

Supporting Information A

Cyclisation reactions of *N*-cinnamoyl-9-aminoanthracenes

Frank D. King, Abil Aliev, Stephen Caddick, Derek Tocher

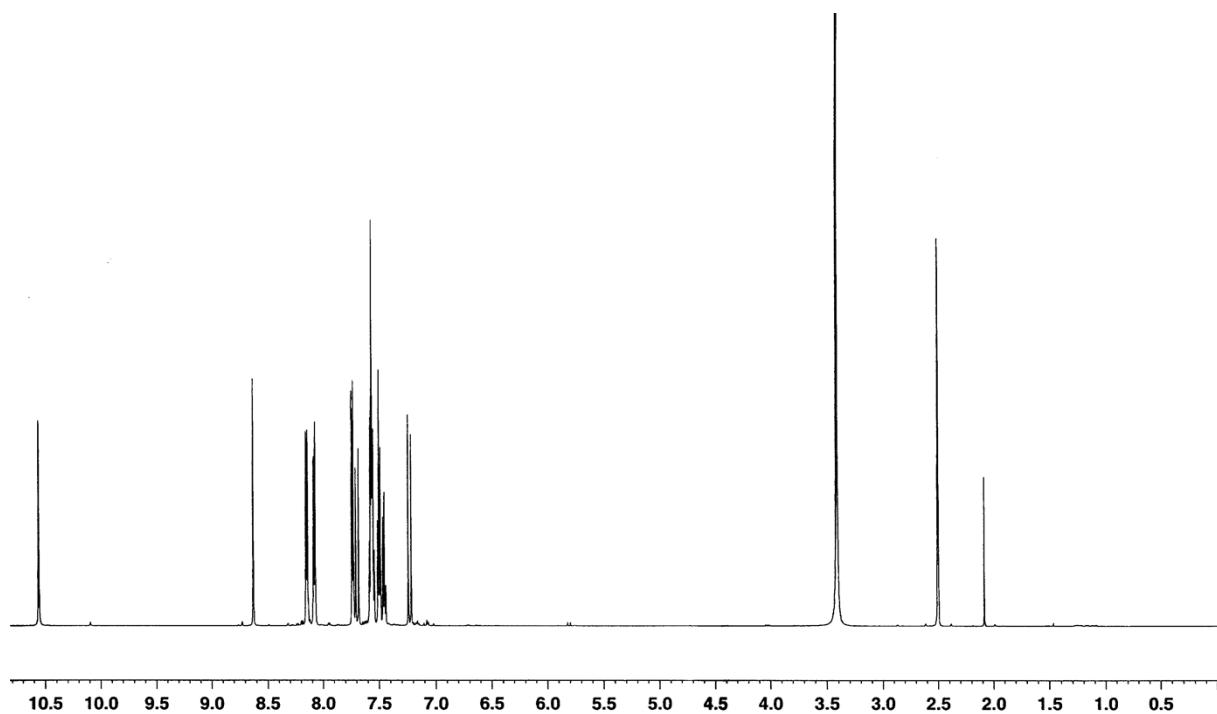
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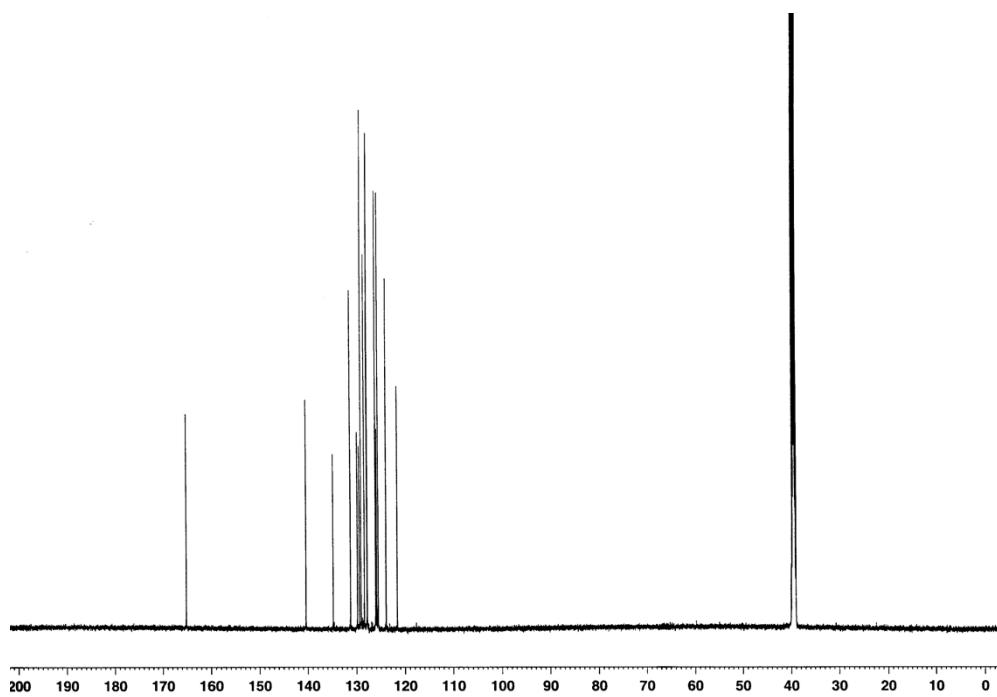
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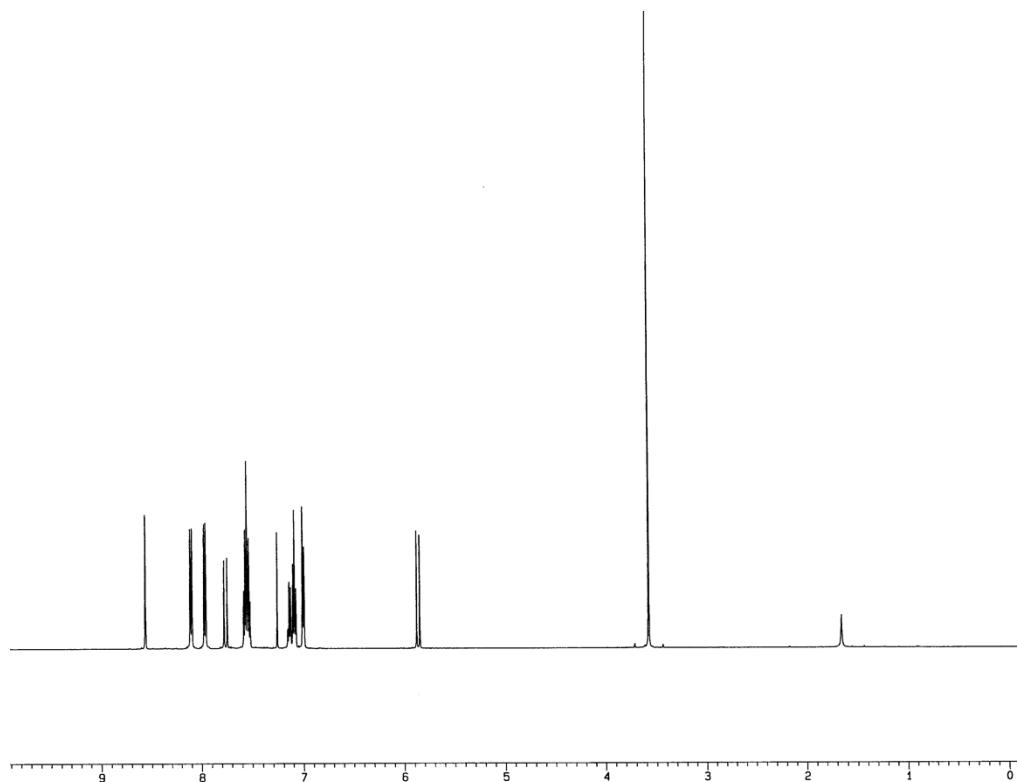
¹H-NMR (600 MHz, d⁶-DMSO) spectrum of *N*-cinnamoyl-9-aminoanthracene **3a**



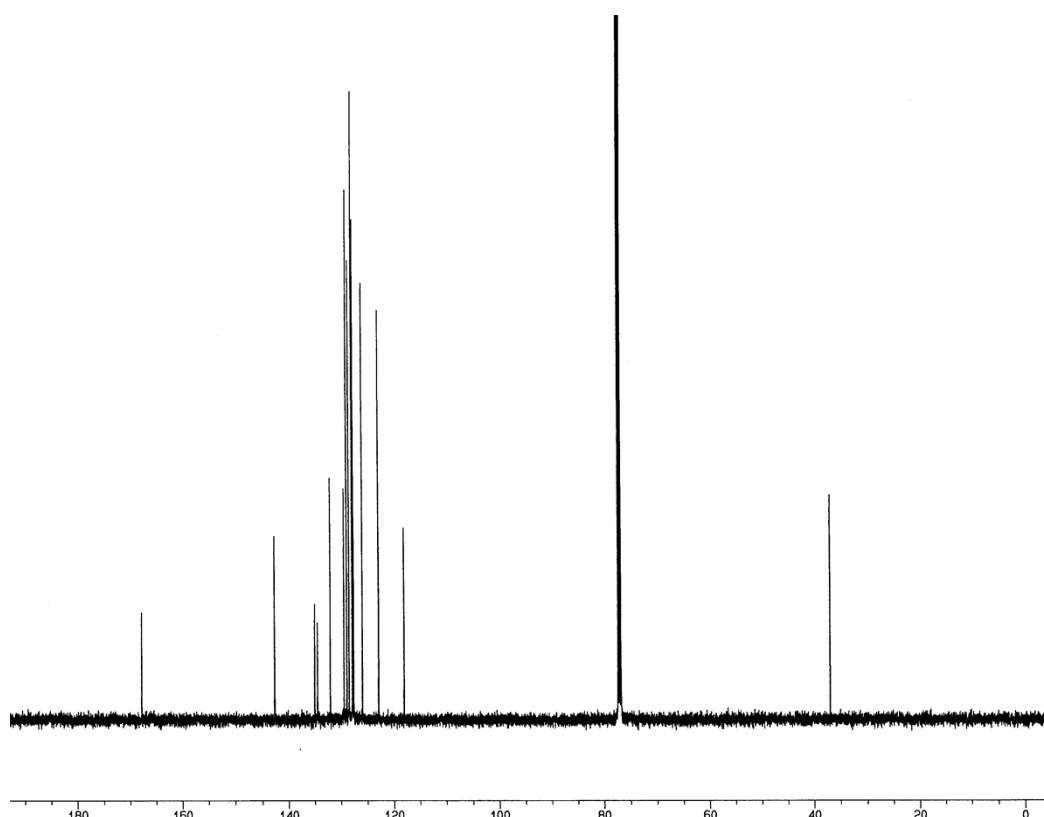
¹³C-NMR (150 MHz, d⁶-DMSO) spectrum of *N*-cinnamoyl-9-aminoanthracene **3a**



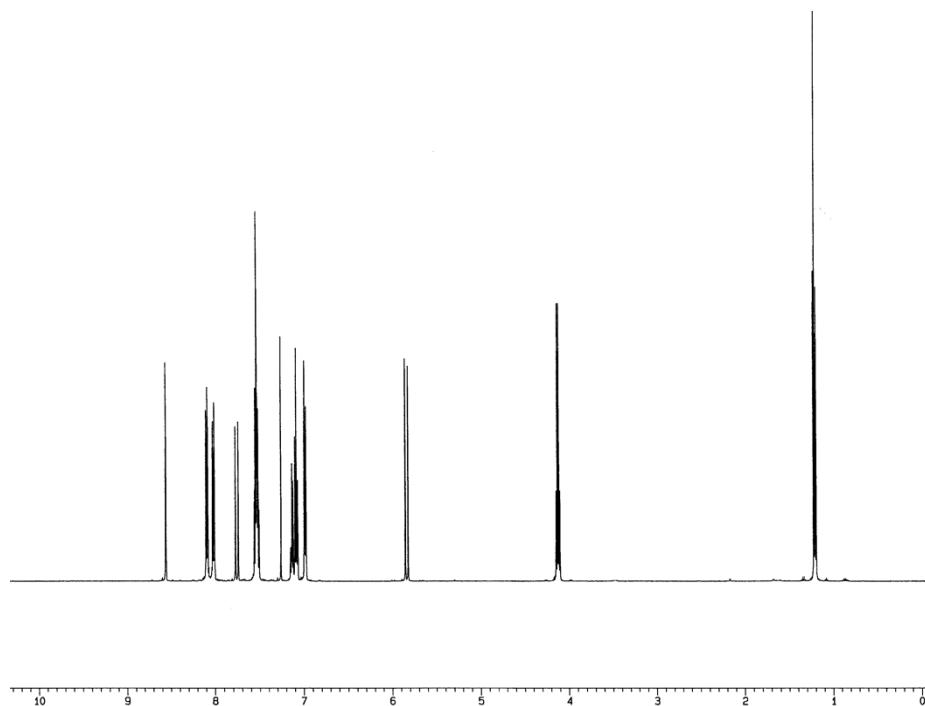
¹H-NMR spectrum (500 MHz, CDCl₃) of *N*-Methyl-*N*-cinnamoyl-9-aminoanthracene **3b**



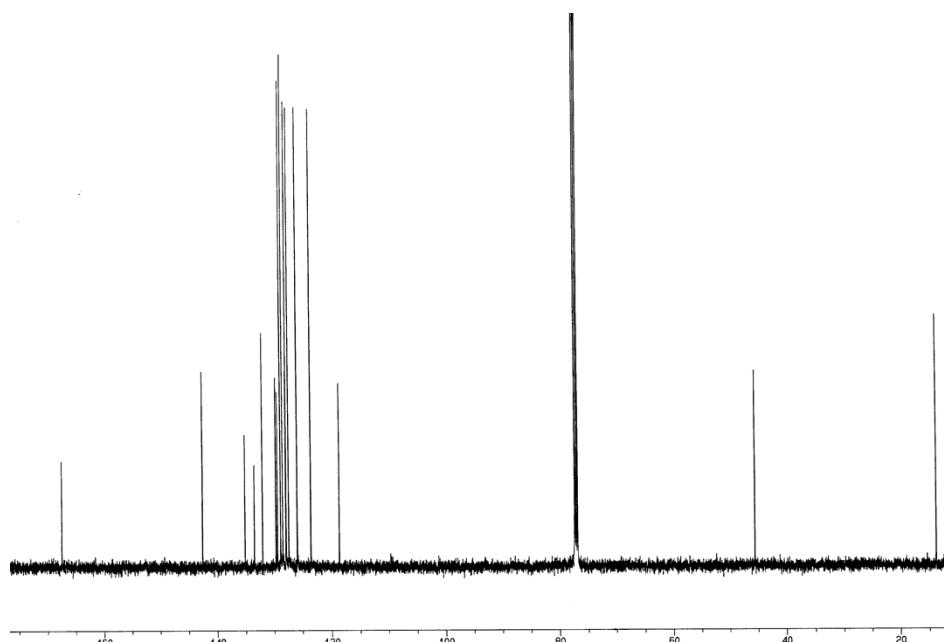
¹³C-NMR spectrum (125 MHz, CDCl₃) of *N*-Methyl-*N*-cinnamoyl-9-aminoanthracene **3b**



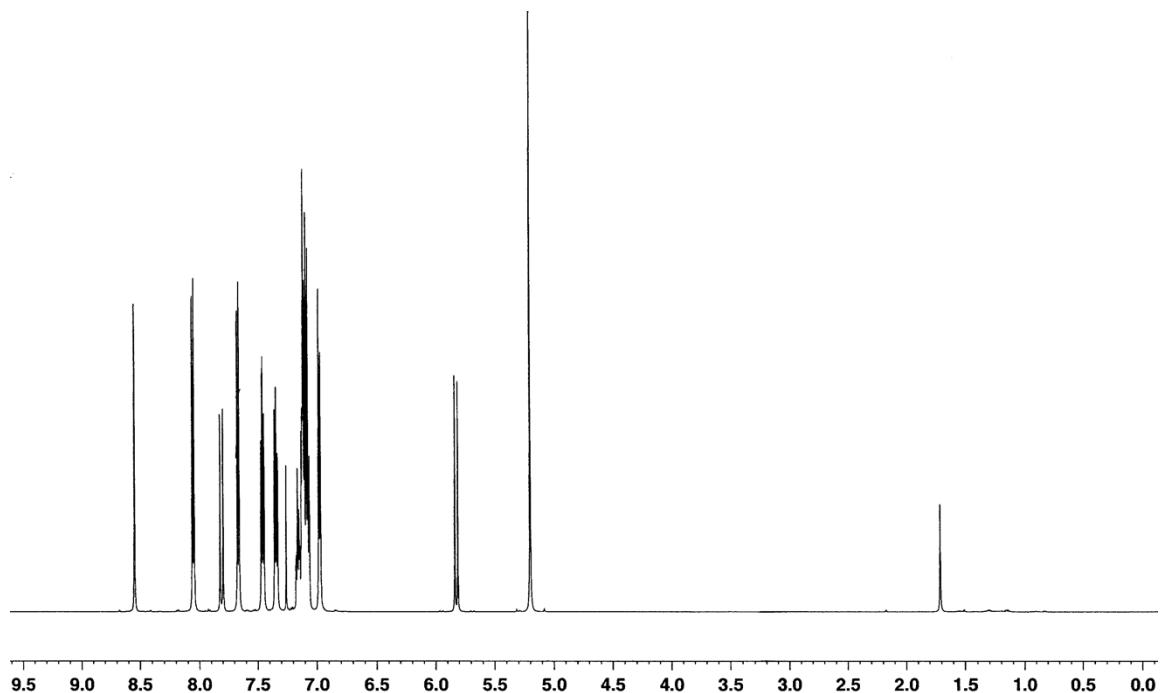
¹H-NMR spectrum of *N*-Ethyl-*N*-cinnamoyl-9-aminoanthracene **3c**



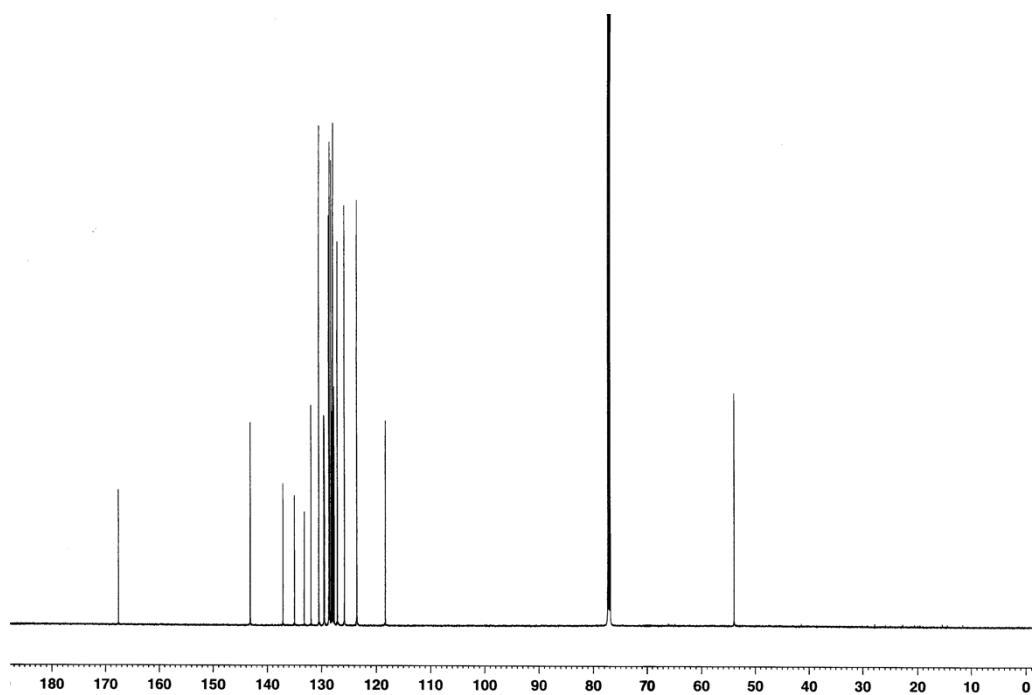
¹³C-NMR spectrum of *N*-Ethyl-*N*-cinnamoyl-9-aminoanthracene **3c**



