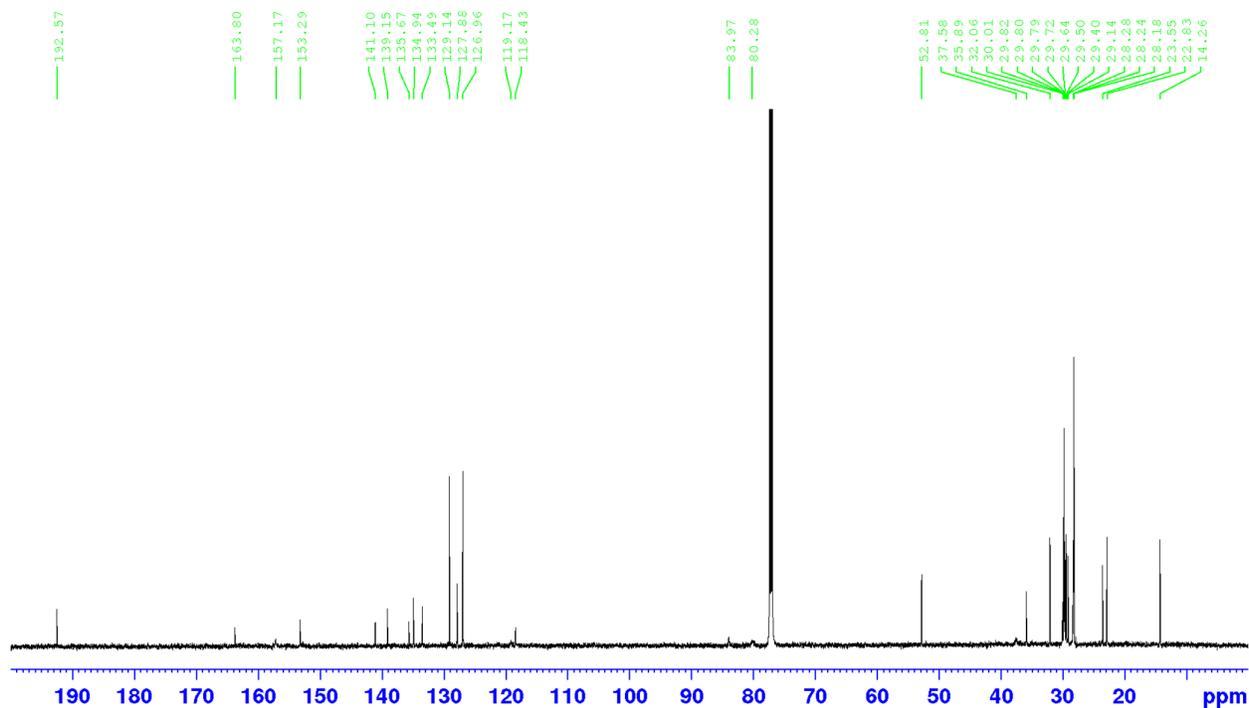


(*E*)-1-*tert*-Butyl-*N*-(*N'*-((*tert*-butyloxidanyl)carbonyl)-*N*-(3-(2-(4-(hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamido)propyl)carbamidoyl)-1-oxidanecarboxamide (**32c**)

^1H NMR (600 MHz, CDCl_3):

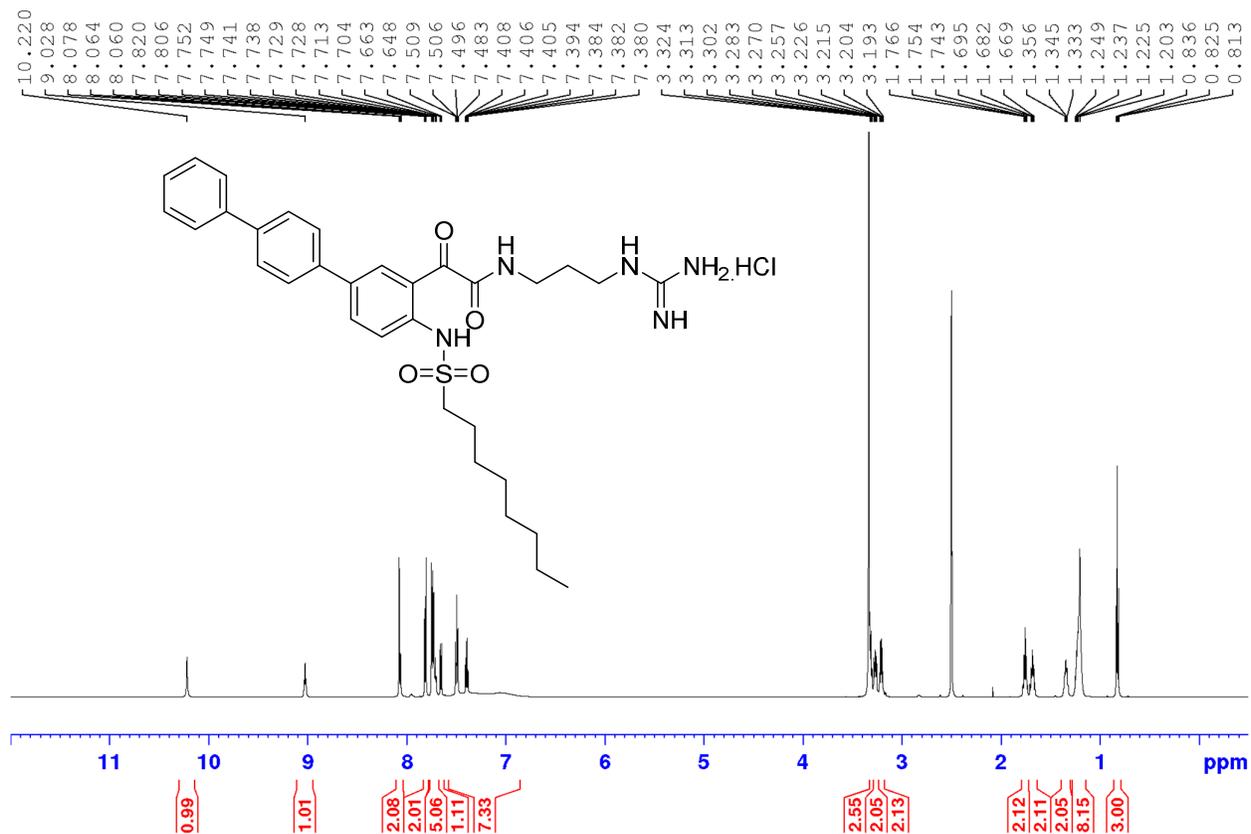


^{13}C NMR (150 MHz, CDCl_3):