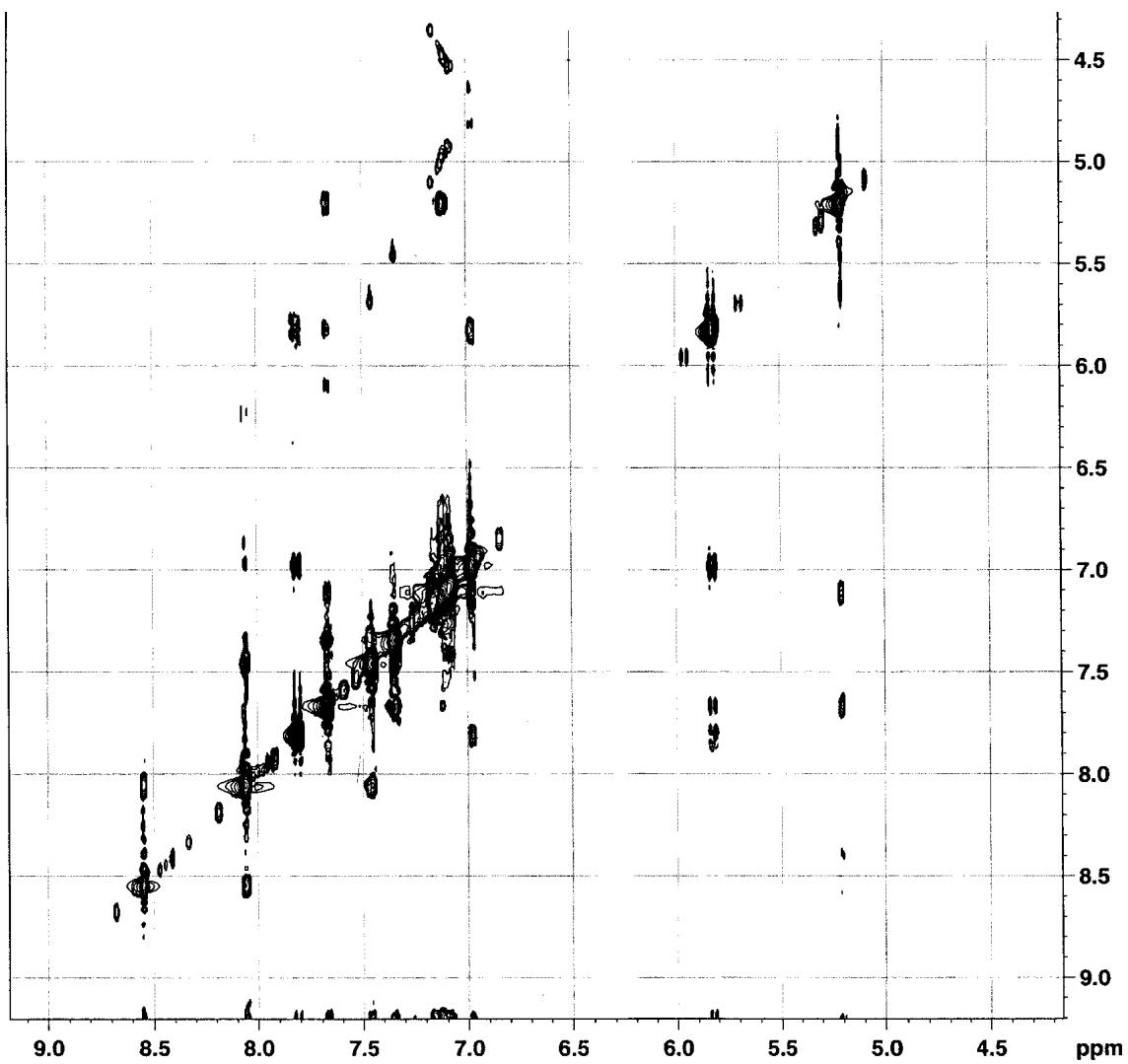
¹H-NMR (600 MHz, CDCl₃) spectrum of *N*-Benzyl-*N*-cinnamoyl-9-aminoanthracene **3d**



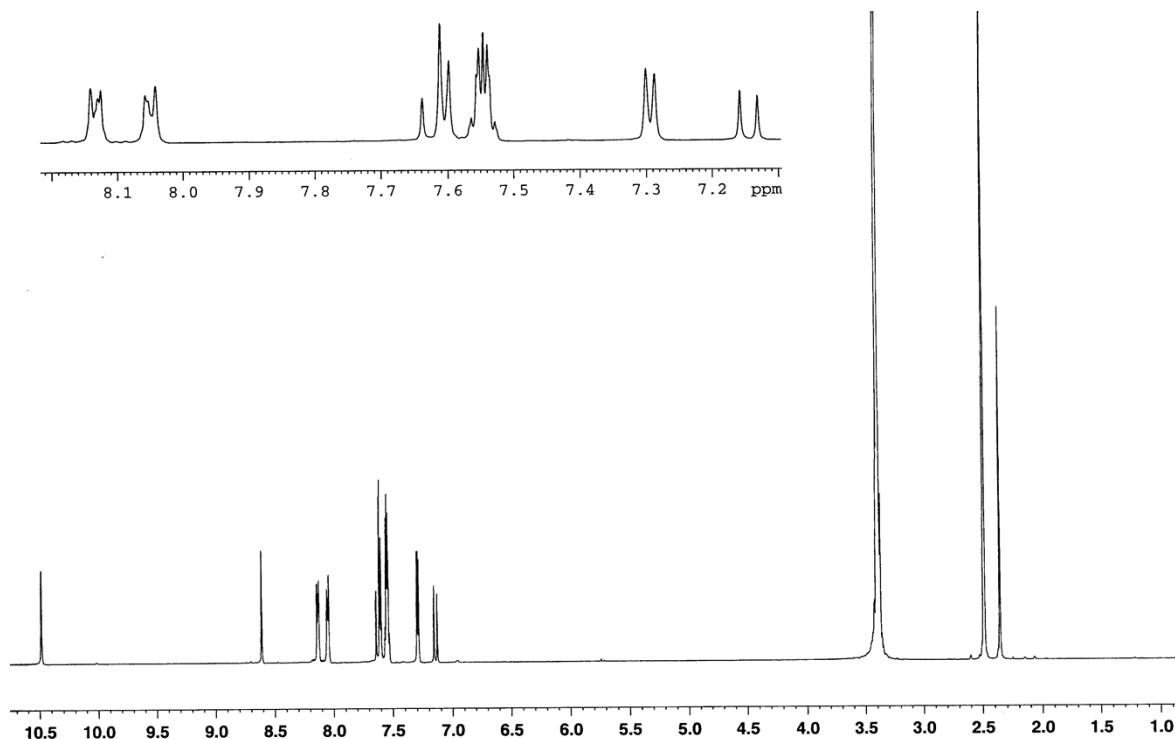
¹³C-NMR (150 MHz, CDCl₃) spectrum of *N*-Benzyl-*N*-cinnamoyl-9-aminoanthracene **3d**



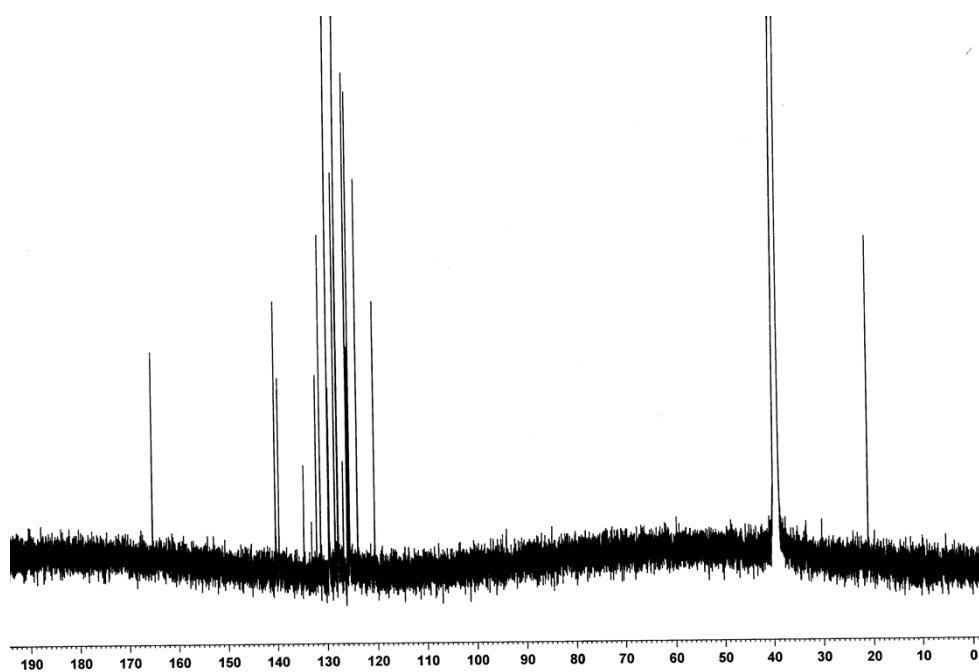
NOESY (600 MHz) spectrum of *N*-Benzyl-*N*-cinnamoyl-9-aminoanthracene **3d**



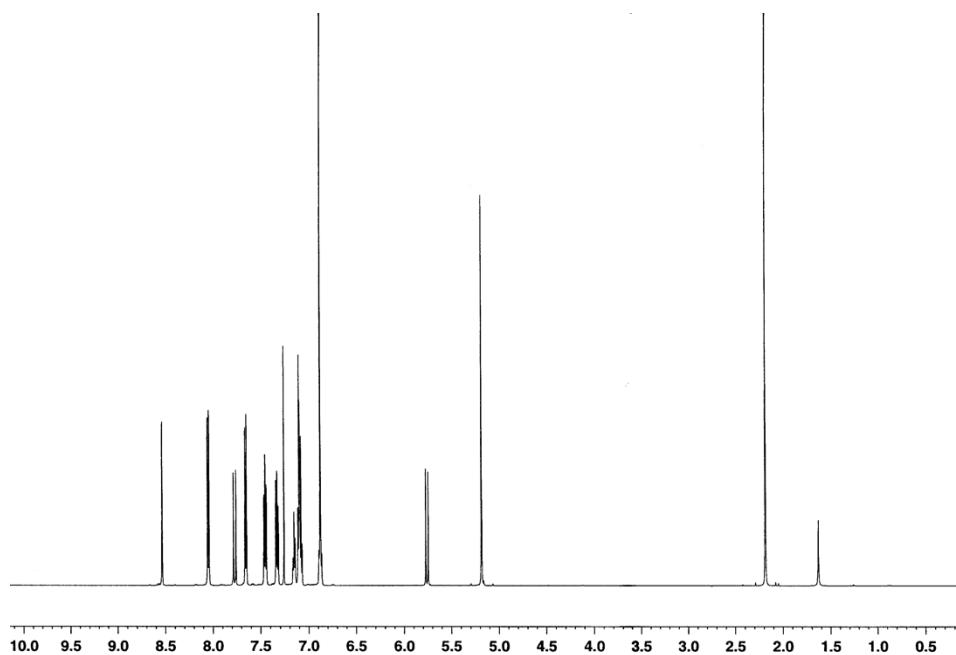
¹H-NMR spectrum (600 MHz, d⁶-DMSO) of *N*-(4-methylcinnamoyl)-9-aminoanthracene **3e**



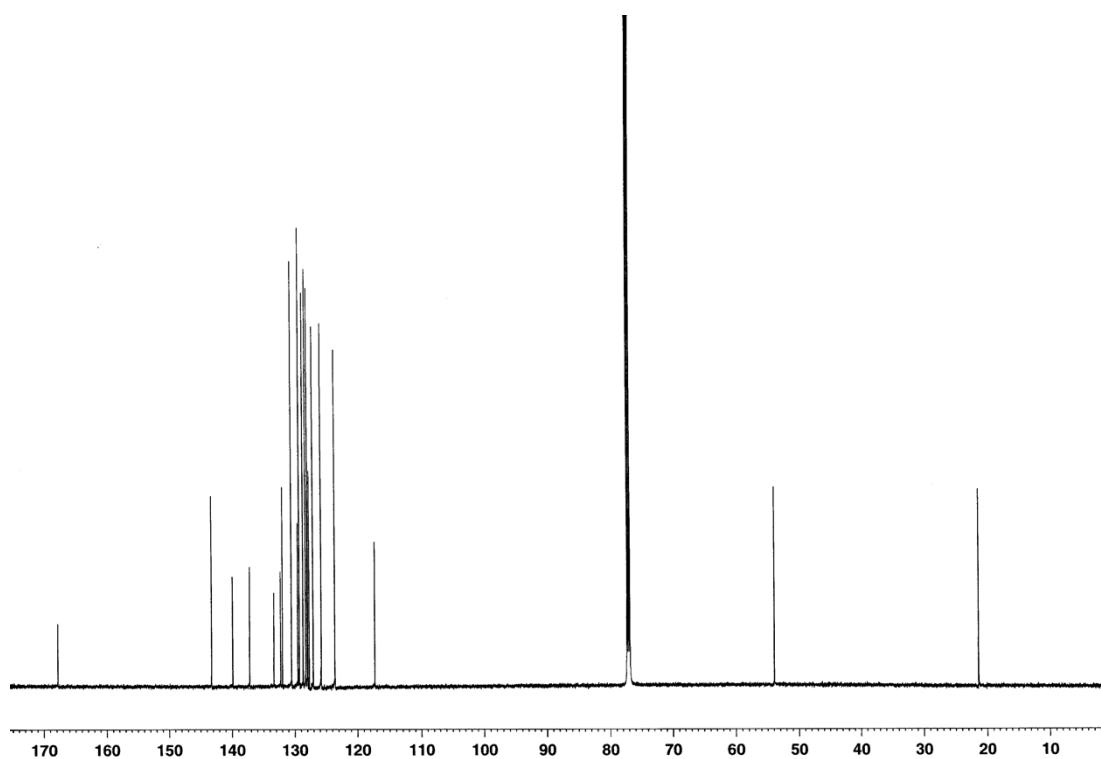
¹³C-NMR spectrum of *N*-(4-methylcinnamoyl)-9-aminoanthracene **3e**



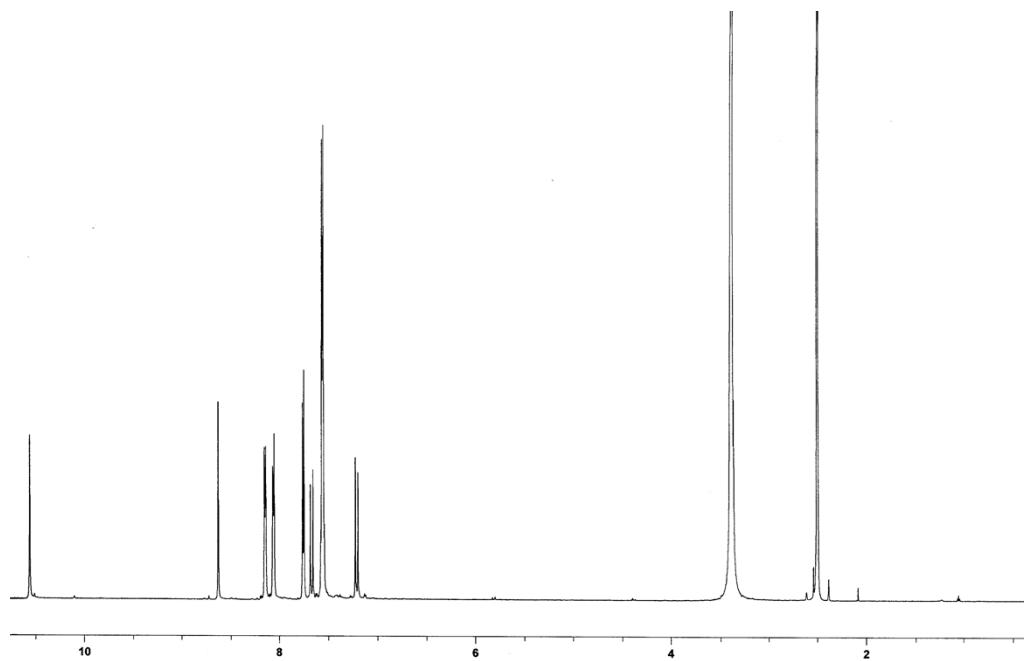
¹H-NMR spectrum (600 MHz, CDCl₃) of *N*-benzyl-*N*-(4-methylcinnamoyl)-9-aminoanthracene **3f**



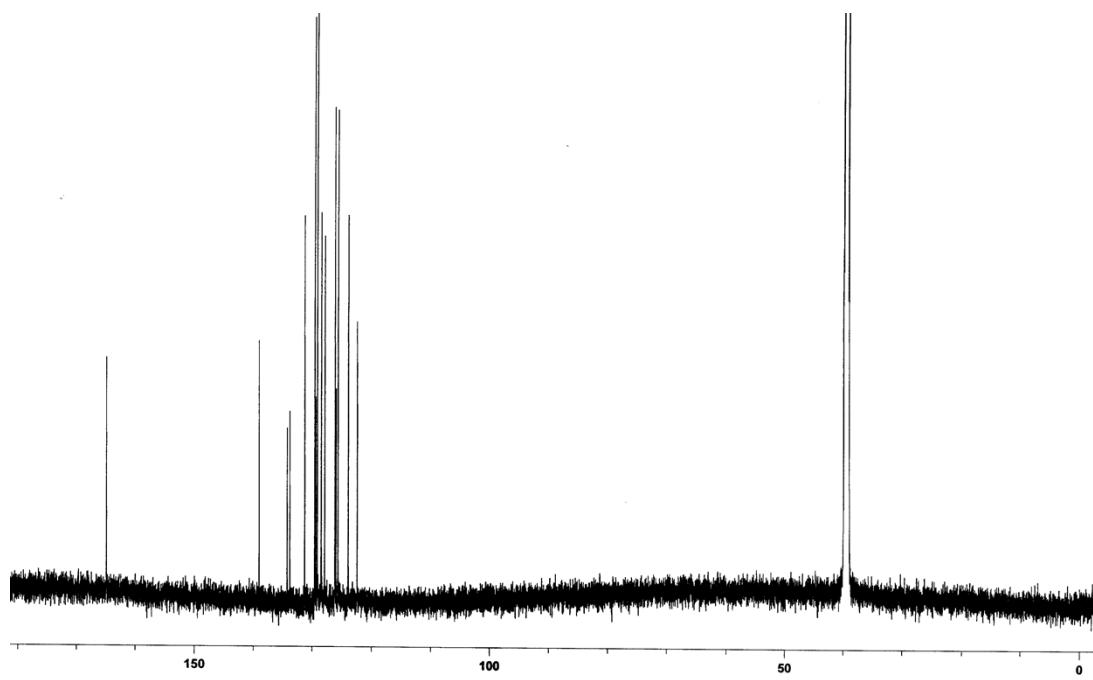
¹³C-NMR spectrum (150 MHz, CDCl₃) of *N*-benzyl-*N*-(4-methylcinnamoyl)-9-aminoanthracene **3f**



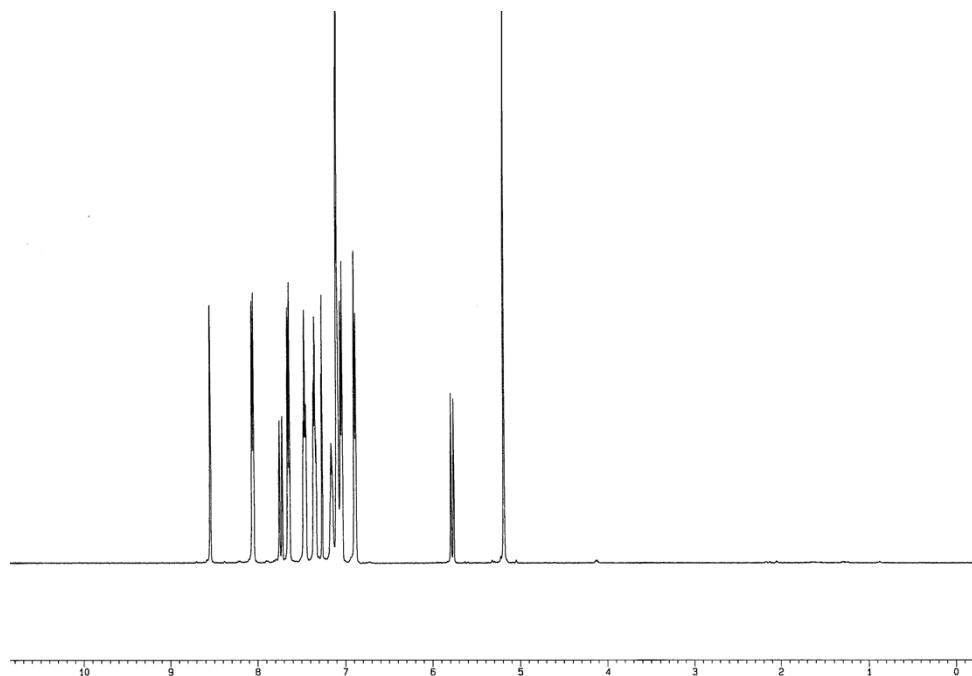
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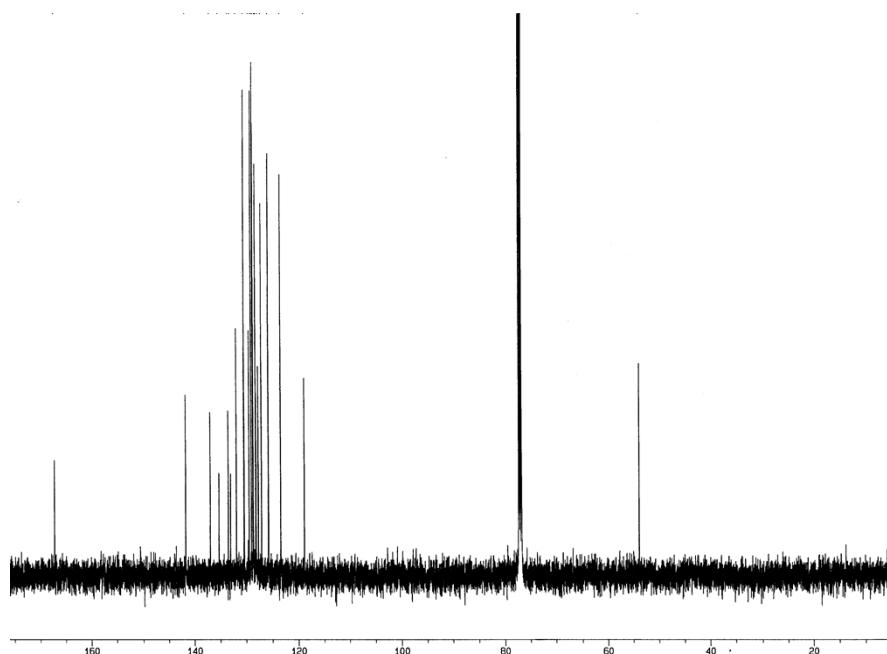
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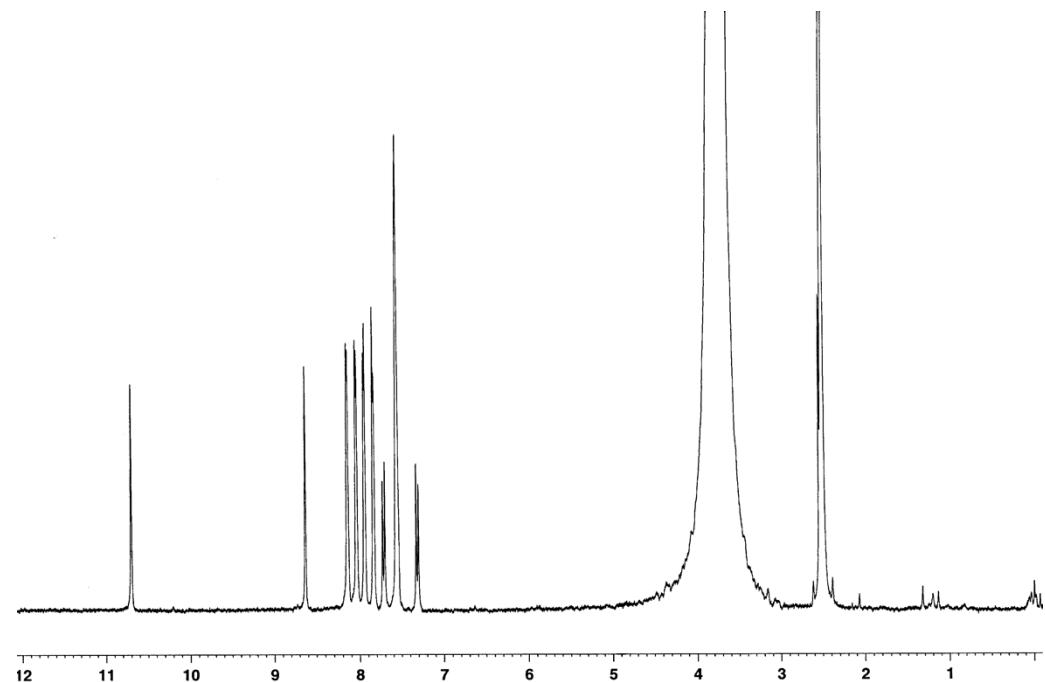
¹H-NMR spectrum of *N*-benzyl-*N*-(4-chlorocinnamoyl)-9-aminoanthracene **3h**



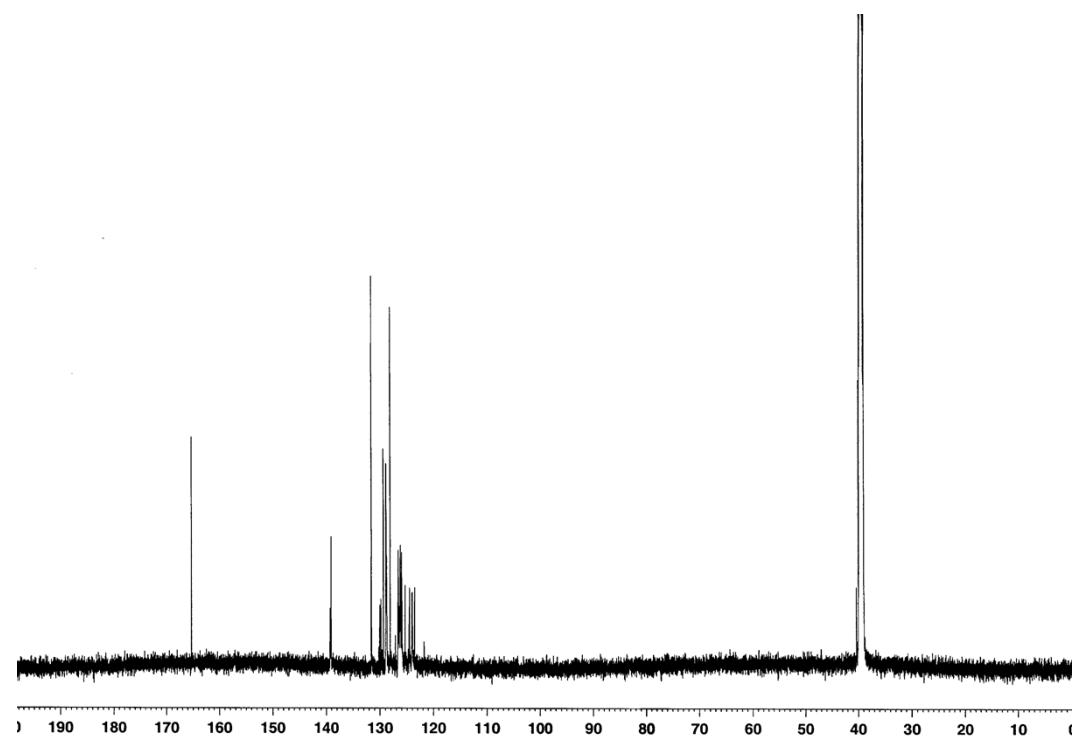
¹³C-NMR spectrum of *N*-benzyl-*N*-(4-chlorocinnamoyl)-9-aminoanthracene **3h**



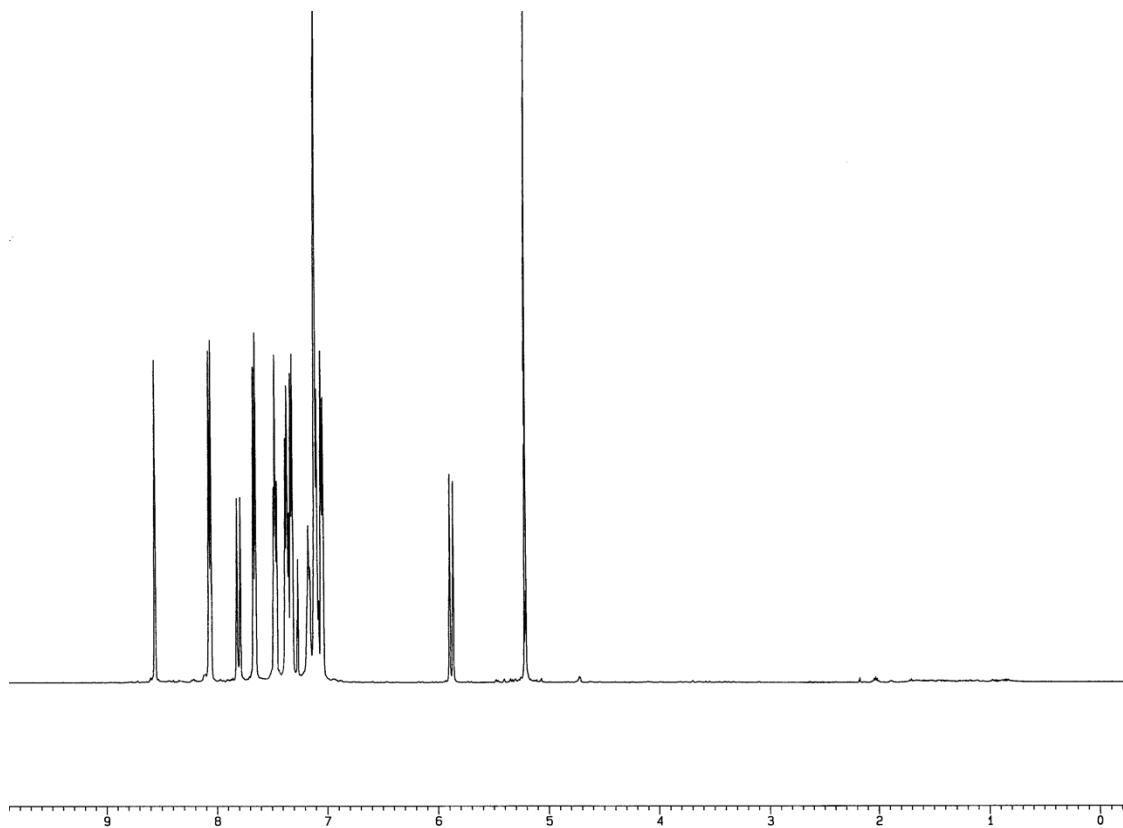
¹H-NMR spectrum (600 MHz, DMSO-d₆) of *N*-(4-trifluoromethylcinnamoyl)-9-aminoanthracene **3i**



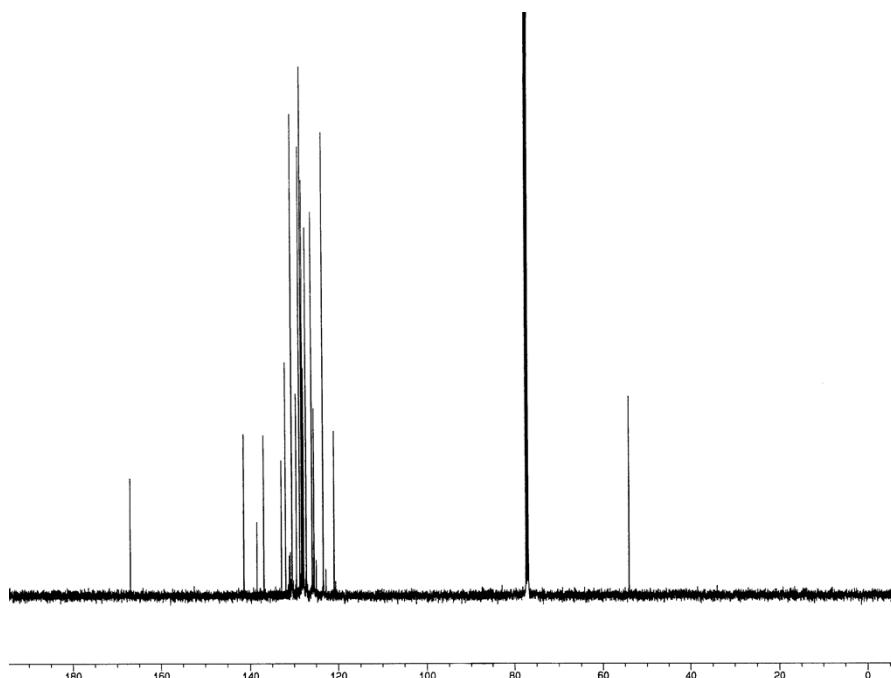
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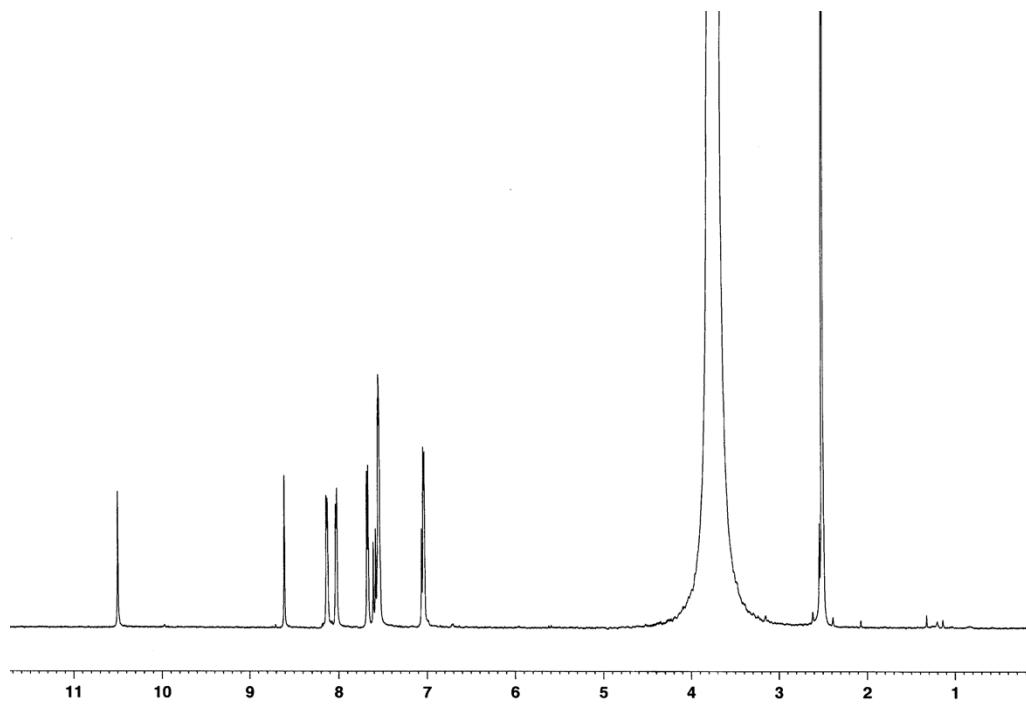
¹H-NMR spectrum (500 MHz, CDCl₃) of *N*-benzyl-*N*-(4-trifluoromethylcinnamoyl)-9-aminoanthracene **3j**



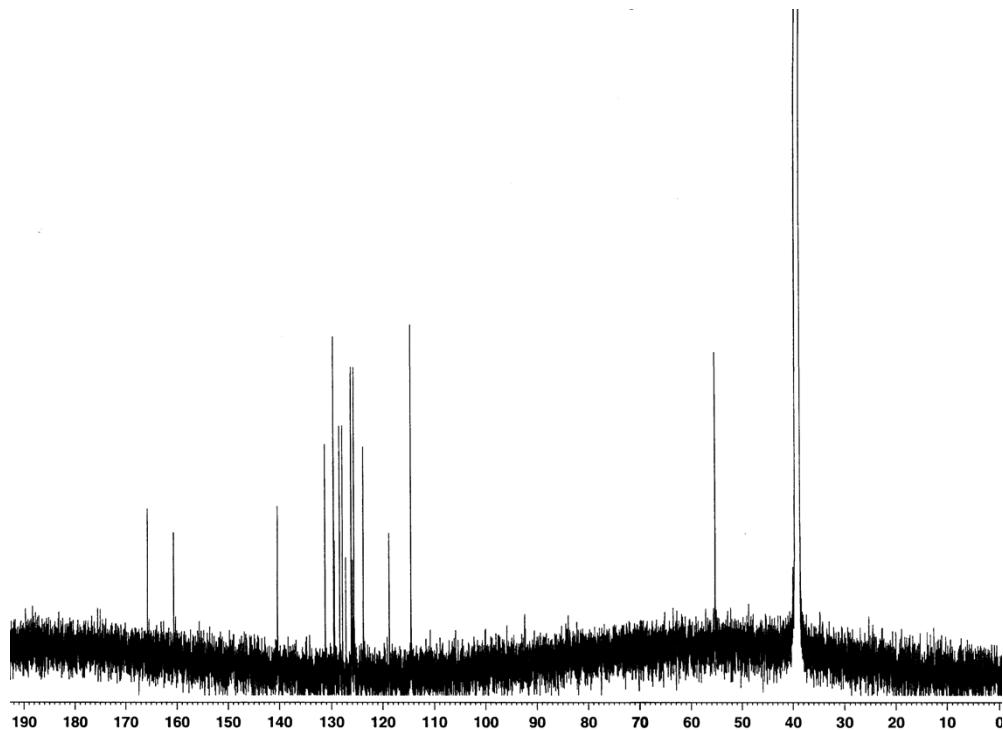
¹³C-NMR spectrum (125 MHz, CDCl₃) of *N*-benzyl-*N*-(4-trifluoromethylcinnamoyl)-9-aminoanthracene **3j**



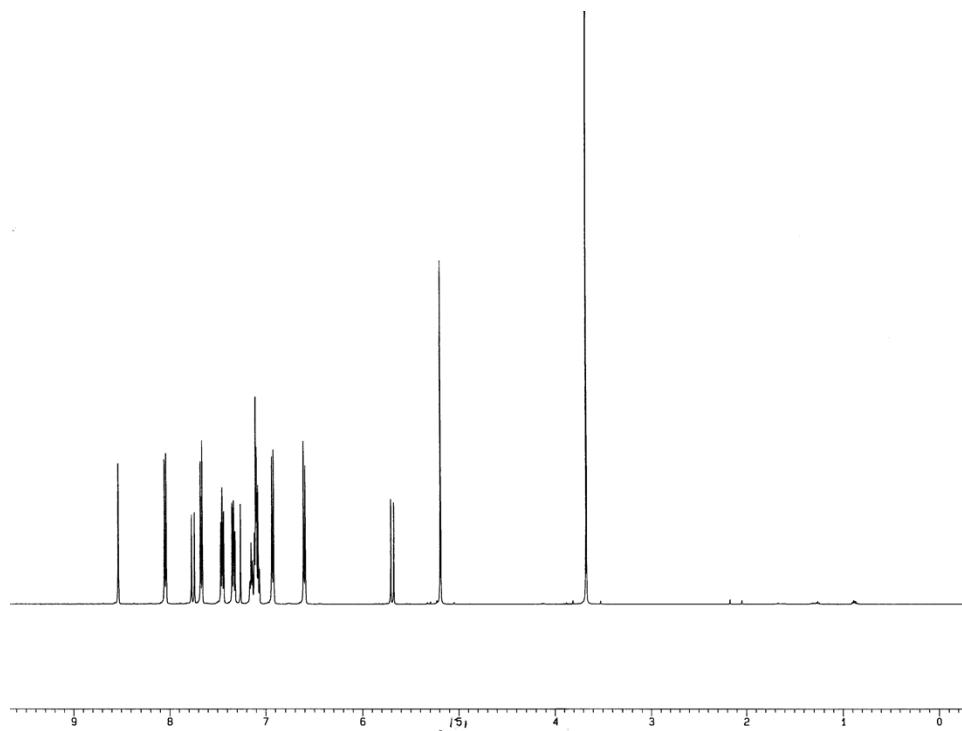
¹H-NMR spectrum (600 MHz, DMSO-d₆) of *N*-(4-methoxycinnamoyl)-9-aminoanthracene **3k**