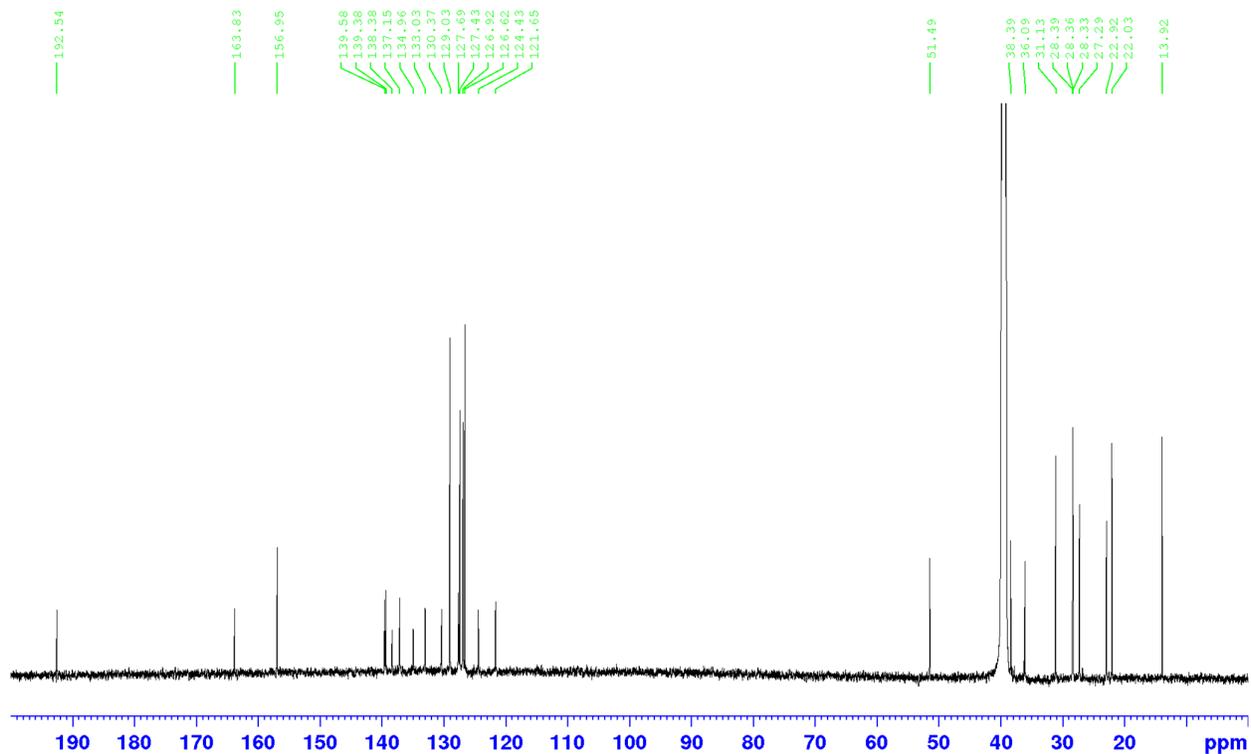


N-(3-Guanidinopropyl)-2-(4-(octylsulfonamido)-[1,1':4',1''-terphenyl]-3-yl)-2-oxoacetamide hydrochloride (**33d**)

¹H NMR (600 MHz, DMSO-*d*₆):