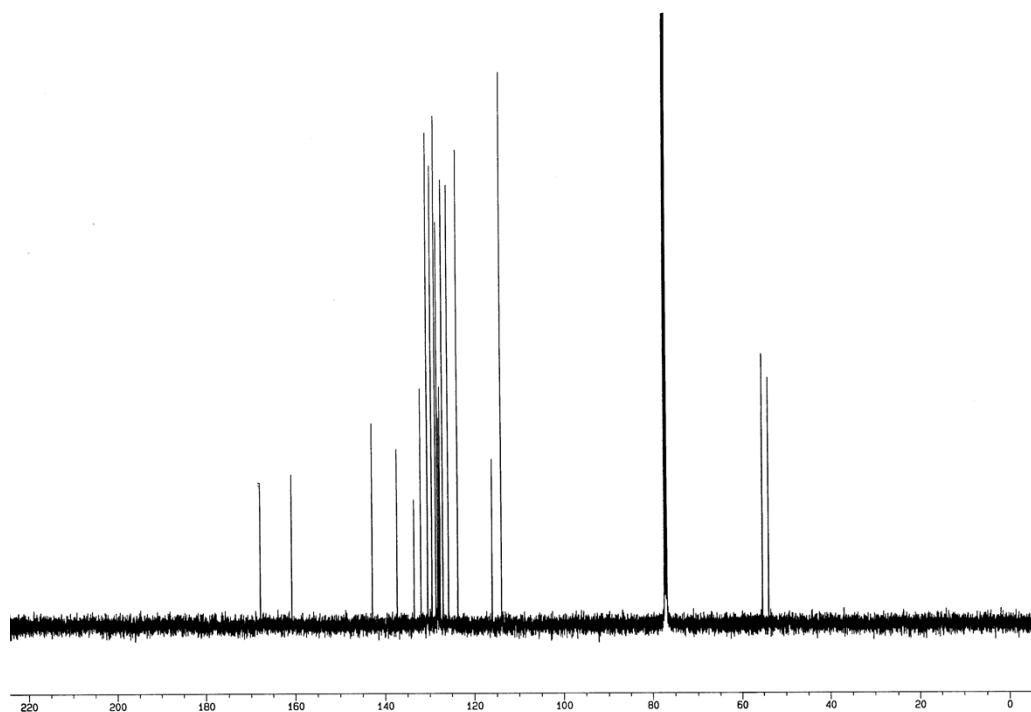
¹³C-NMR spectrum (150 MHz, DMSO-d₆) of *N*-(4-methoxycinnamoyl)-9-aminoanthracene **3k**



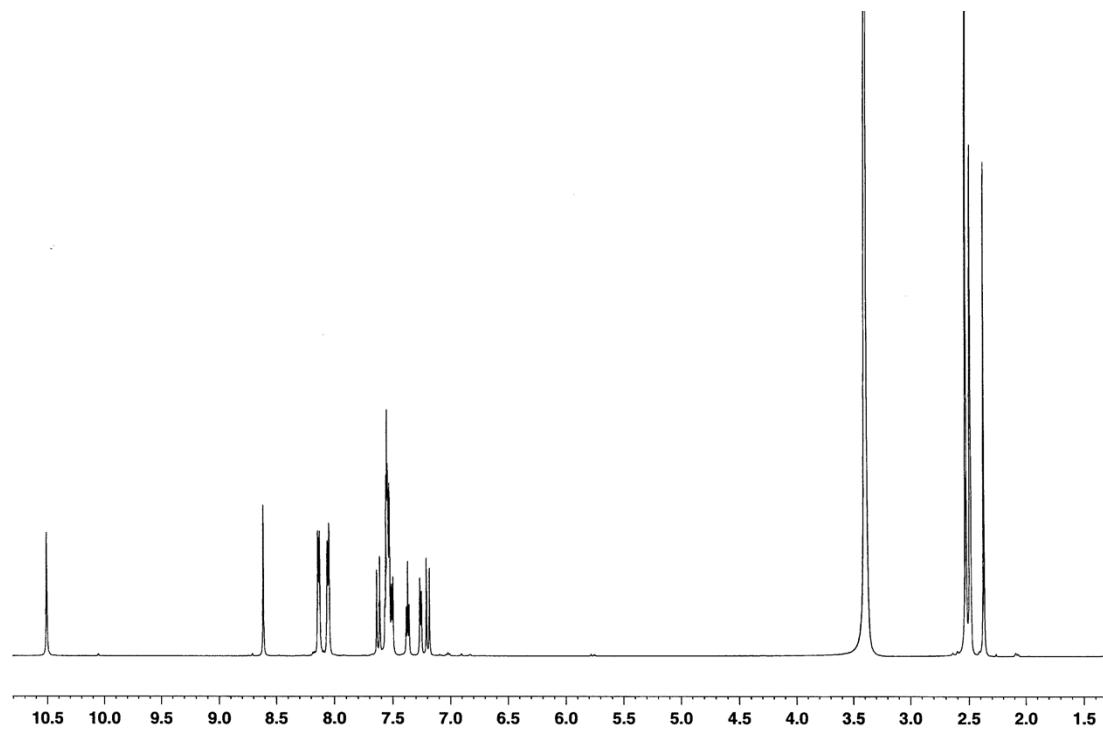
¹H-NMR spectrum (500 MHz, CDCl₃) of *N*-Benzyl-*N*-(4-methoxycinnamoyl)-9-aminoanthracene **3I**



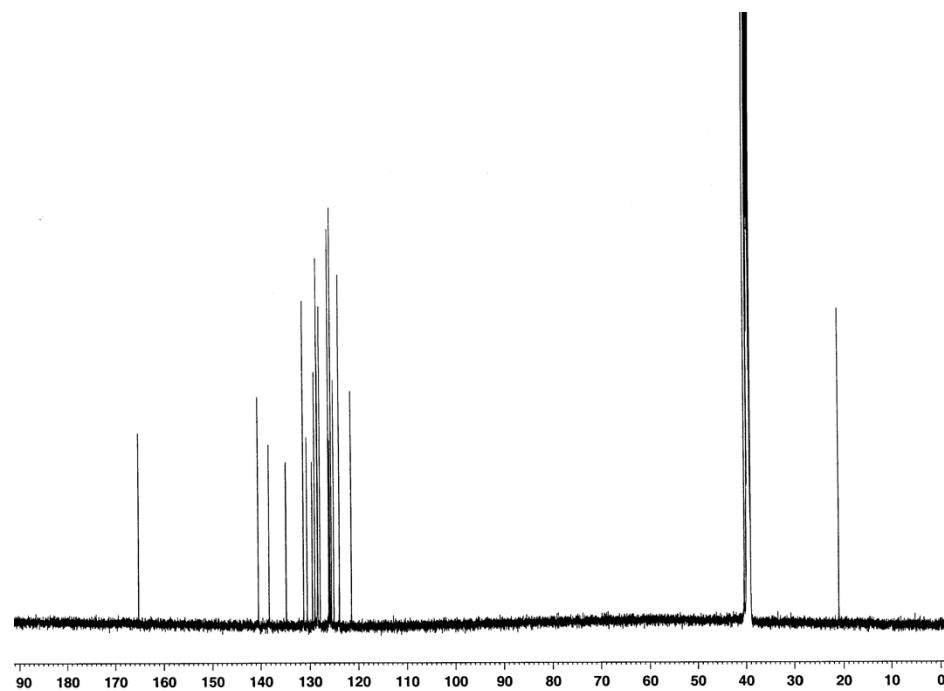
¹³C-NMR spectrum (125 MHz, CDCl₃) of *N*-Benzyl-*N*-(4-methoxycinnamoyl)-9-aminoanthracene **3I**



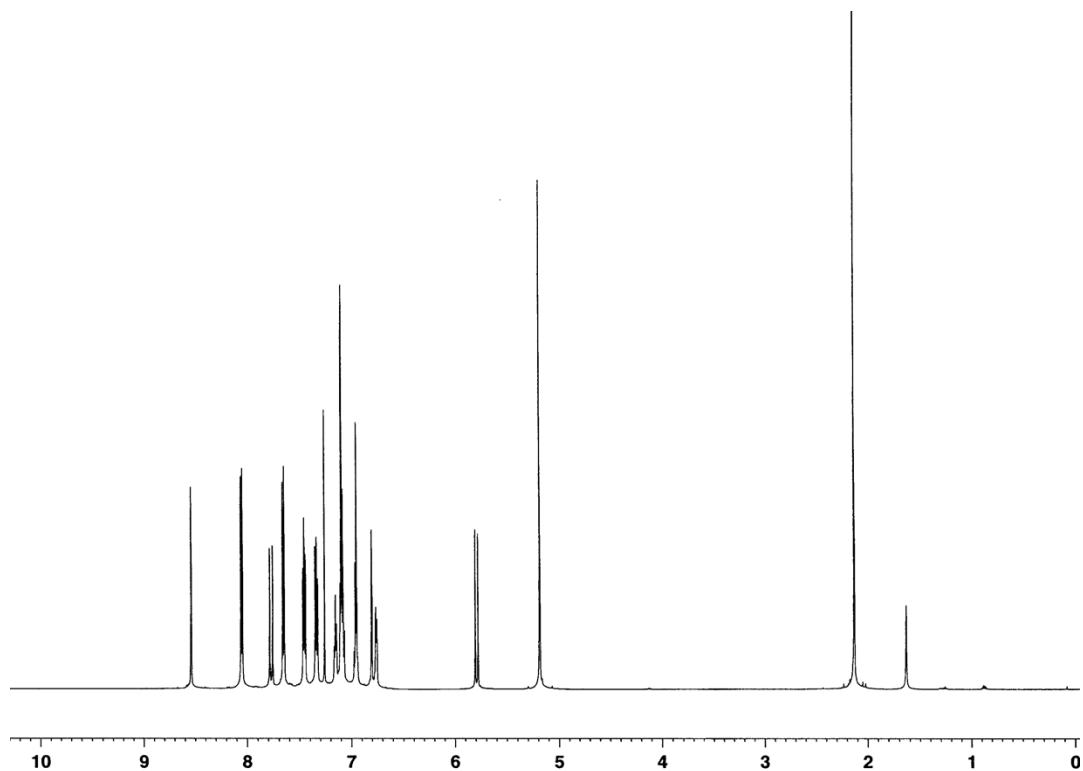
¹H-NMR spectrum (600 MHz, d⁶-DMSO) of *N*-(3 methylcinnamoyl)-9-aminoanthracene **3m**



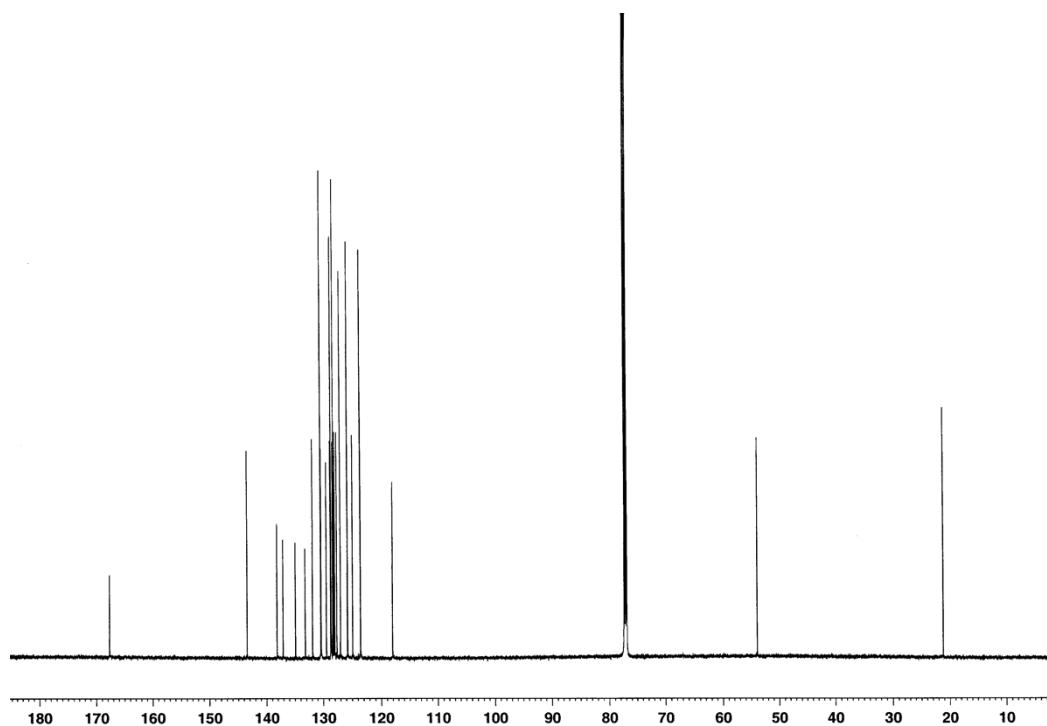
¹³C-NMR spectrum (150 MHz, d⁶-DMSO) of *N*-(3 methylcinnamoyl)-9-aminoanthracene **3m**



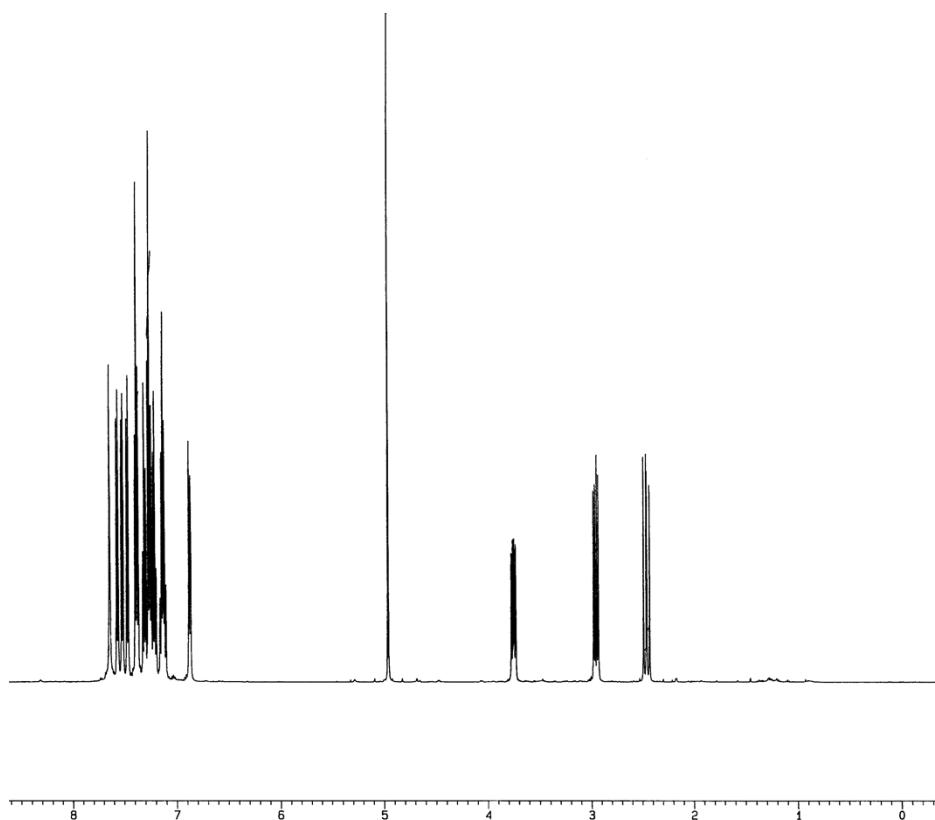
¹H-NMR spectrum (600 MHz, CDCl₃) of *N*-benzyl-*N*-(3-methylcinnamoyl)-9-aminoanthracene **3n**



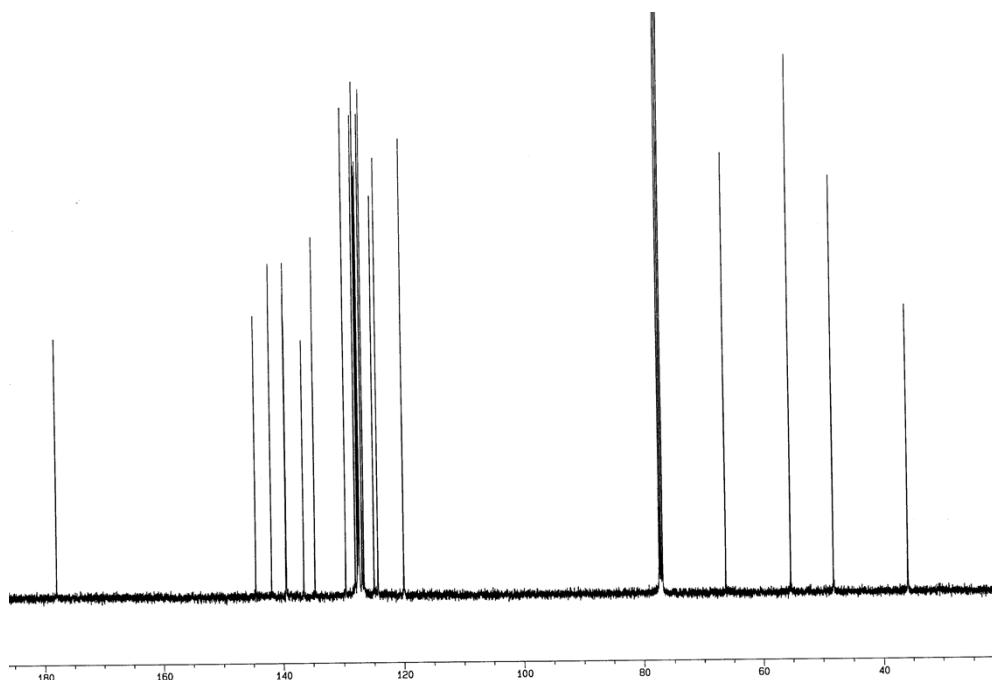
¹³C-NMR spectrum (150 MHz, CDCl₃) of *N*-benzyl-*N*-(3-methylcinnamoyl)-9-aminoanthracene **3n**



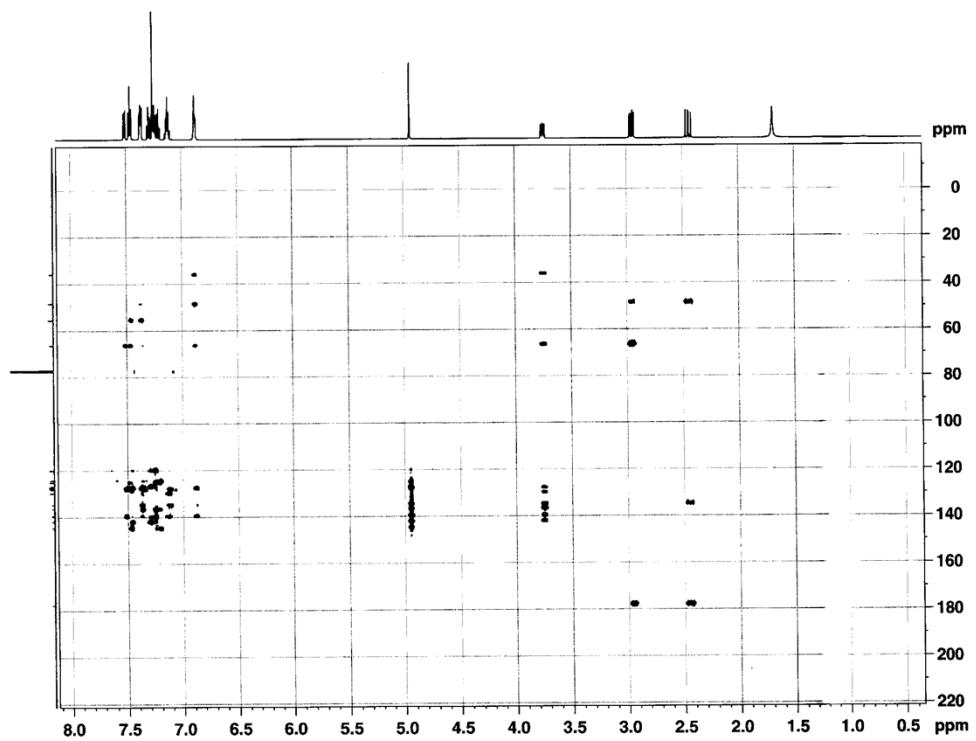
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4a**