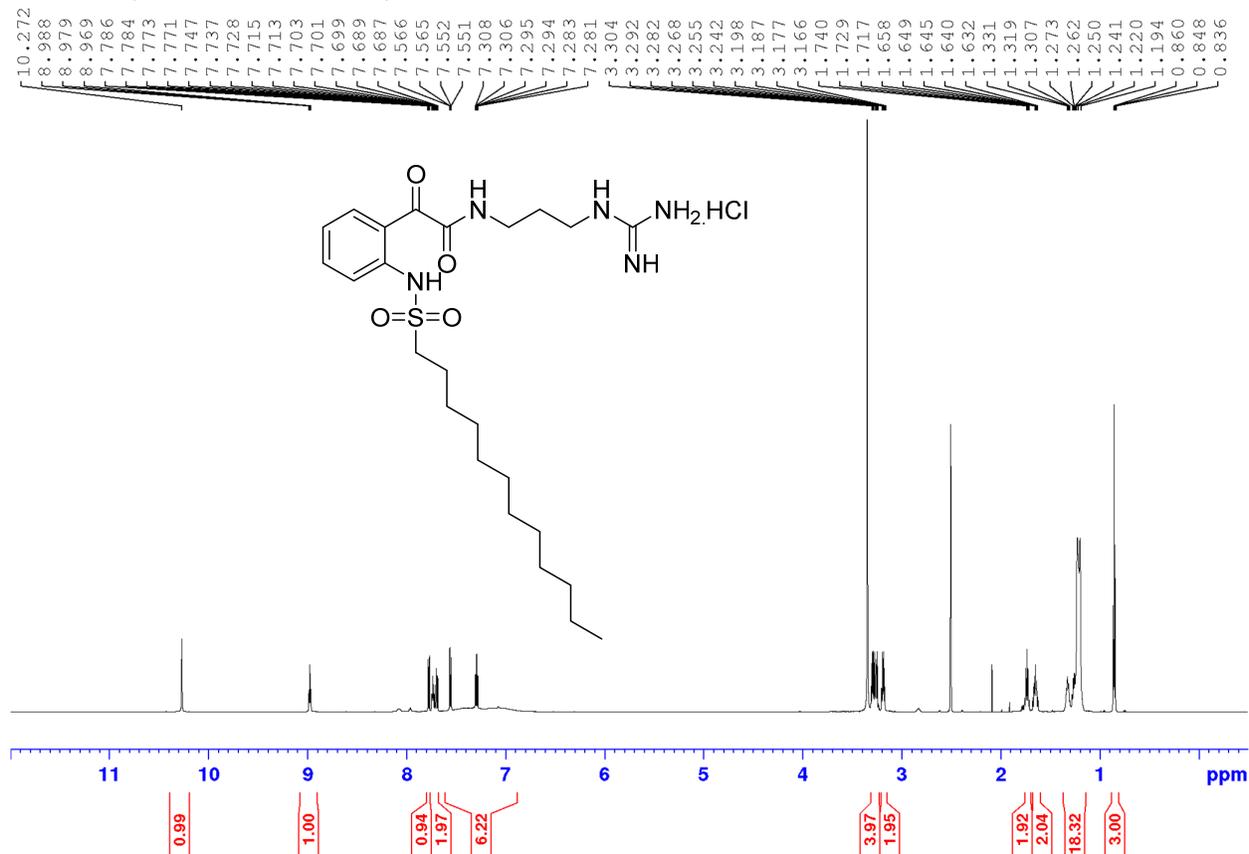


¹³C NMR (150 MHz, DMSO-*d*₆):

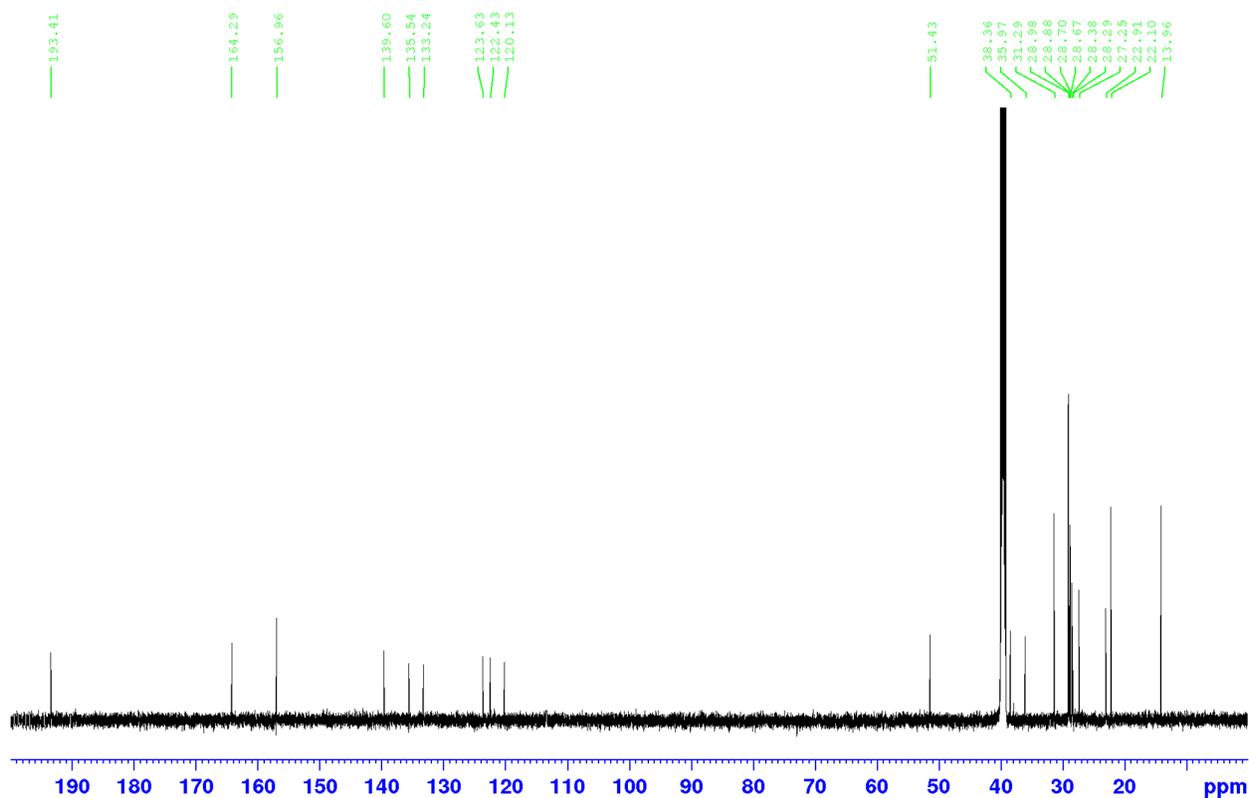


2-(2-(Dodecylsulfonamido)phenyl)-N-(3-guanidinopropyl)-2-oxoacetamide hydrochloride (**34a**)

¹H NMR (600 MHz, DMSO-*d*₆):

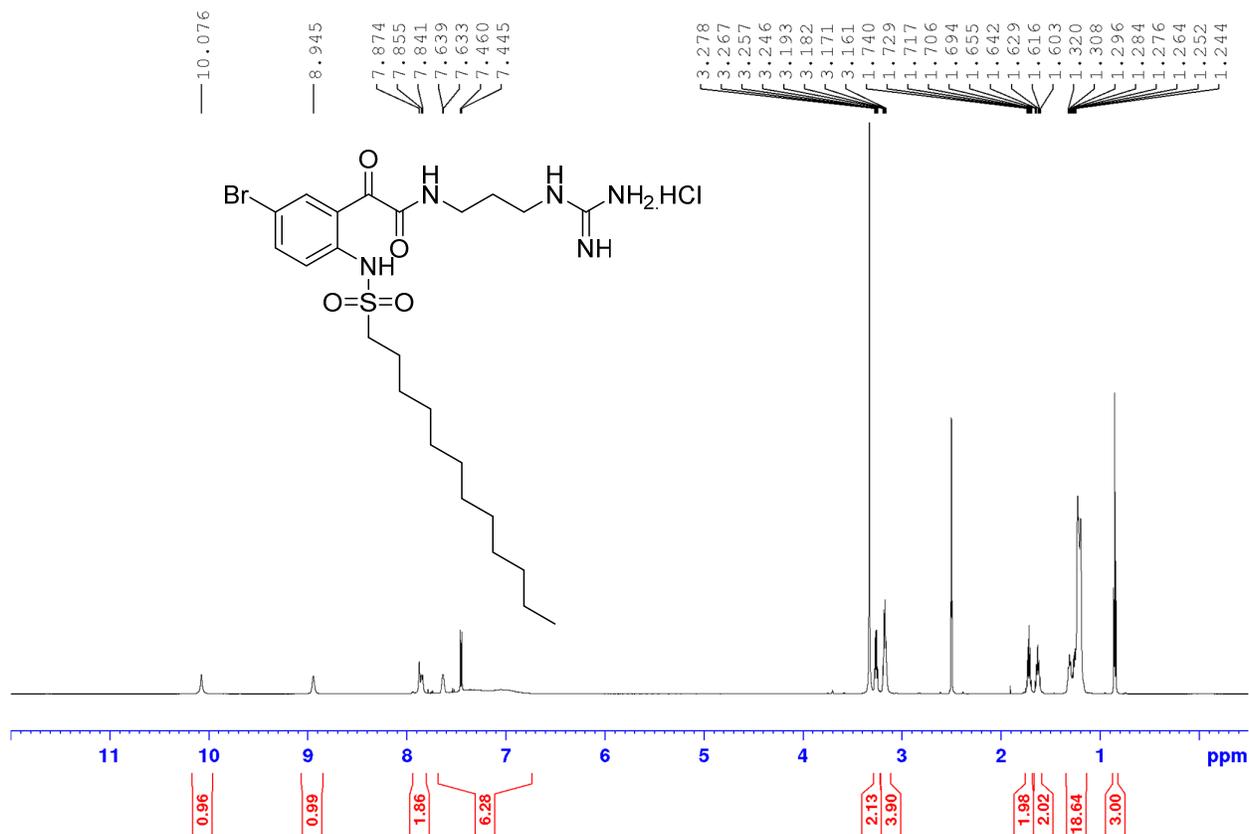


¹³C NMR (150 MHz, DMSO-*d*₆):

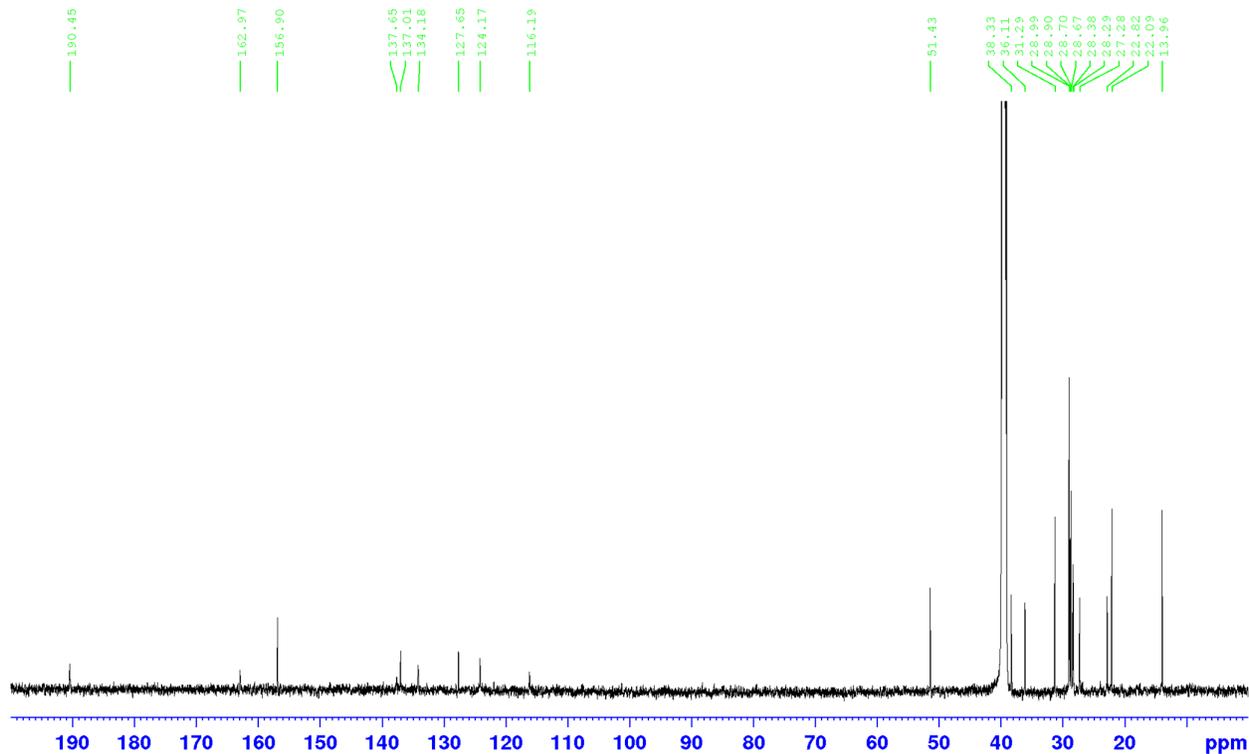


2-(5-Bromo-2-(dodecylsulfonamido)phenyl)-*N*-(3-guanidinopropyl)-2-oxoacetamide hydrochloride
(34b)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