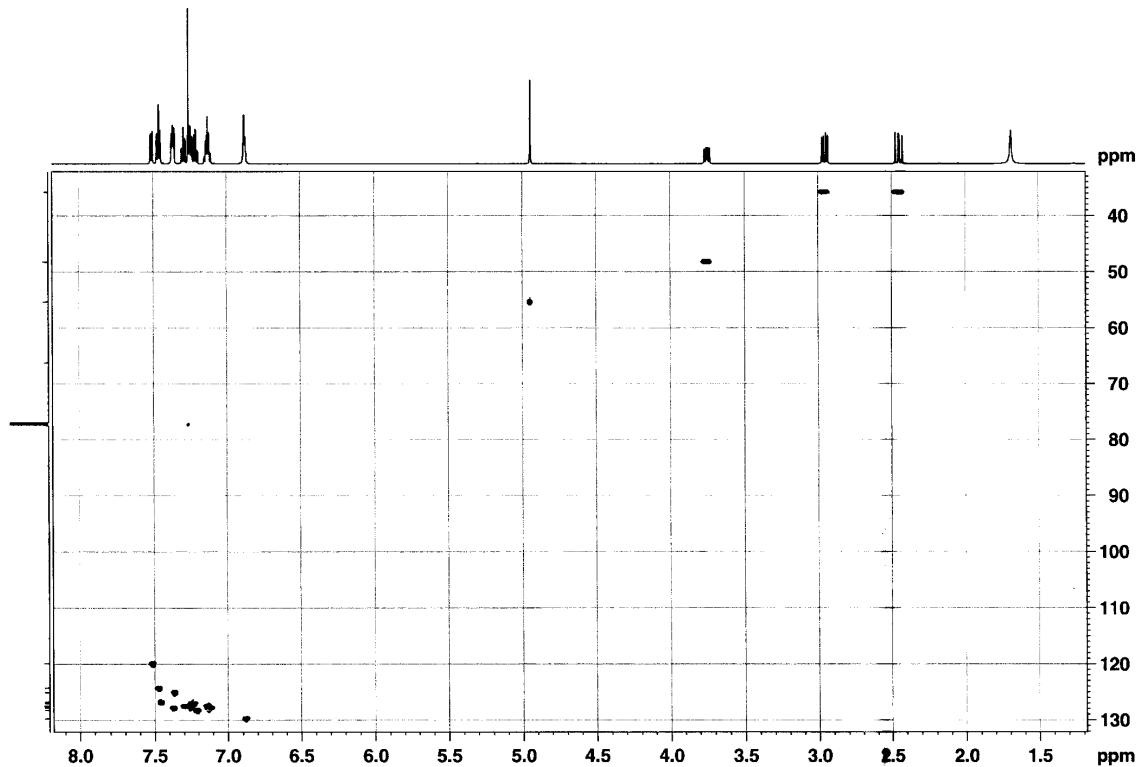
¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4a**



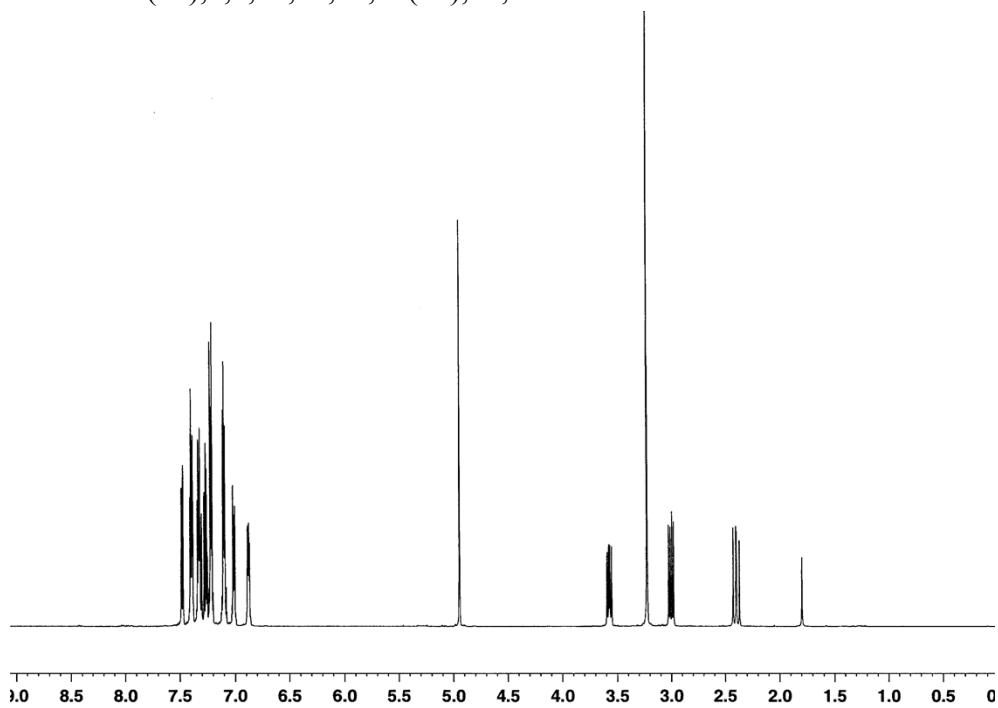
HMBC NMR spectrum (600MHz, CDCl₃) of (\pm) 2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa- 6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4a**



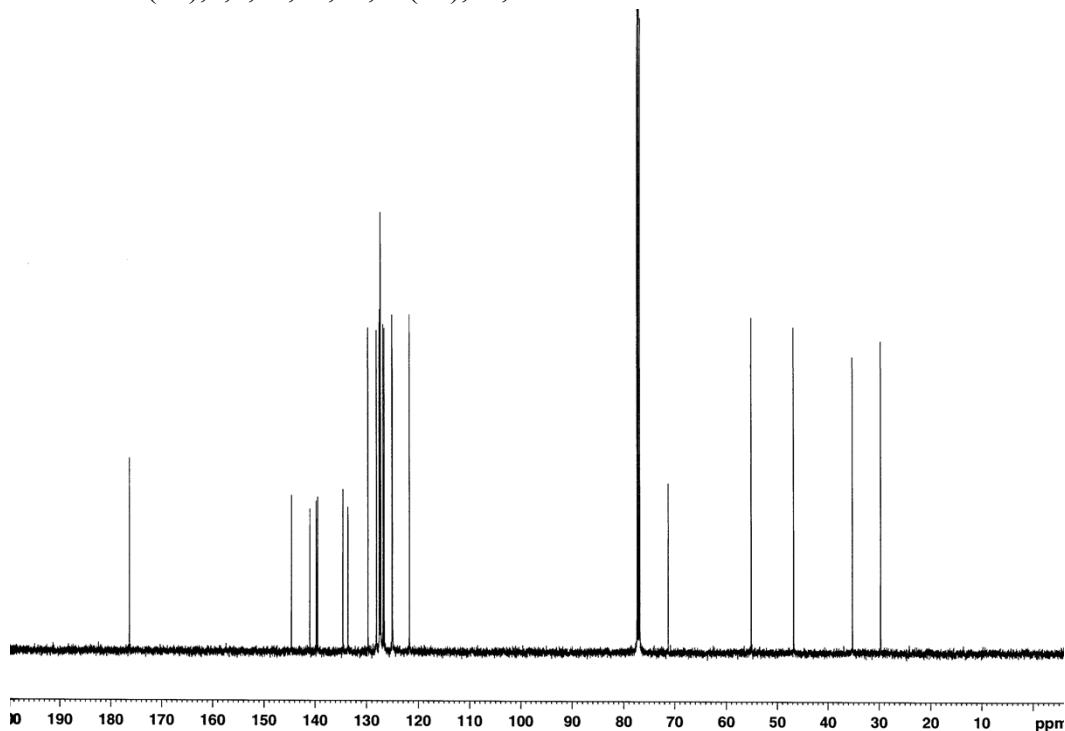
HSQC NMR spectrum (600MHz, CDCl₃) of (\pm) 2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa- 6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4a**



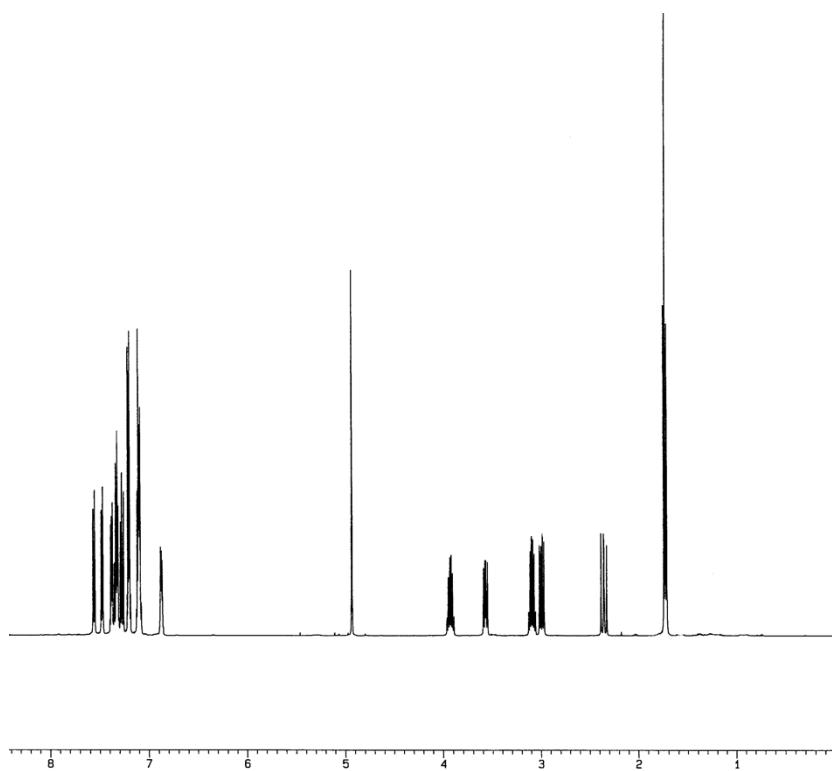
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 2-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4b**



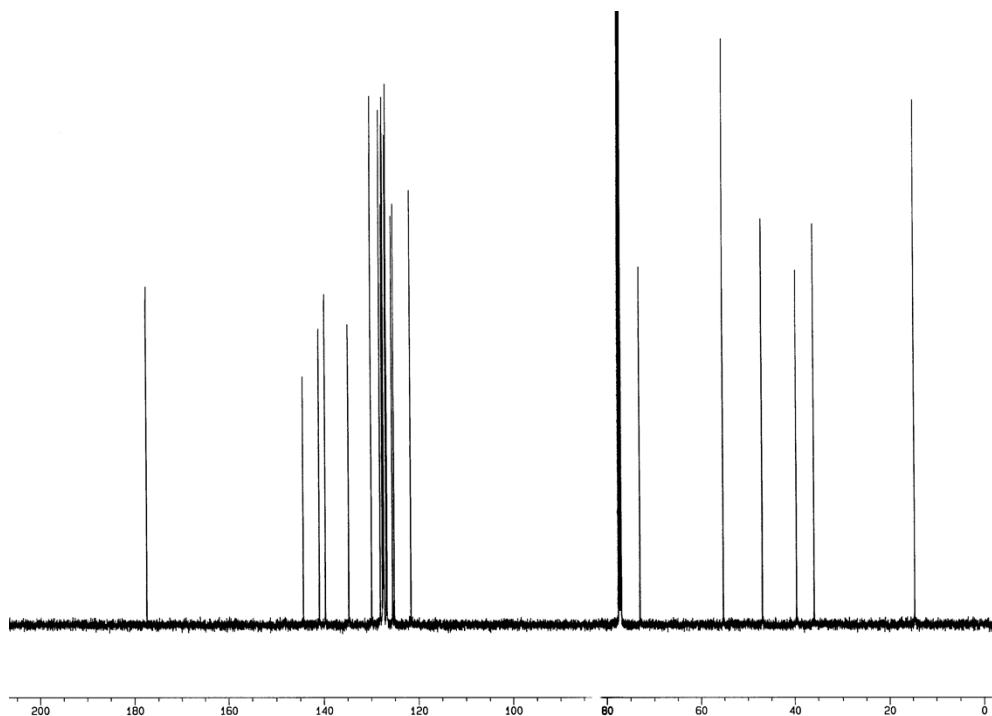
¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 2-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4b**



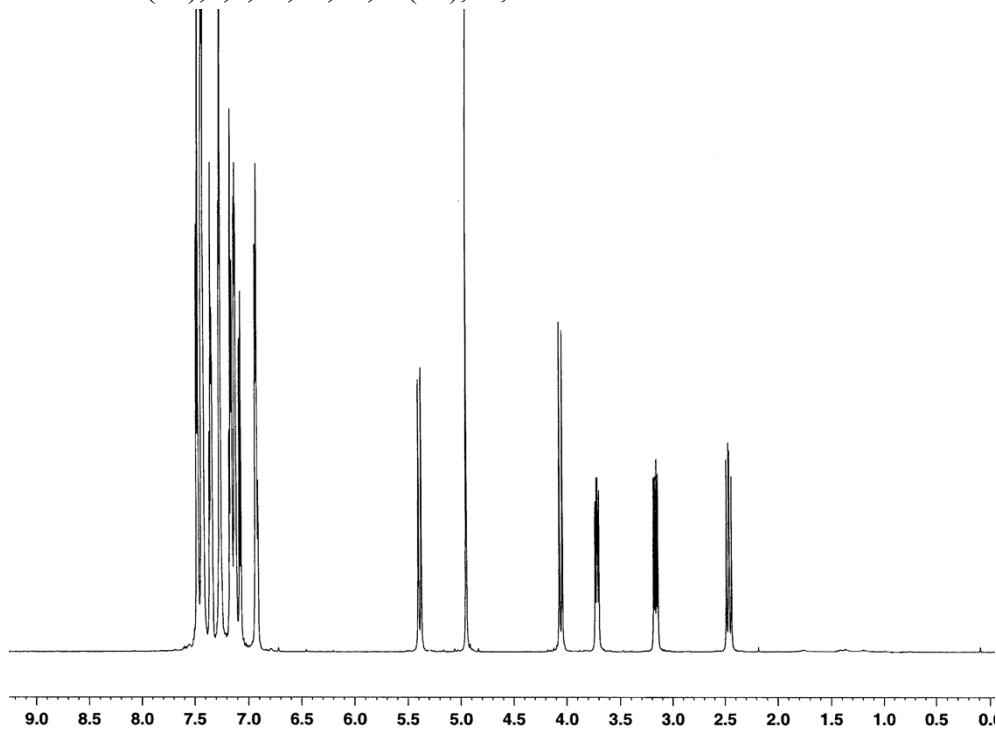
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 2-ethyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4c**



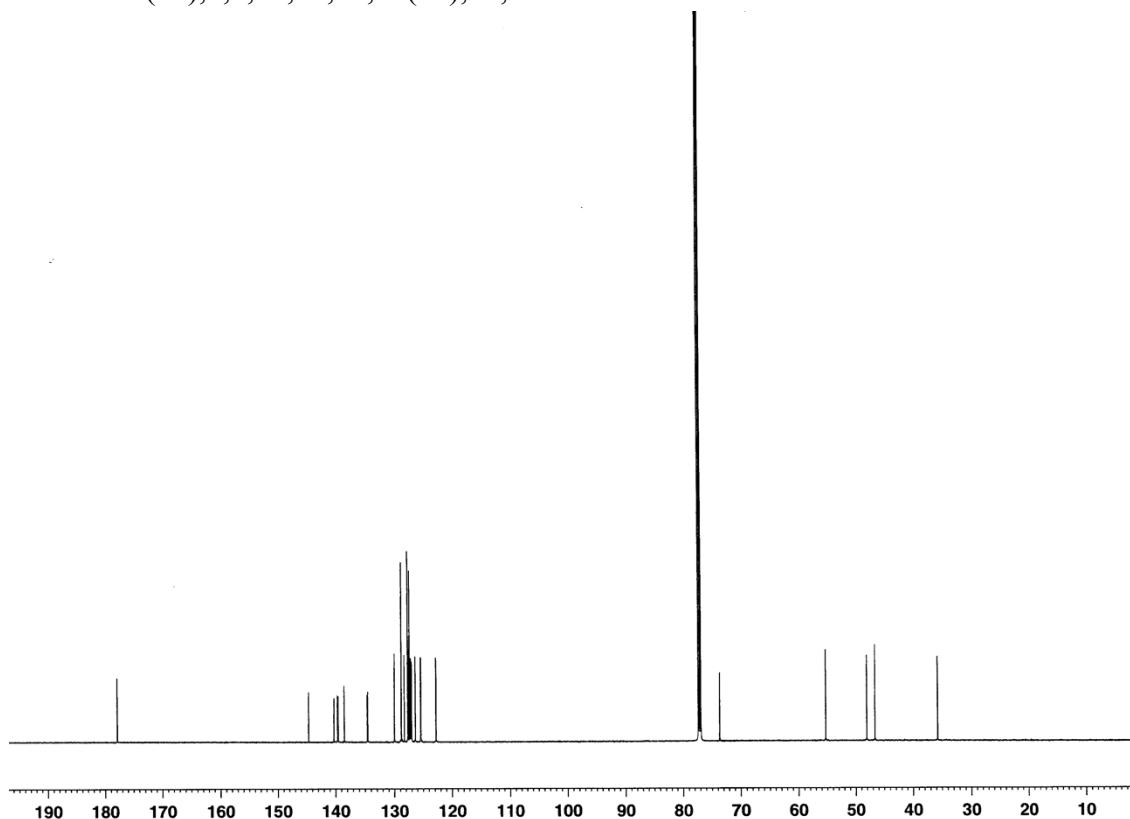
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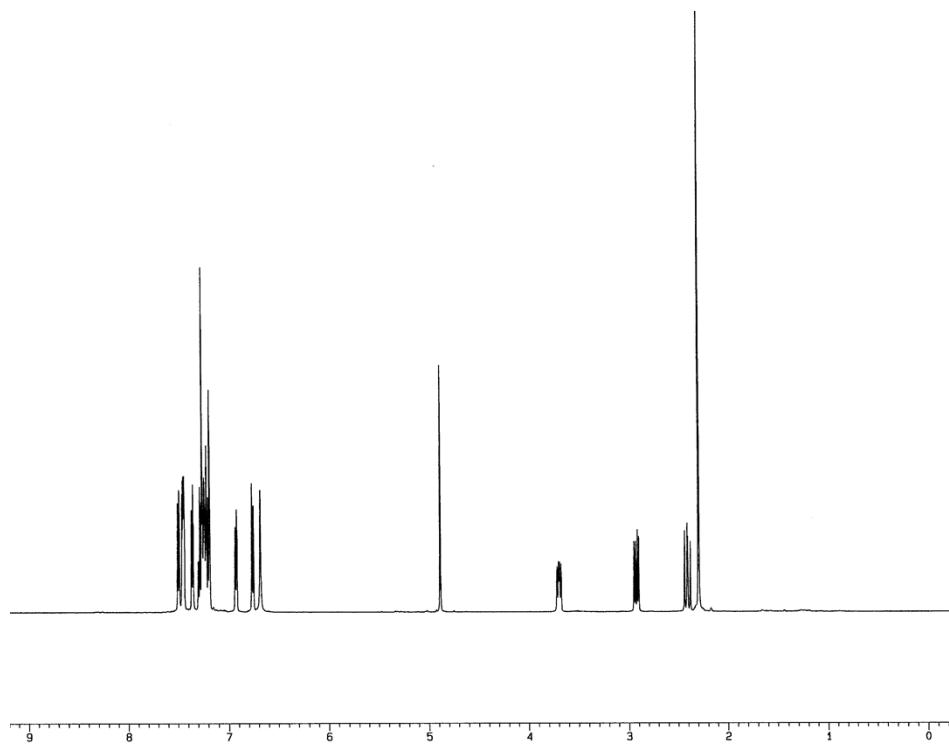
¹H-NMR spectrum (600MHz, CDCl₃) of (\pm) 2-benzyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}] tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4d**



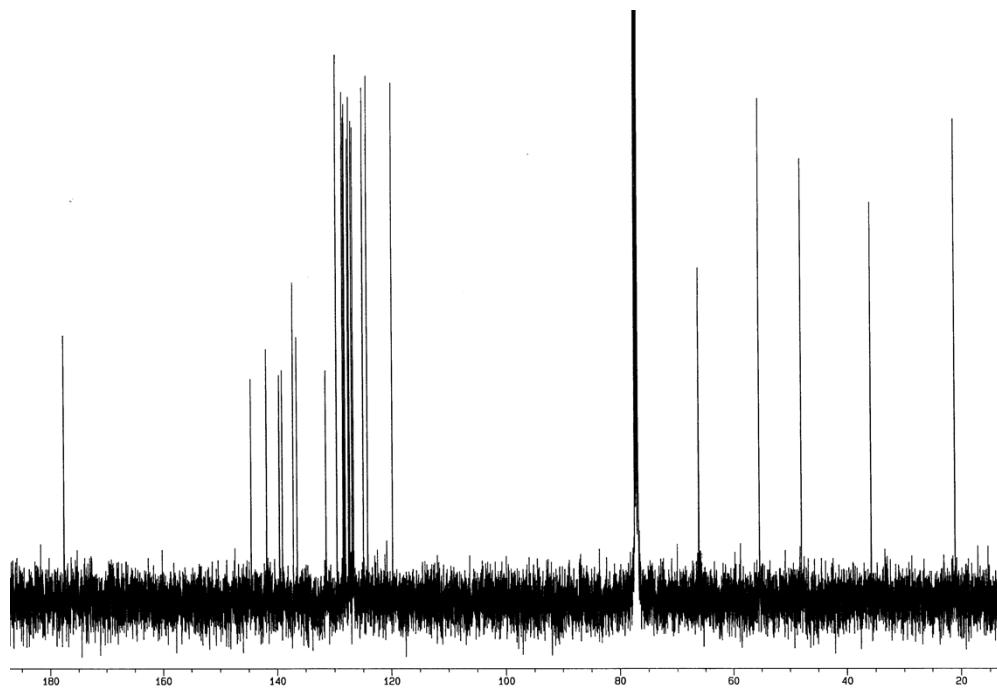
¹³C-NMR spectrum (150 MHz, CDCl₃) of (\pm) 2-benzyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}] tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4d**