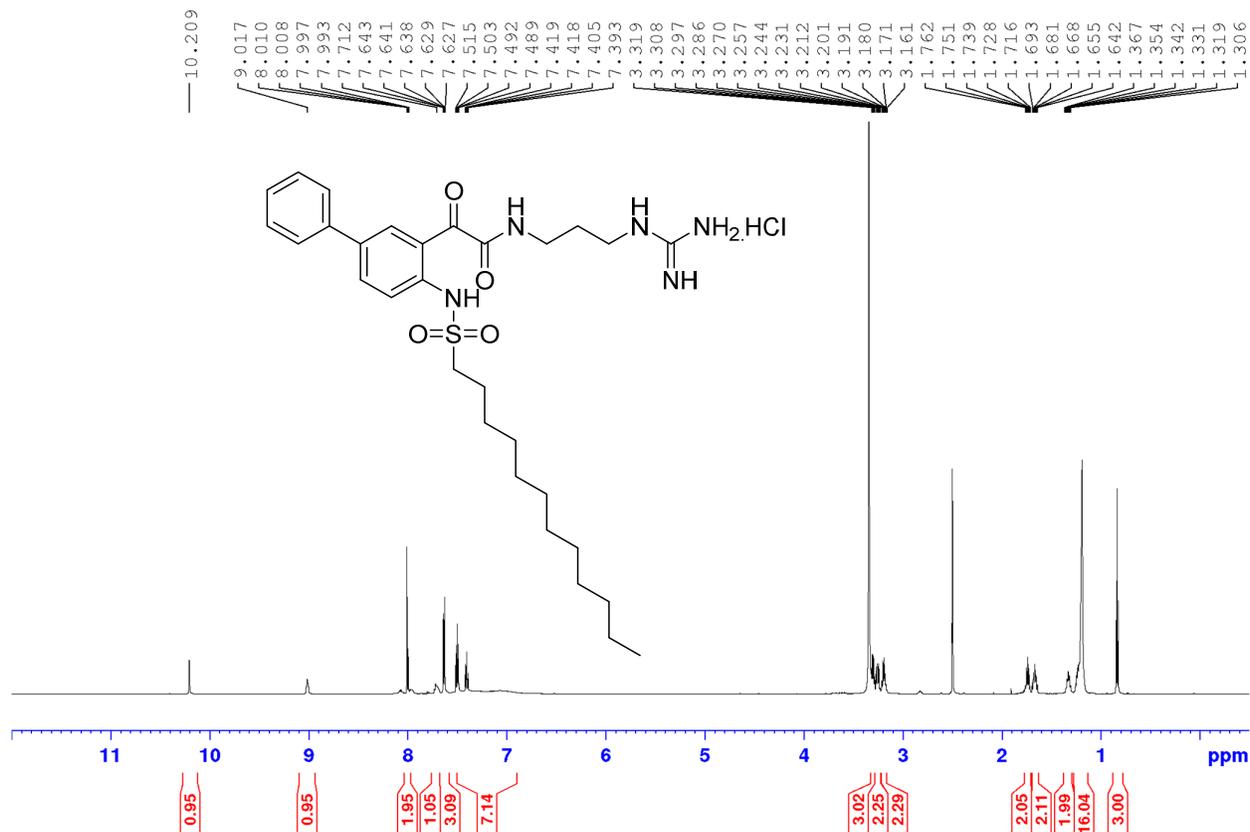


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

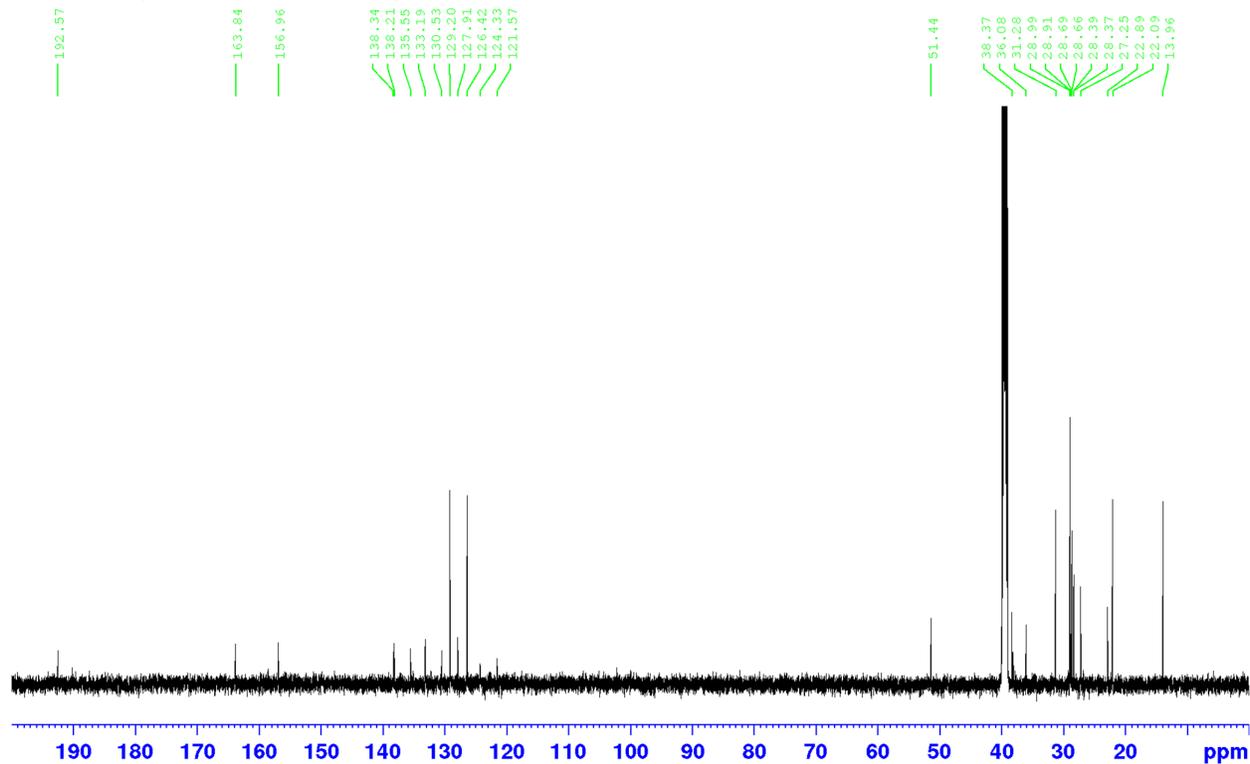


2-(4-(Dodecylsulfonamido)-[1,1'-biphenyl]-3-yl)-*N*-(3-guanidinopropyl)-2-oxoacetamide hydrochloride (**34c**)

¹H NMR (600 MHz, DMSO-*d*₆):

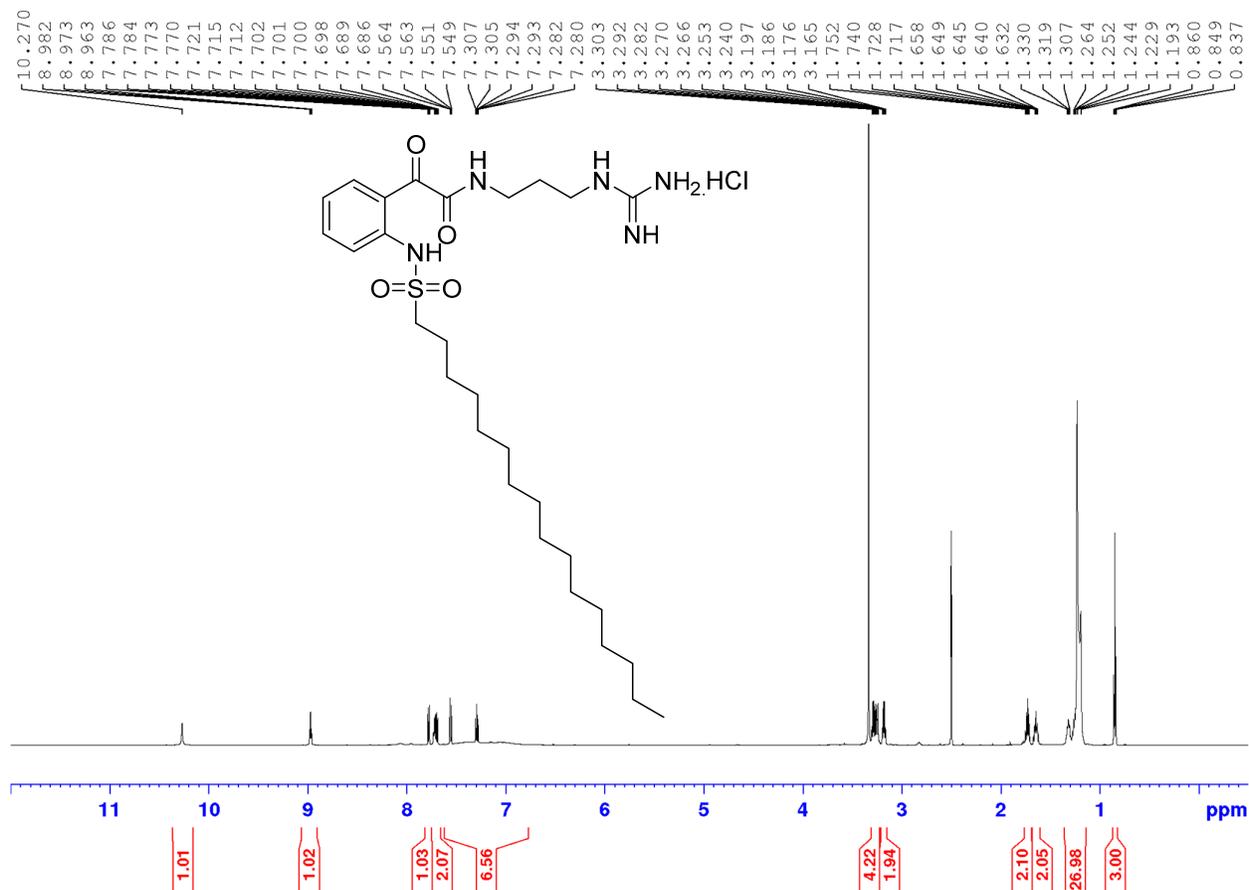


¹³C NMR (150 MHz, DMSO-*d*₆):