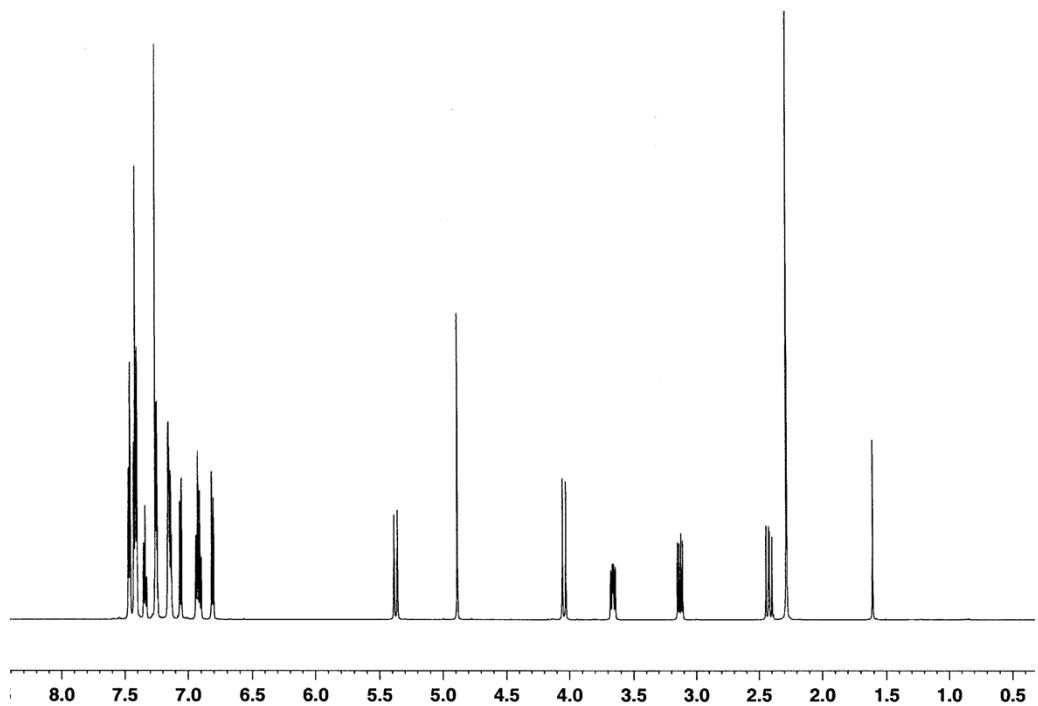
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 9-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa- 6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4e**



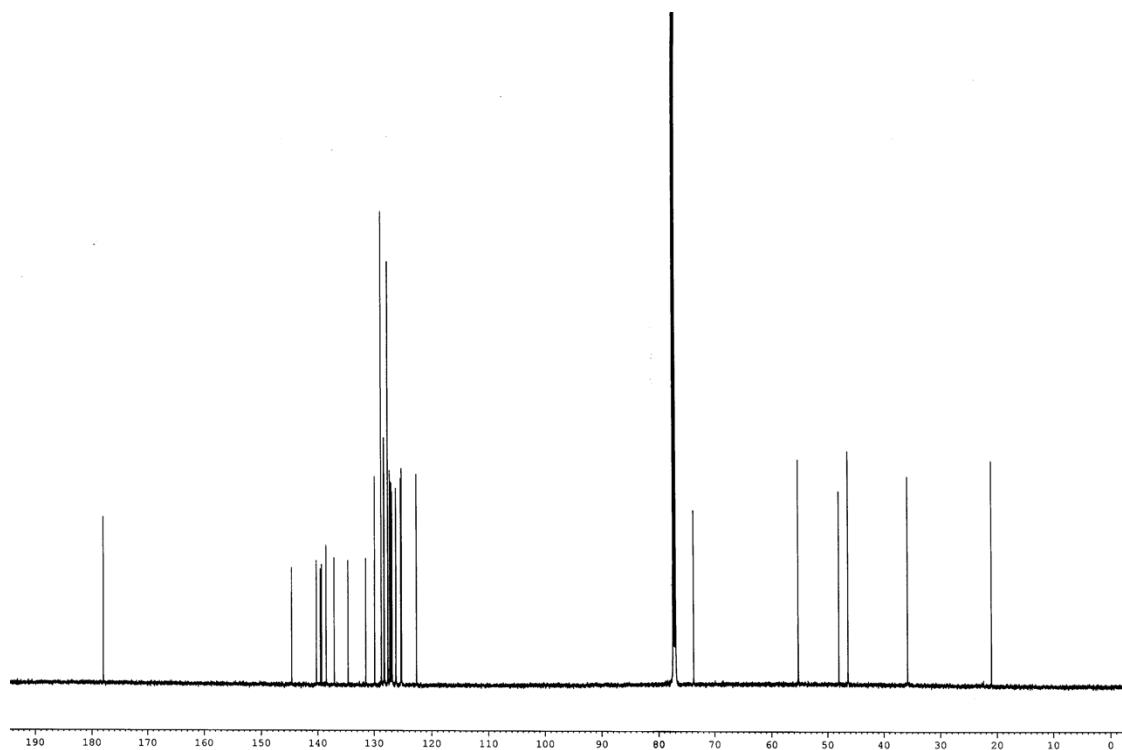
¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 9-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa- 6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4e**



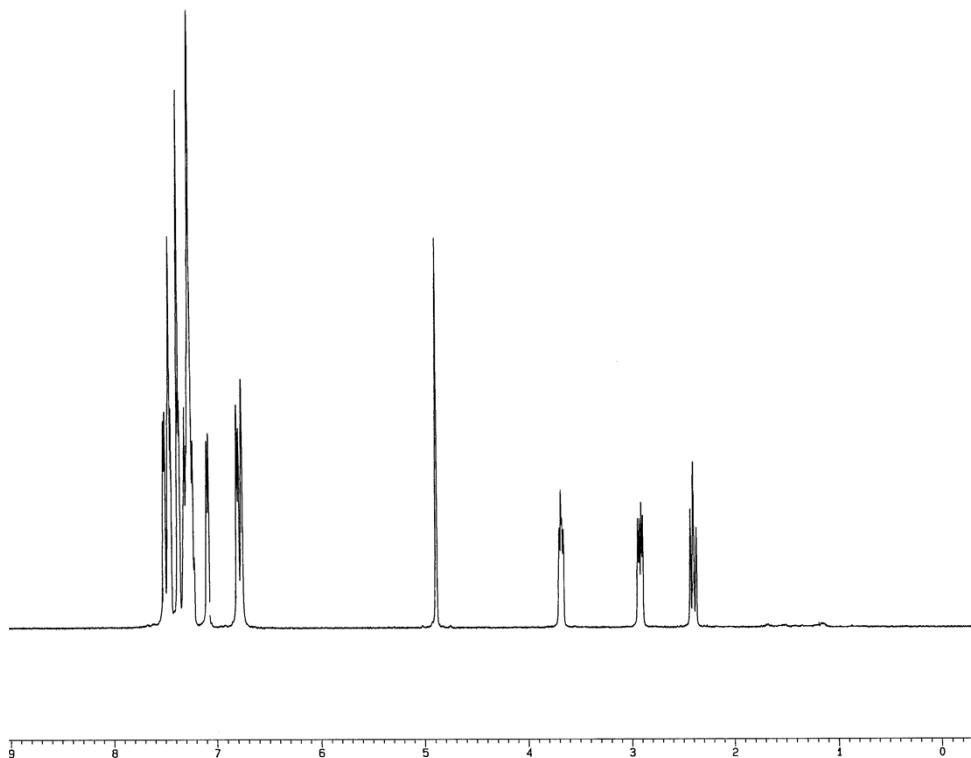
¹H-NMR spectrum (600MHz, CDCl₃) of (\pm) 2-benzyl-9-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4f**



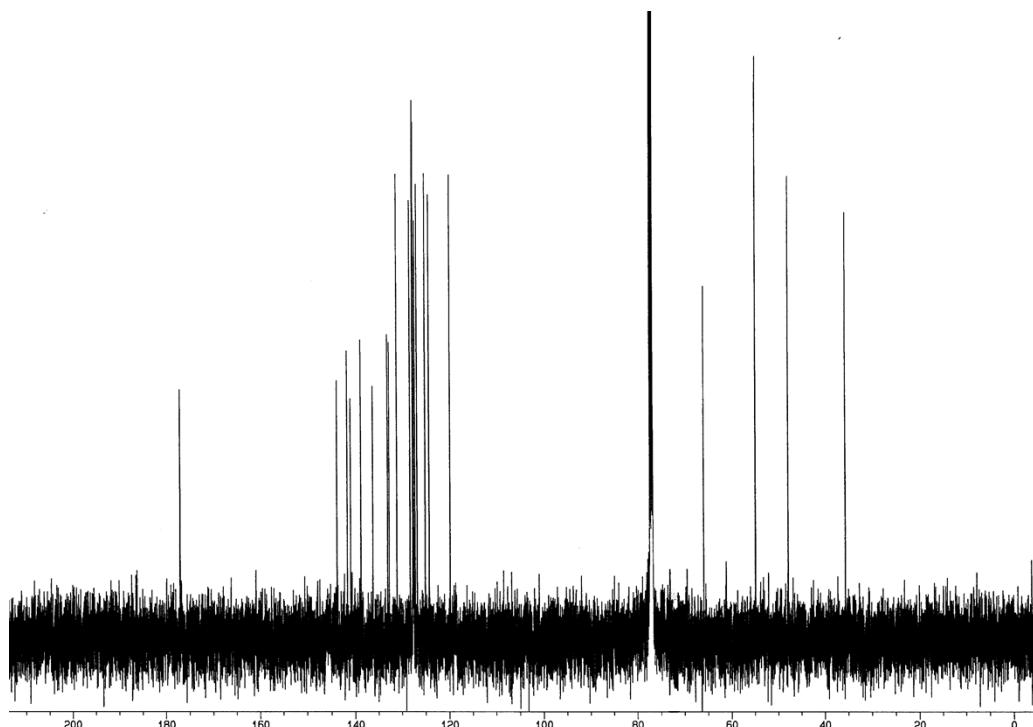
¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 2-benzyl-9-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4f**



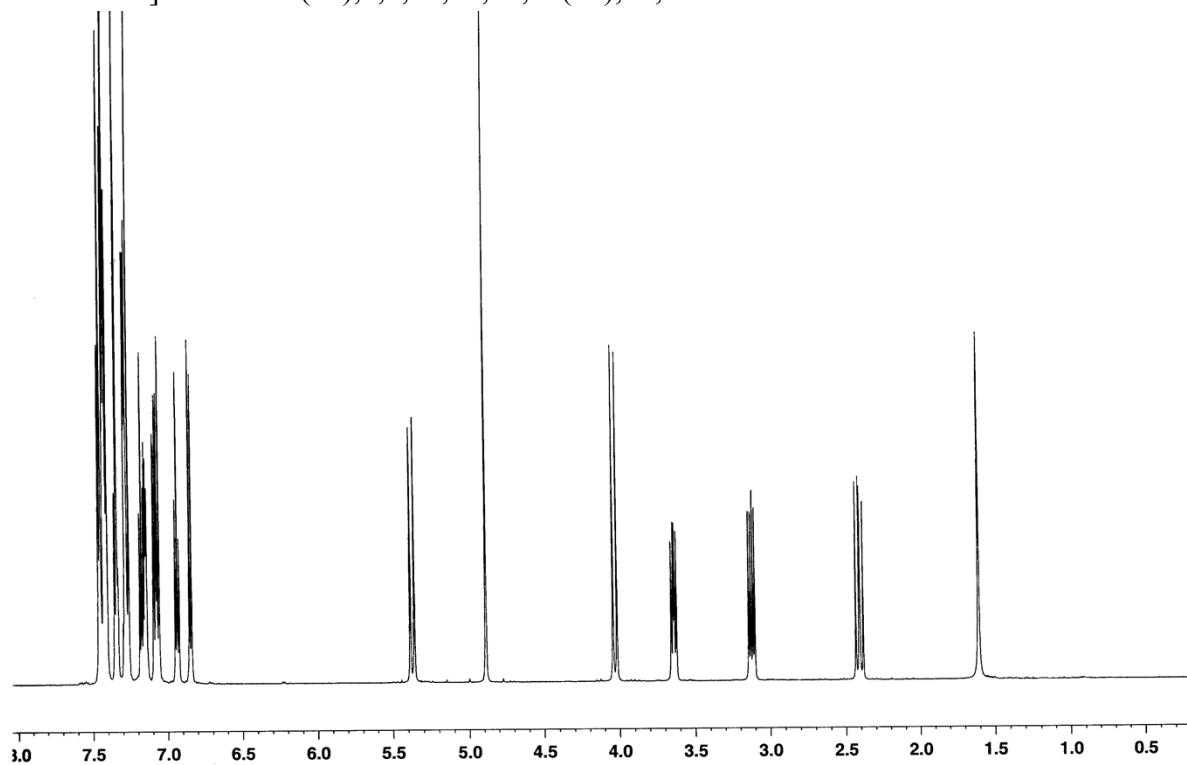
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 9-chloro-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4g**



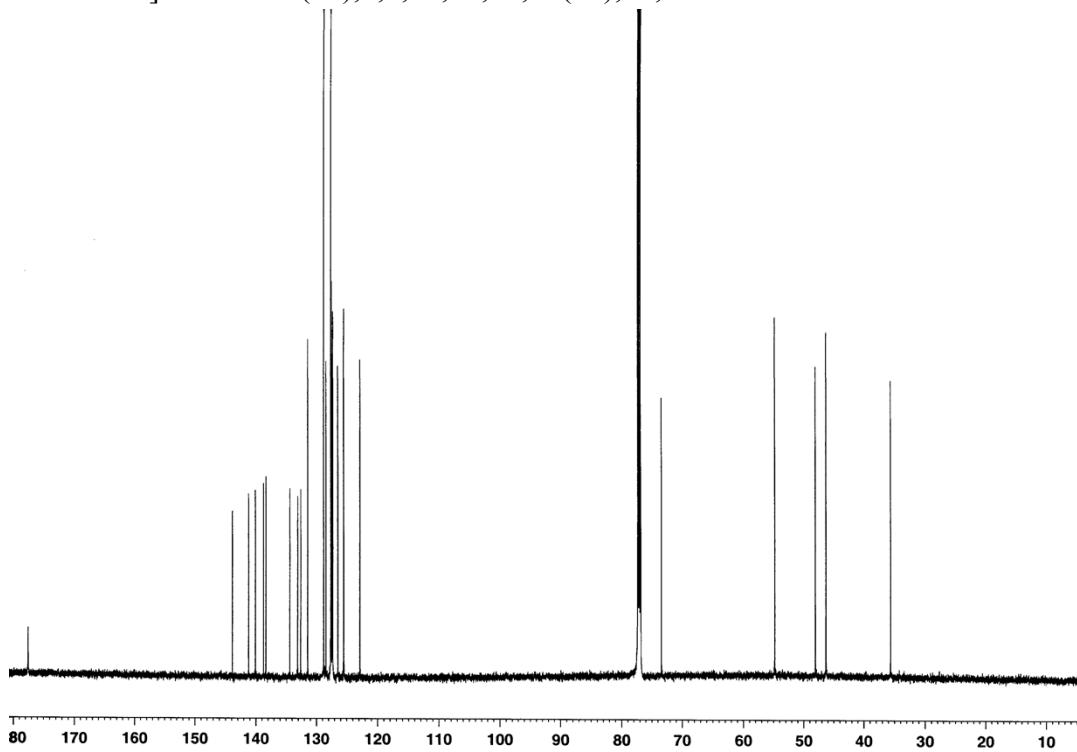
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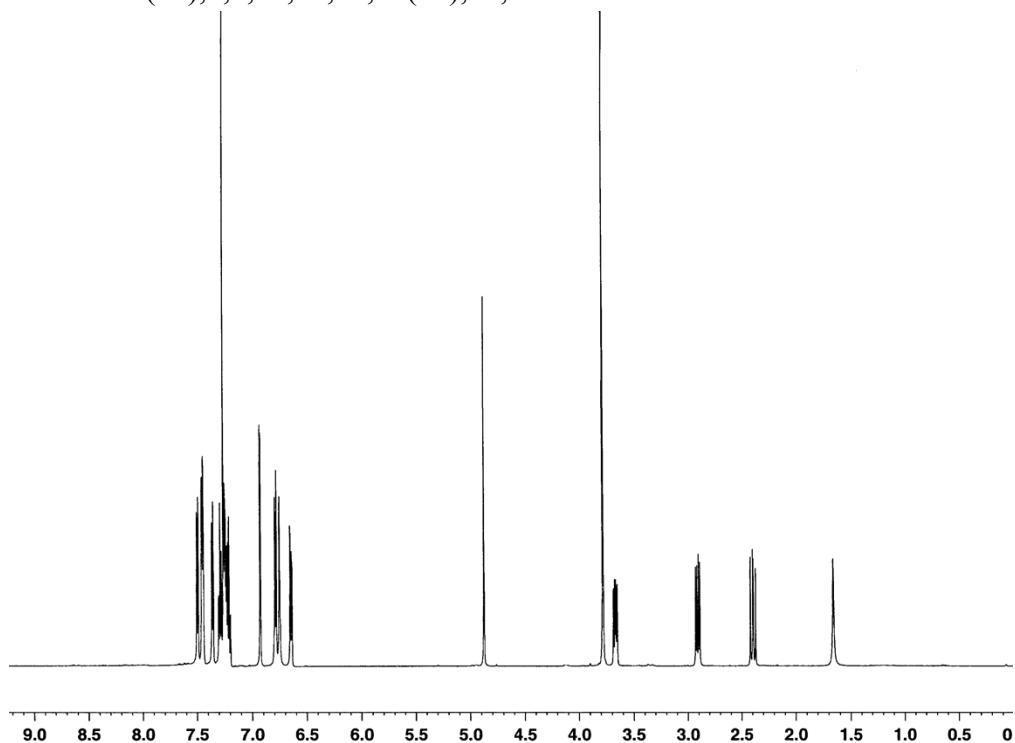
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 2-benzyl-9-chloro-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4h**



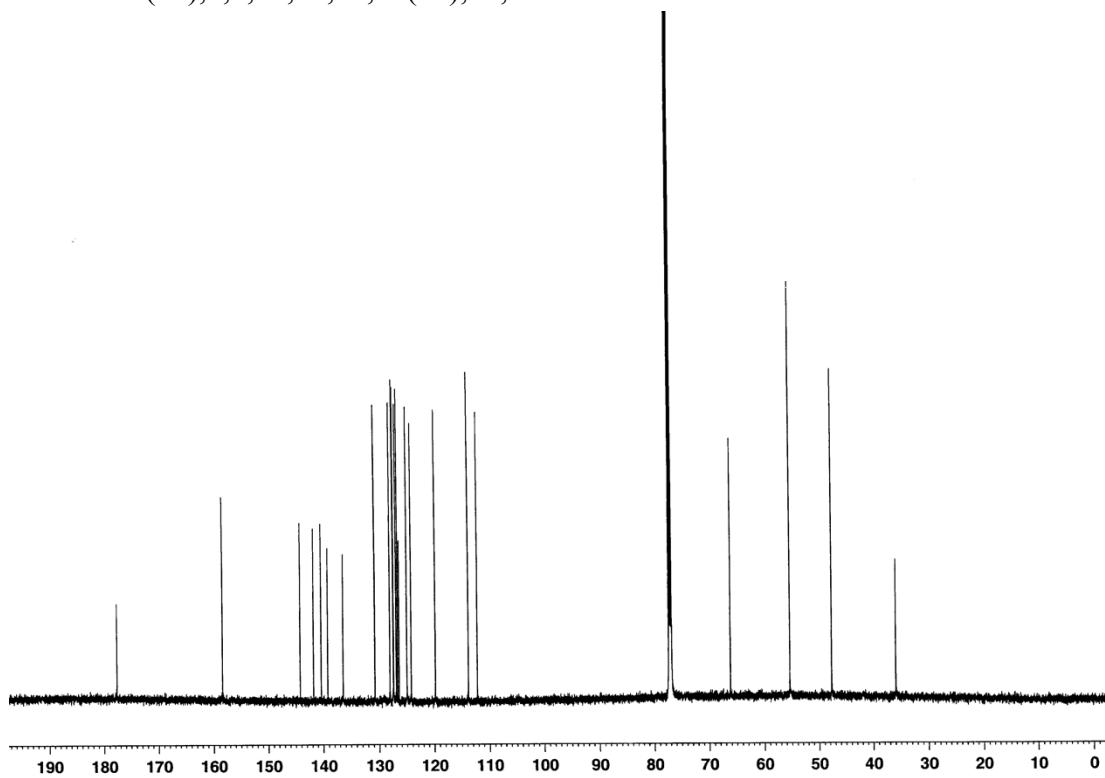
¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 2-benzyl-9-chloro-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4h**



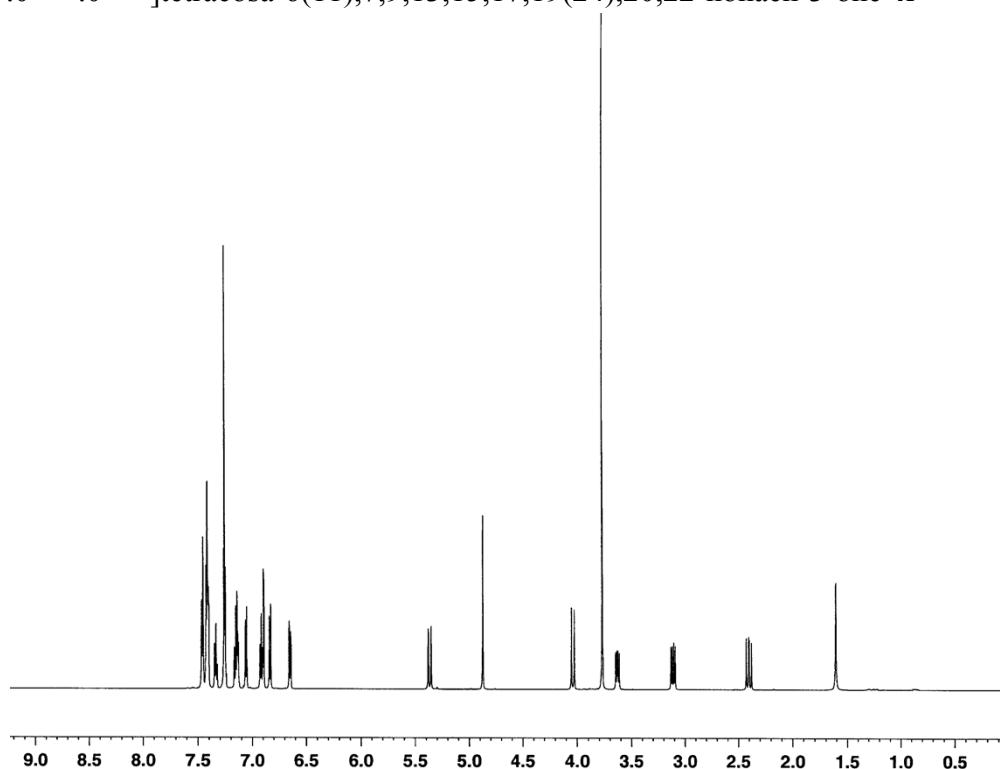
¹H-NMR spectrum (600MHz, CDCl₃) of (\pm) 9-methoxy-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}] tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4k**



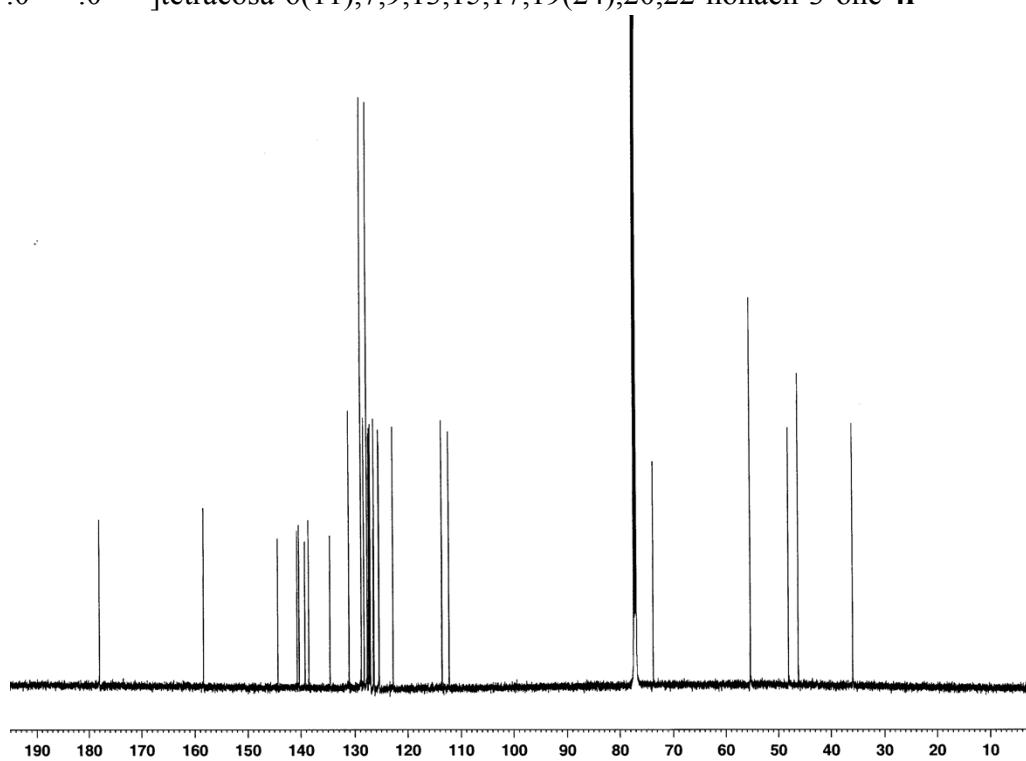
¹³C-NMR spectrum (150MHz, CDCl₃) of (\pm) 9-methoxy-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}] tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4k**



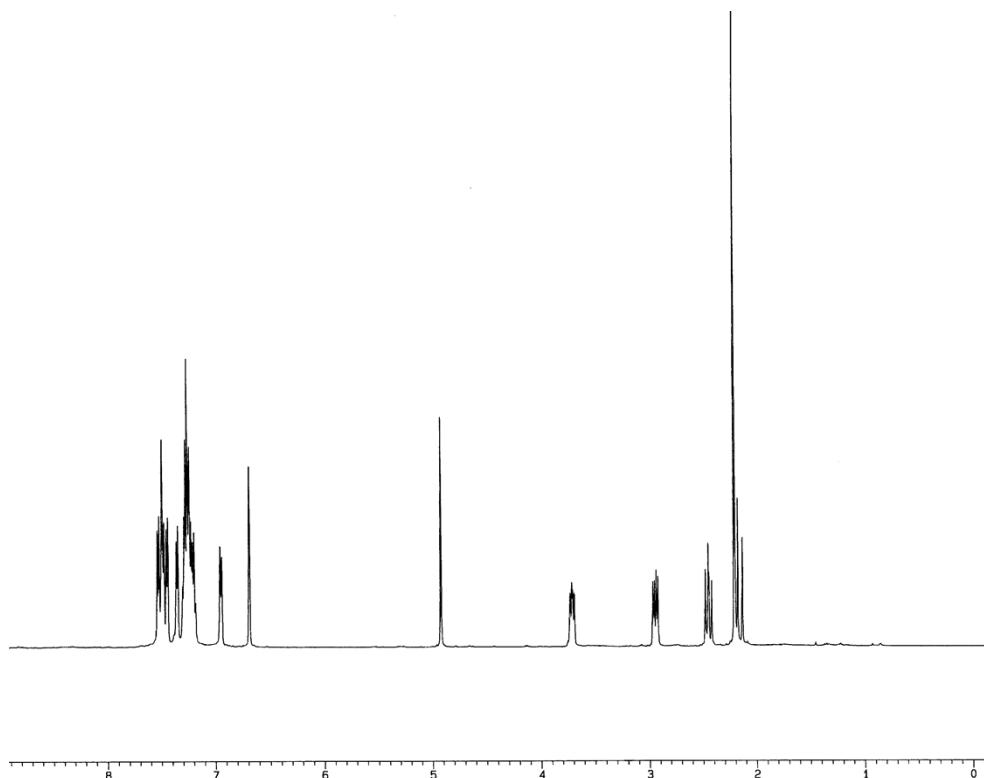
¹H-NMR spectrum (600MHz, CDCl₃) of (\pm) 2-benzyl-9-methoxy-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4l**



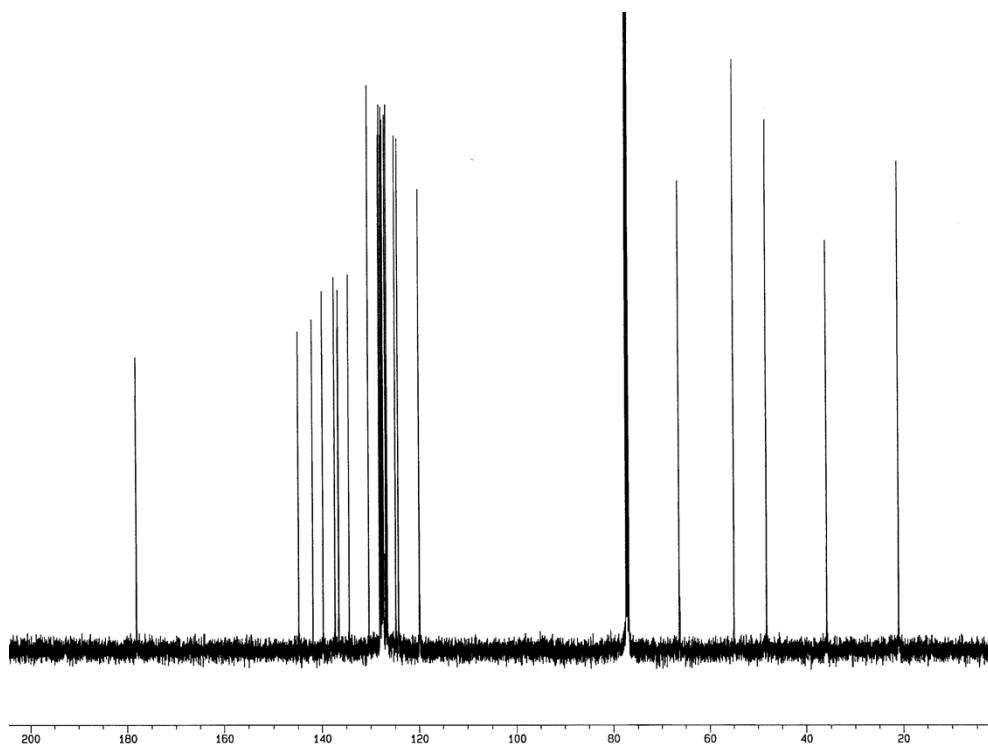
¹³C-NMR spectrum (150MHz, CDCl₃) of (\pm) 2-benzyl-9-methoxy-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4l**



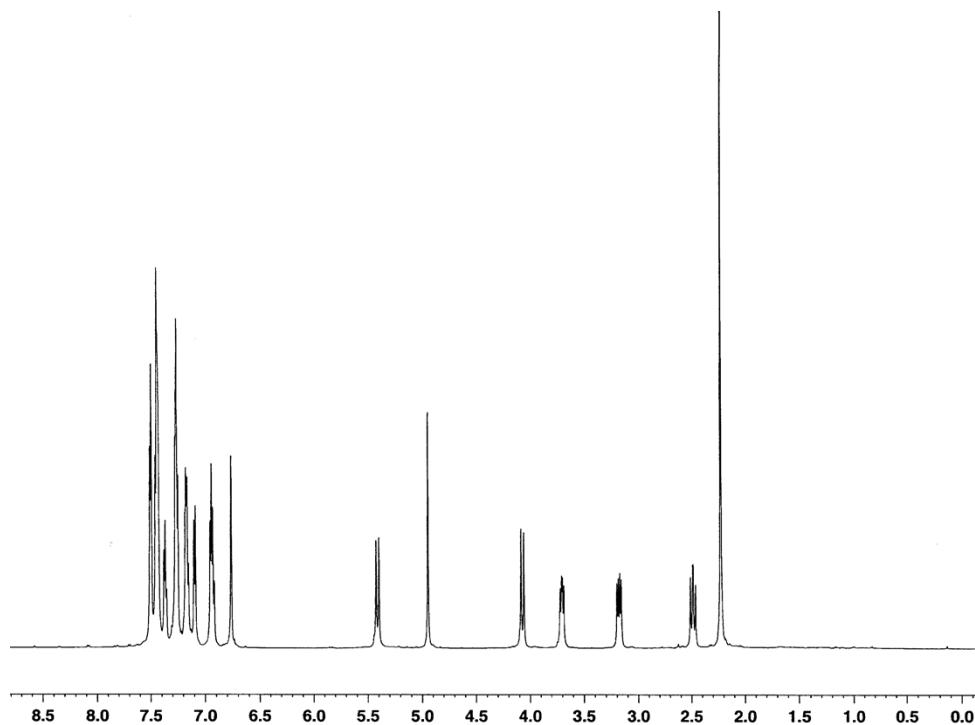
¹H-NMR spectrum (500MHz, CDCl₃) of (\pm) 8-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4m**



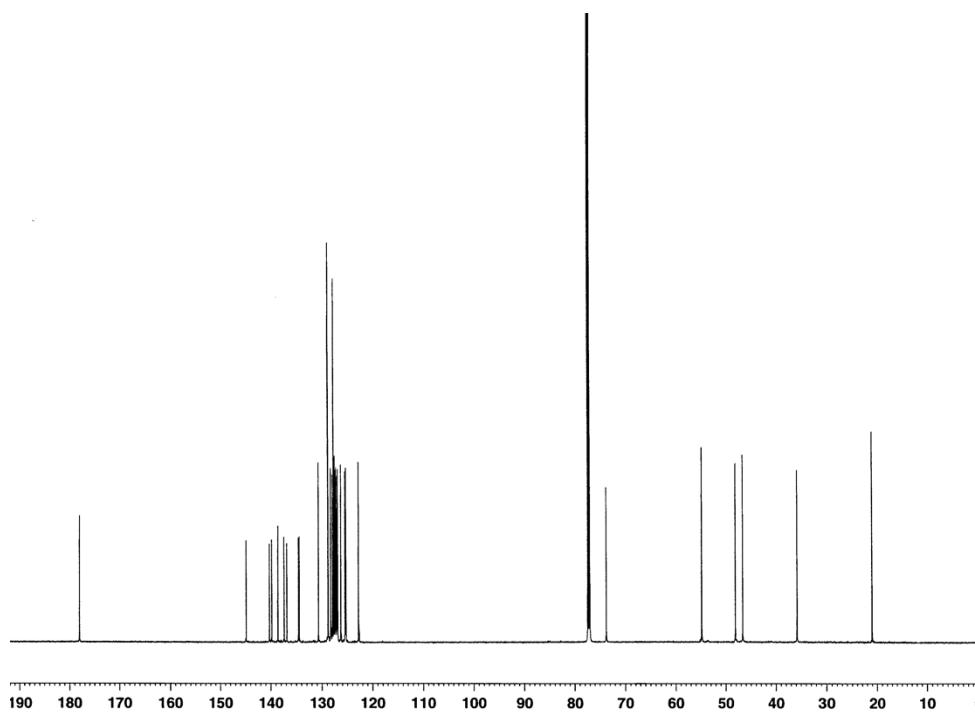
¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 8-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4m**



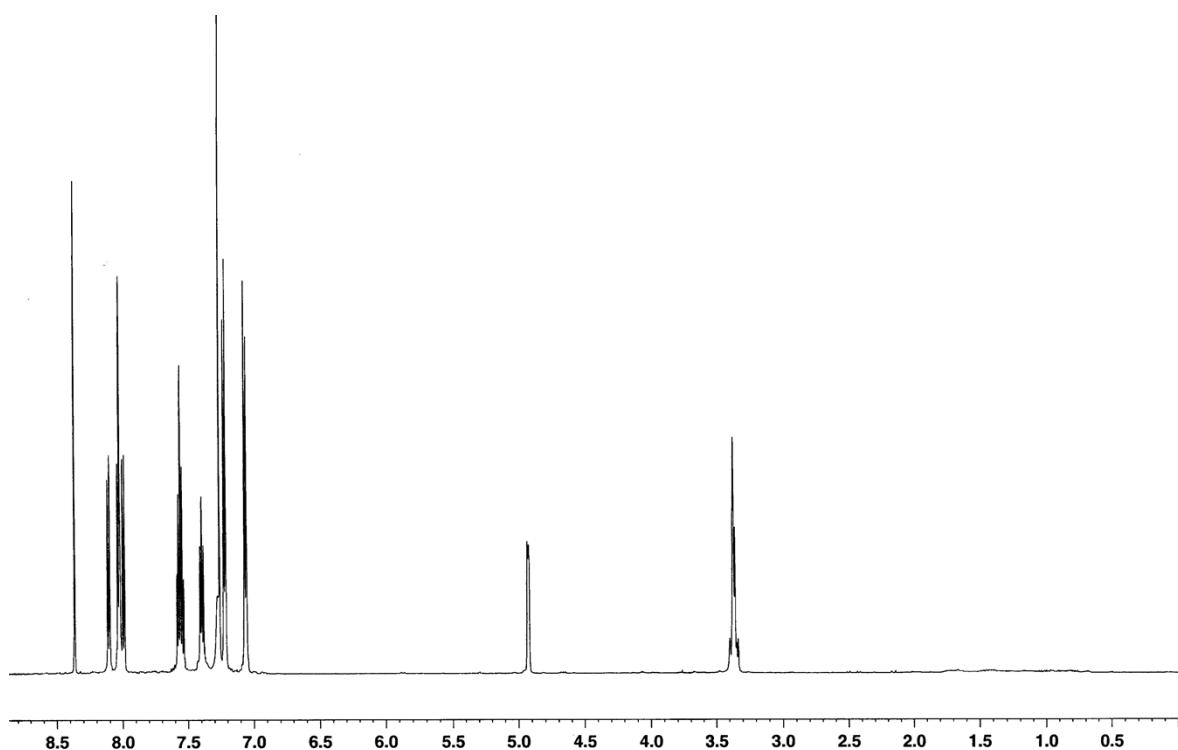
¹H-NMR spectrum (600MHz, CDCl₃) of (\pm) 2-benzyl-8-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4n**



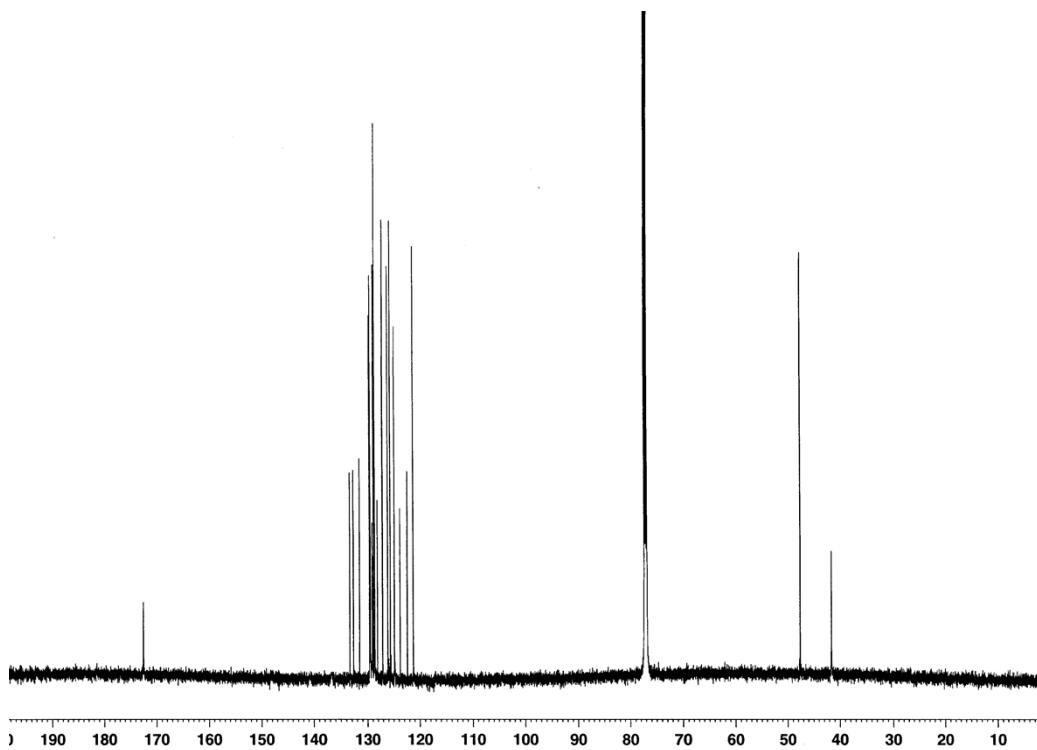
¹³C-NMR spectrum (150MHz, CDCl₃) of (\pm) 2-benzyl-8-methyl-2-azahexacyclo[10.6.6.0^{1,5}.0^{6,11}.0^{13,18}.0^{19,24}]tetracosa-6(11),7,9,13,15,17,19(24),20,22-nonaen-3-one **4n**