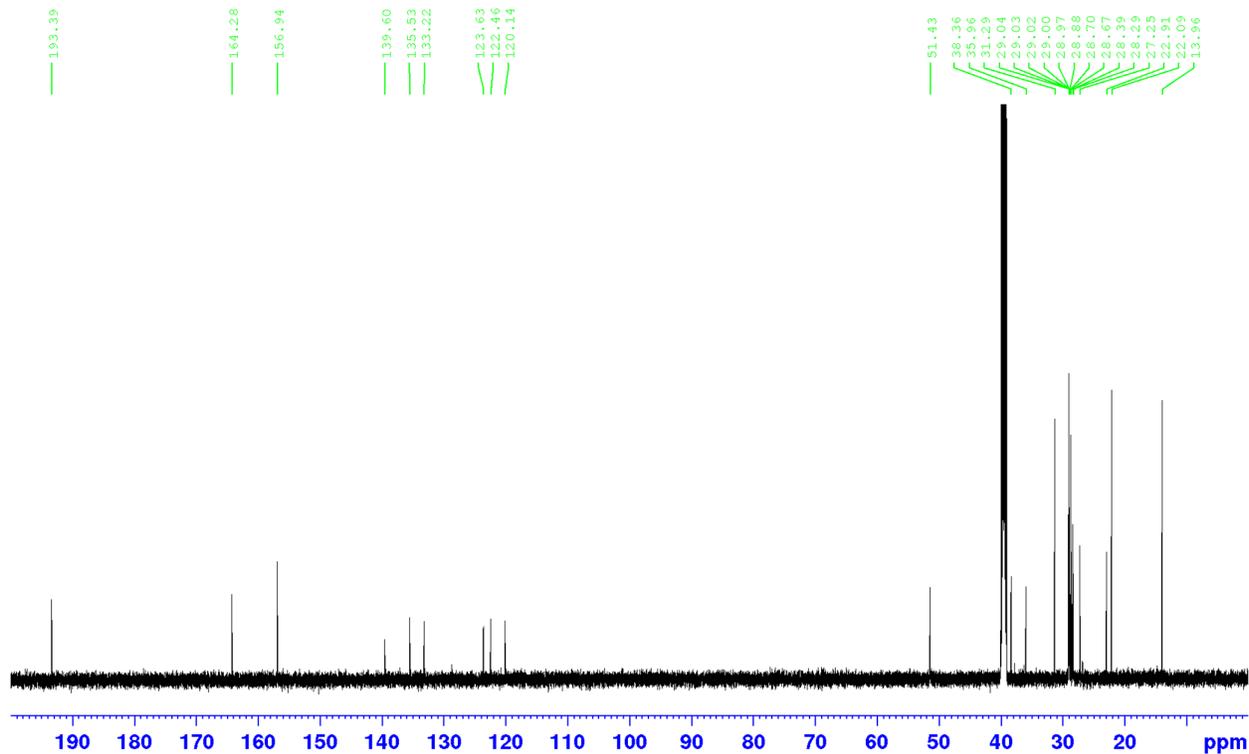


N-(3-Guanidinopropyl)-2-(2-(hexadecylsulfonamido)phenyl)-2-oxoacetamide hydrochloride (**35a**)

^1H NMR (600 MHz, $\text{DMSO-}d_6$):

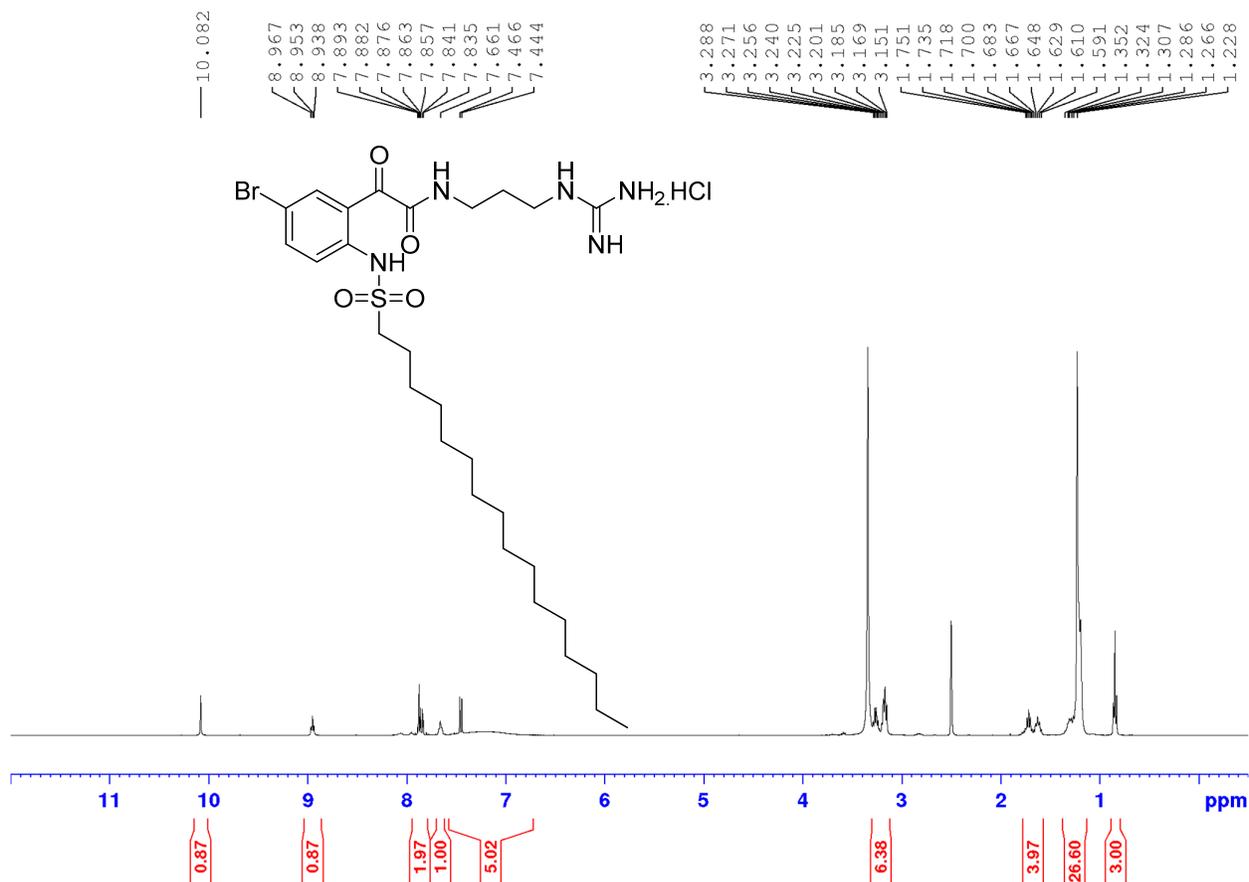


^{13}C NMR (150 MHz, $\text{DMSO-}d_6$):

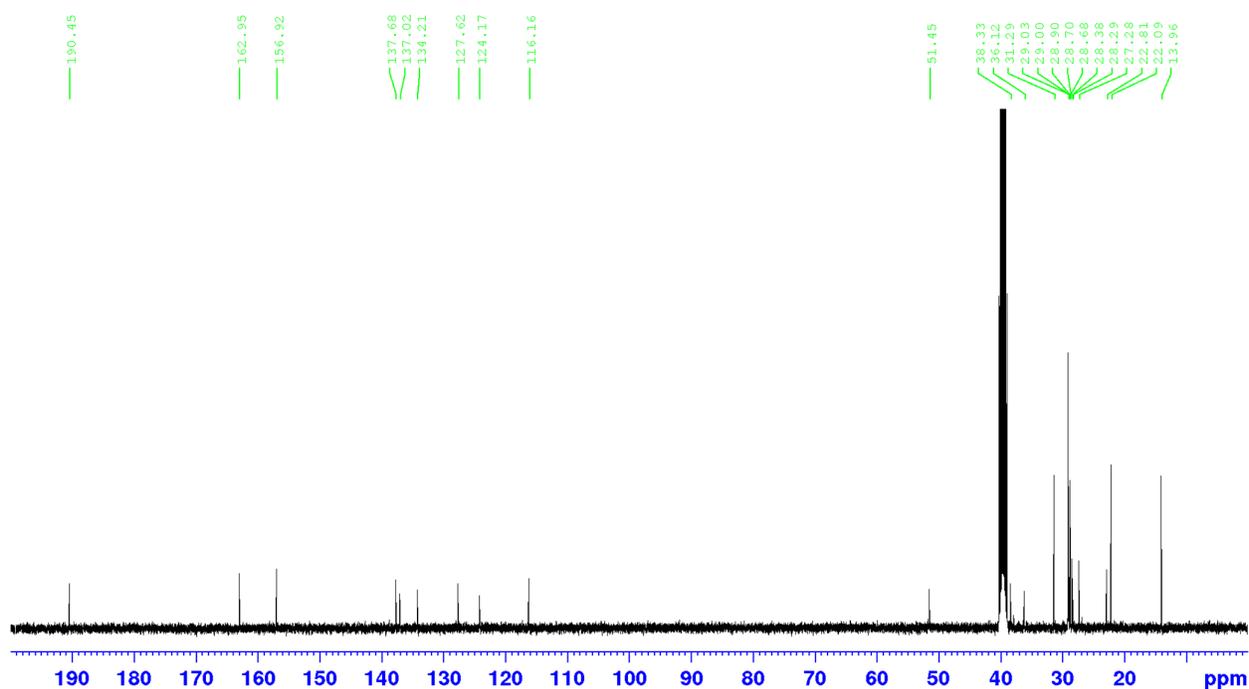


2-(5-Bromo-2-(hexadecylsulfonamido)phenyl)-*N*-(3-guanidinopropyl)-2-oxoacetamide hydrochloride
(35b)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

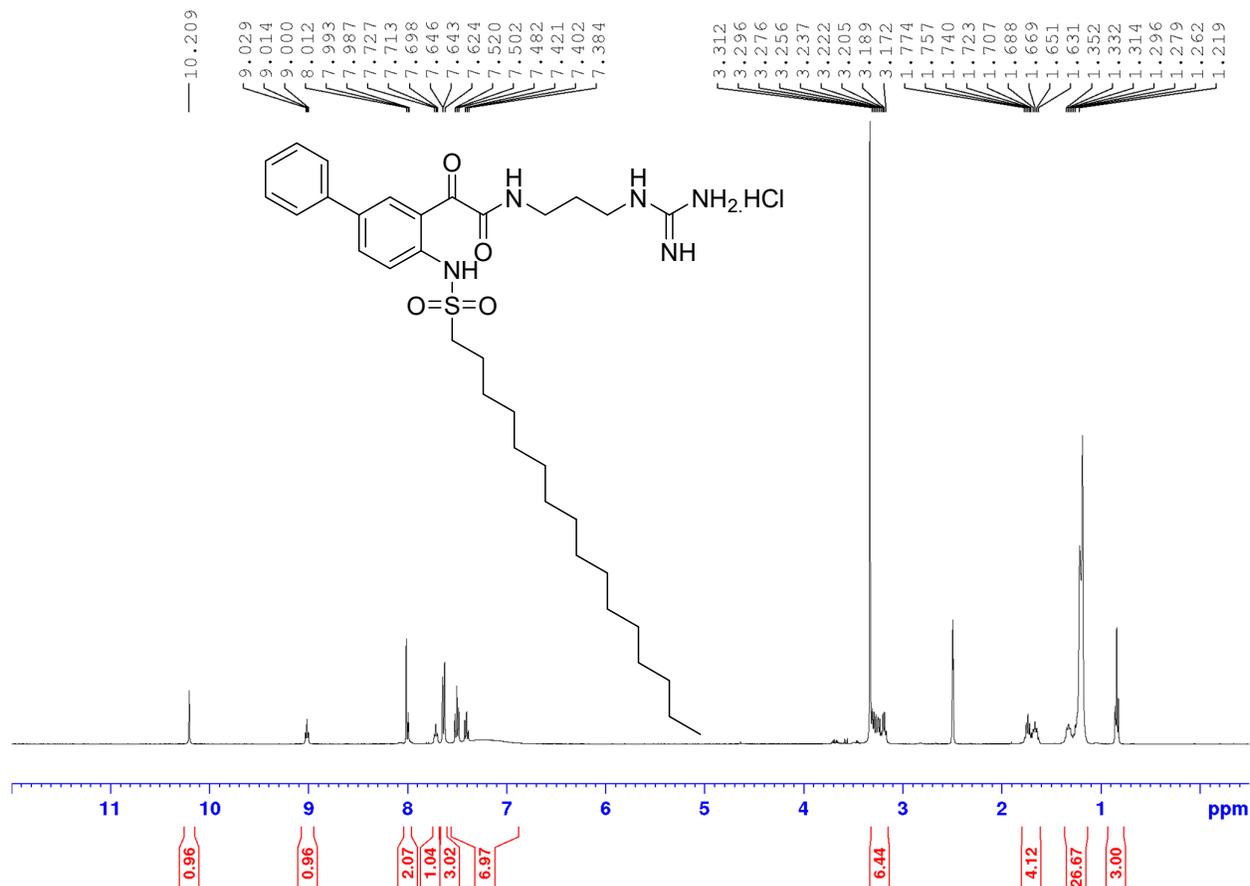


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):



N-(3-Guanidinopropyl)-2-(4-(hexadecylsulfonamido)-[1,1'-biphenyl]-3-yl)-2-oxoacetamide hydrochloride (**35c**)

¹H NMR (400 MHz, DMSO-*d*₆):



¹³C NMR (100 MHz, DMSO-*d*₆):