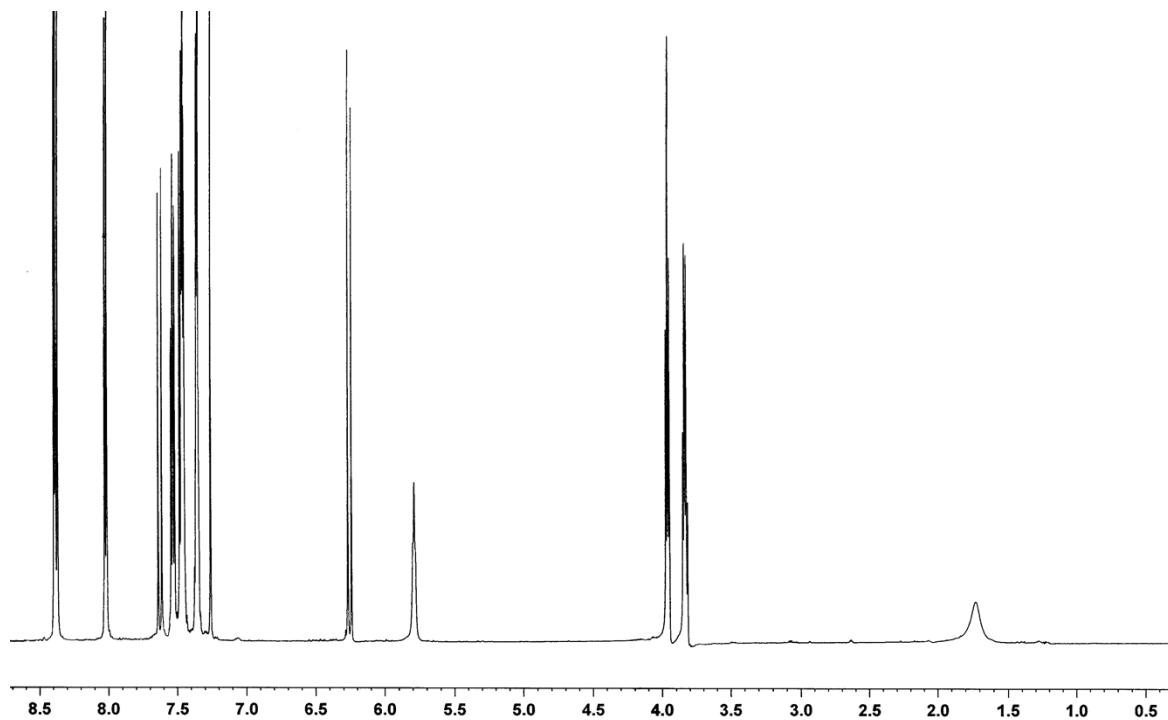
^1H -NMR spectrum (600MHz, CDCl_3) of (\pm) 4-phenyl-3,4-dihydro-1H-1-azacyclohept[de]anthracen-2-one 7



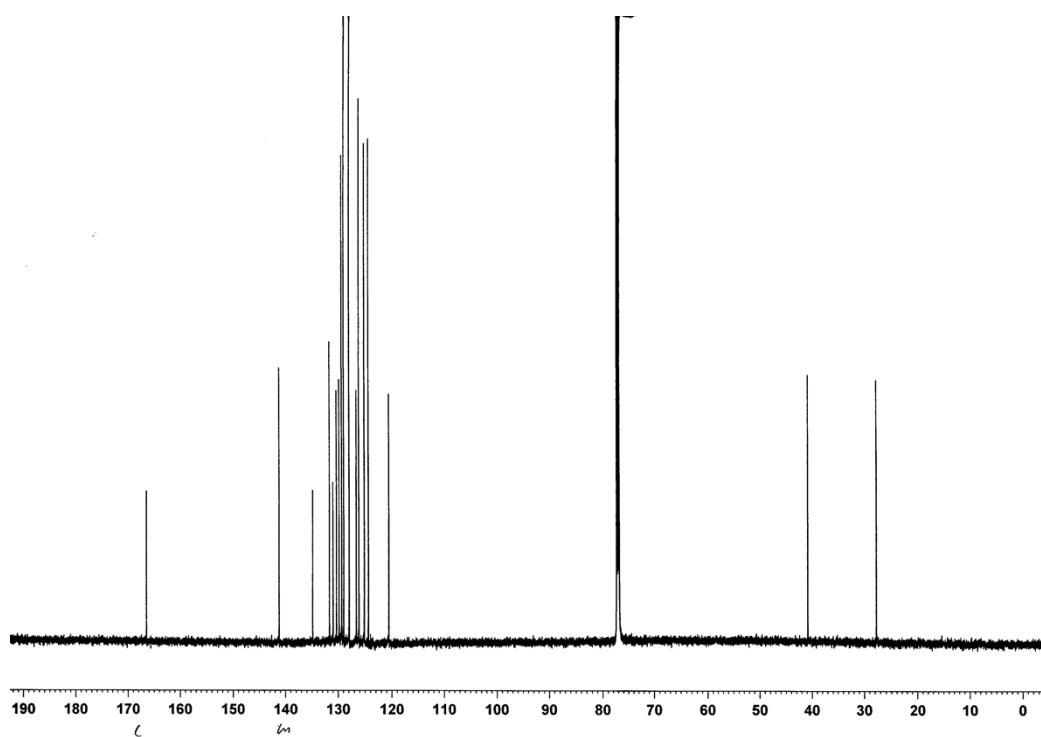
^{13}C -NMR spectrum (125MHz, CDCl_3) of (\pm) 4-phenyl-3,4-dihydro-1H-1-azacyclohept[de]anthracen-2-one 7



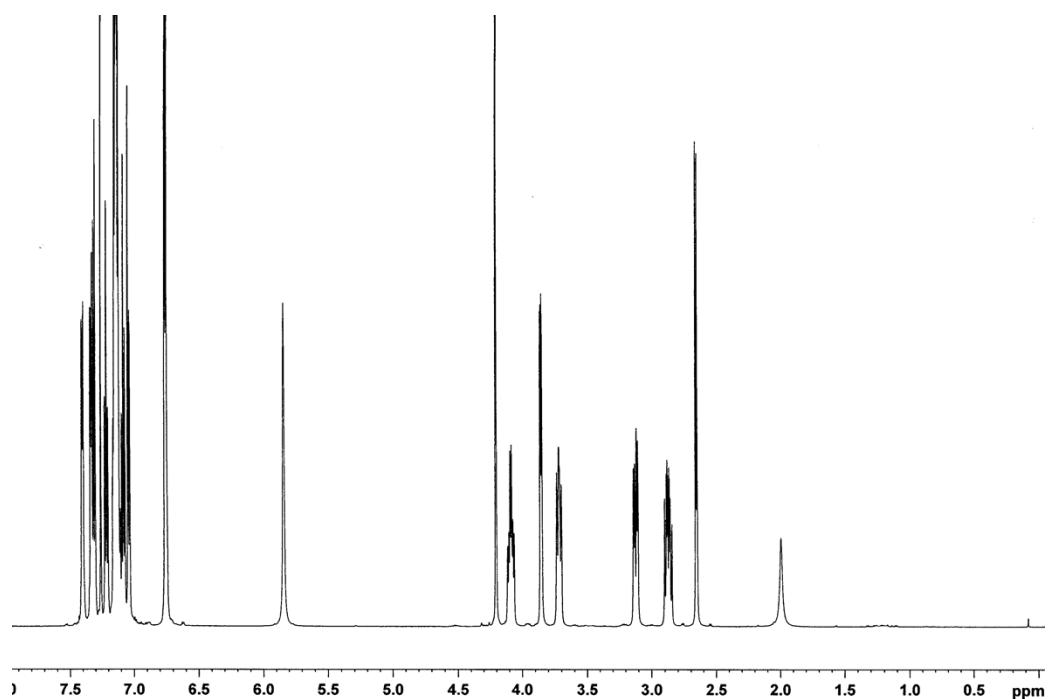
¹H-NMR spectrum (600MHz, CDCl₃) of *N*-(anthracen-9-yl-ethyl)-3-phenylacrylamide **8**



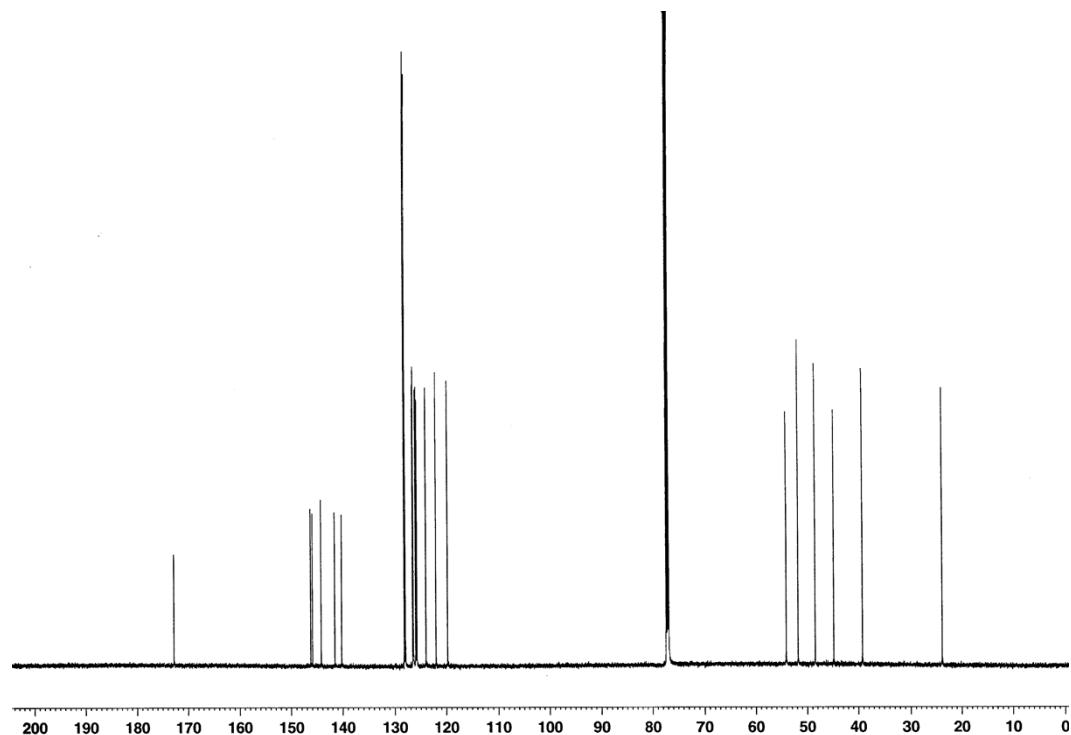
¹³C-NMR spectrum (125MHz, CDCl₃) of *N*-(anthracen-9-yl-ethyl)-3-phenylacrylamide **8**



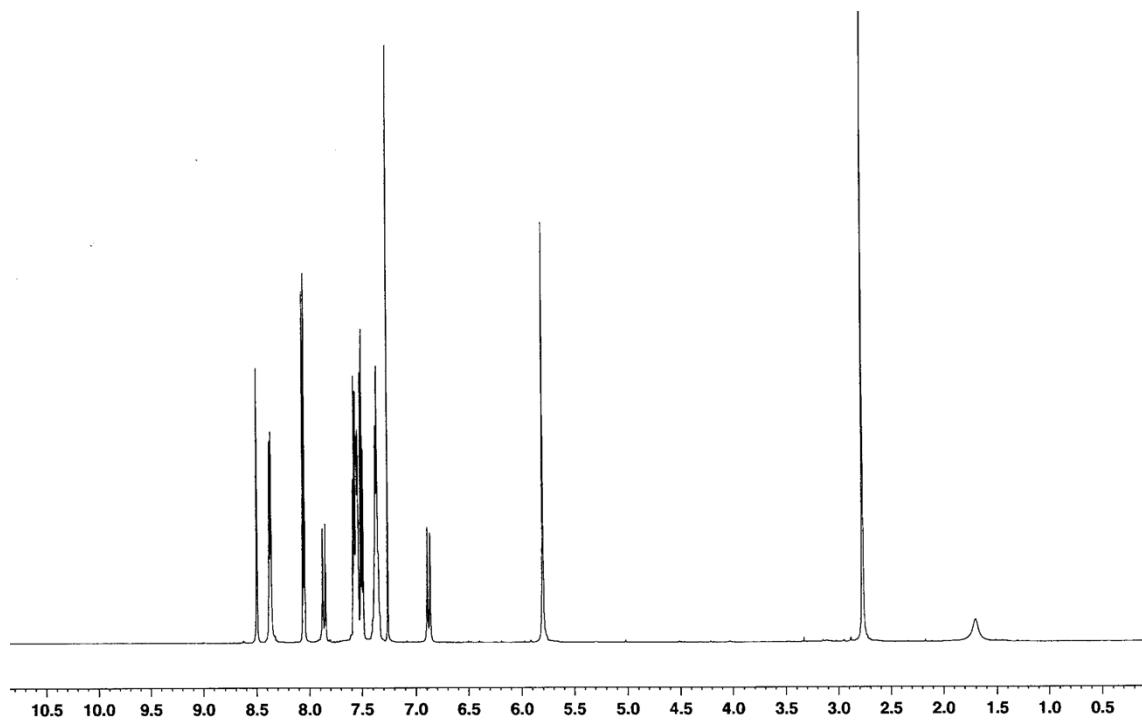
¹H-NMR spectrum (600MHz, CDCl₃) of (19S,20R)(19R,20S)-20-phenyl-17-azapentacyclo[6.-6.-6.-0^{1,19}.0^{2,7}.0^{9,14}]icosa- 2,4,6,9(14),10,12-hexaen-18-one **9**



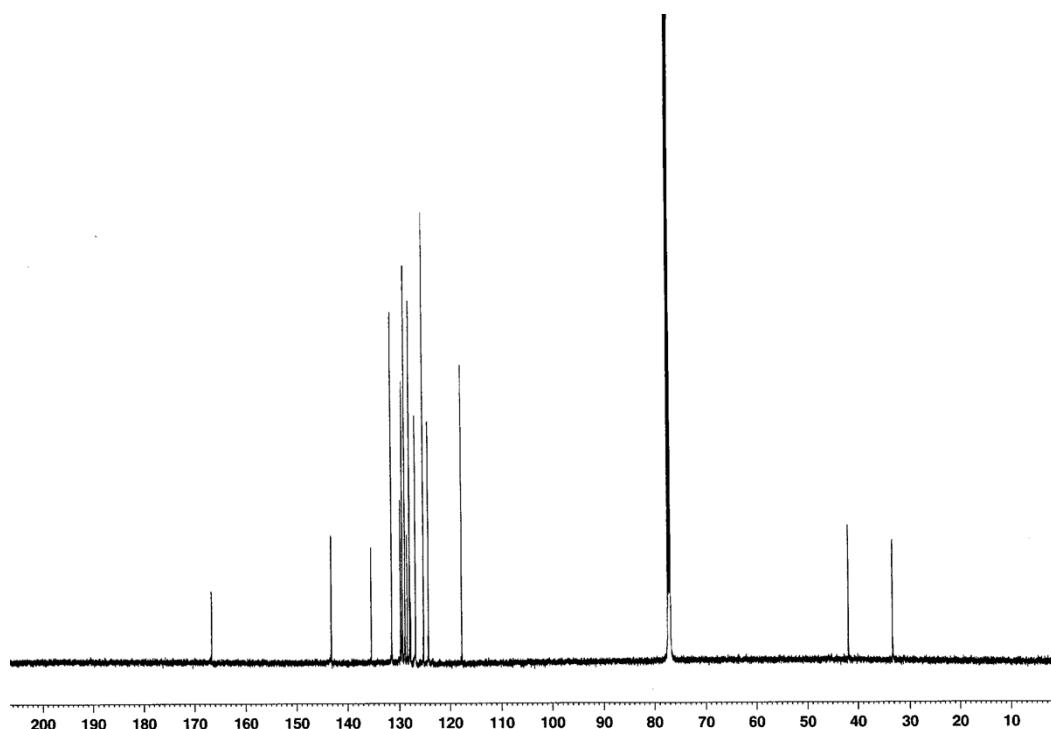
¹³C-NMR spectrum (125MHz, CDCl₃) of (19S,20R)(19R,20S)-20-phenyl-17-azapentacyclo[6.-6.-6.-0^{1,19}.0^{2,7}.0^{9,14}]icosa- 2,4,6,9(14),10,12-hexaen-18-one **9**



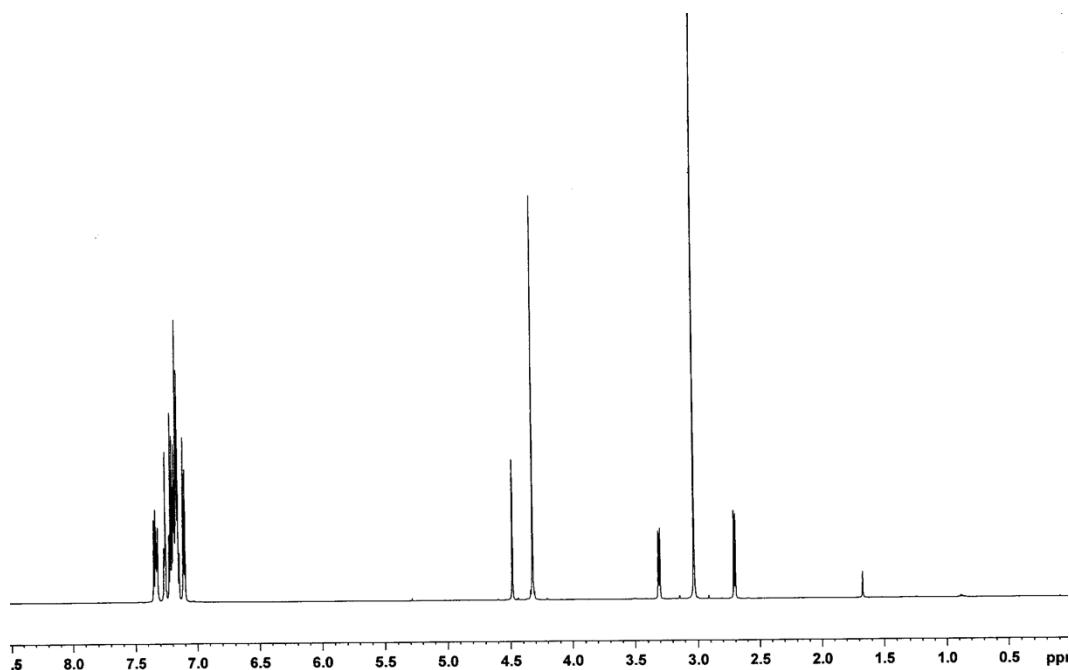
¹H-NMR spectrum (600MHz, CDCl₃) of *N*-(anthracen-9-yl-methyl)-*N*-methyl-3-phenylacryl-amide **10**



¹³C-NMR spectrum (125MHz, CDCl₃) of *N*-(anthracen-9-yl-methyl)-*N*-methyl-3-phenylacryl-amide **10**



¹H-NMR spectrum (600MHz, CDCl₃) of (\pm) 16-methyl-19-phenyl-16-azapentacyclo[6.6.5.0^{1,18}.0^{2,7}.0^{9,14}]nonadeca-2,4,6,9(14),10,12-hexaen-17-one **11**



¹³C-NMR spectrum (125MHz, CDCl₃) of (\pm) 16-methyl-19-phenyl-16-azapentacyclo[6.6.5.0^{1,18}.0^{2,7}.0^{9,14}]nonadeca-2,4,6,9(14),10,12-hexaen-17-one **11**

