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Supporting Information

Aza-aromatic polycycles based on triphenylene and acridine or acridone: synthesis and properties

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Table of Contents

General information and crystallographic details p. S2

Experimental procedures and analyses of intermediate compounds p. S3

NMR spectra of compounds **1**, **2**, **3a-c**, **4a-c**, **5**, **6**, **7**, **8**, **9**, **10**, **11**, **12** and **13** p. S7

Highest occupied Hückel molecular orbitals (HOMO) of the compounds **A**, **B**, **C**, **1**, **3a-c**, **5**, **10** and **12** p. S32

Qualitative evaluation of **8** and **9** as matrices for MALDI-MS p. S37

References and notes p. S45

General information

Column chromatography separations were achieved on silica gel (40-63 μm). Melting points were measured on a Kofler apparatus. IR spectra were taken on a Perkin-Elmer Spectrum 100 spectrometer. ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectra were recorded either on a Bruker Avance III spectrometer at 300 MHz and 75 MHz respectively, or on a Bruker Avance III HD spectrometer at 500 MHz and 126 MHz respectively. ^{1}H chemical shifts (δ) are given in ppm relative to the solvent residual peak and ^{13}C chemical shifts are relative to the central peak of the solvent signal.[1] Unless otherwise specified, mass spectra (HRMS) were recorded on an Ultraflex III apparatus in Matrix Assisted Laser Desorption (MALDI) positive mode (Matrix: *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile, DCTB).

Unless otherwise stated, all reagents are commercially available and used as received. After distillation, dimethylsulfoxyde and dimethylformamide were stored on 3Å molecular sieves. Activated copper,[2] 2-iodotriphenylene,[3] 2-aminobenzaldehyde[4] and 9-aminoacridine (9AA)[5] were prepared as reported previously. All reactions involving moisture-sensitive reactants were performed under argon atmosphere. Before use, $CDCl_3$ was neutralized by passing through a short plug of anhydrous, activated basic alumina.

Crystallographic details

The X-ray diffraction data of the compounds **2** and **8** were collected at 150(2) K on a D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector by using Mo-Kα radiation (λ = 0.71073 Å, multilayered monochromator). The structures were solved by dual-space algorithm using the *SHELXT* program,[6] and then refined with full-matrix least-square methods based on F^2 (*SHELXL*).[7] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. The molecular diagrams were generated by ORTEP-3 (version 2.02).[8]

Experimental procedures and analyses of the compounds

Synthesis of the compounds 1 and 3 (General procedure).

They were prepared under an argon atmosphere by adapting a procedure reported previously.[9] To a solution of either 2-aminobenzaldehyde[4] (0.12 g, 1.0 mmol), or the commercial 2-aminophenone (1.0 mmol), and 2-iodotriphenylene[3] (0.35 g, 1.0 mmol) in degassed Bu_2O (1 mL) were successively added activated Cu^2 (0.20 equiv, 13 mg, 0.20 mmol) and K_2CO_3 (2 equiv, 0.29 g, 2.0 mmol). The mixture was degassed and refluxed under argon for 12 h. During this time, activated Cu^2 (4 x 13 mg, 4 x 0.2 mmol) was added after 2, 4, 6 and 8 h of heating. After cooling to room temperature, the mixture was concentrated and purified as specified in the product description.

2-(2-Triphenylenyl)aminobenzaldehyde (1). It was prepared according to the general procedure by starting from 2-aminobenzaldehyde.[4] Purification by column chromatography on silica gel (eluent: petroleum ether-AcOEt 90:10; R_f = 0.46) gave **1** in 86% yield (0.31 g) as a yellow solid: mp 182 °C; IR (ATR): 664, 717, 749, 802, 857, 869, 968, 998, 1042, 1052, 1117, 1150, 1185, 1199, 1241, 1319, 1400, 1432, 1452, 1492, 1509, 1581, 1605, 1652, 2751, 2850, 2920, 3053, 3282 cm^{-1}; ^1H NMR ($CDCl_3$) δ 6.88-6.93 (m, 1H), 7.44 (d, 2H, *J* = 3.4 Hz), 7.59-7.71 (m, 6H), 8.52-8.68 (m, 6H), 9.98 (s, 1H, CHO), 10.32 (br s, 1H, NH); ^{13}C NMR ($CDCl_3$) δ 113.2 (CH), 116.5 (CH), 117.6 (CH), 119.8 (C), 122.7 (CH), 123.1 (CH), 123.4 (CH), 123.4 (CH), 123.5 (CH), 124.7 (CH), 126.5 (C), 126.9 (CH), 127.3 (CH), 127.4 (CH), 127.6 (CH), 129.3 (C), 129.4 (C), 129.7 (C), 130.2 (C), 131.1 (C), 135.8 (CH), 136.8 (CH), 138.9 (C), 147.7 (C), 194.4 (CH, CHO).

Phenyl 2-(2-triphenylenyl)aminophenyl ketone (3a). It was prepared according to the general procedure by starting from 2-aminobenzophenone (0.20 g). Purification by column chromatography on silica gel (eluent: petroleum ether-AcOEt 90:10; R_f = 0.50) gave **3a** in 71% yield (0.31 g) as an orange solid: mp 100 °C; IR (ATR): 750, 804, 819, 855, 911, 939, 1001,

1028, 1050, 1075, 1108, 1154, 1246, 1317, 1448, 1490, 1509, 1569, 1599, 2919, 3062, 3277 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 6.83 (t, 1H, *J* = 7.5 Hz), 7.44 (td, 1H, *J* = 7.6 and 1.4 Hz), 7.53-7.64 (m, 9H), 7.70 (dd, 1H, *J* = 8.0 and 1.3 Hz), 7.89 (d, 2H, *J* = 6.7 Hz), 8.49-8.59 (m, 6H), 10.55 (s, 1H, NH); ^{13}C NMR ($CDCl_3$) δ 114.8 (CH), 114.9 (CH), 117.0 (CH), 120.2 (C), 121.6 (CH), 122.8 (CH), 123.1 (CH), 123.2 (CH), 123.2 (CH), 124.5 (CH), 125.6 (C), 126.5 (CH), 127.0 (CH), 127.1 (CH), 127.2 (CH), 128.1 (2CH), 129.0 (C), 129.2 (C), 129.5 (2CH), 129.6 (C), 130.0 (C), 130.9 (C), 131.4 (CH), 134.3 (CH), 135.0 (CH), 139.5 (C), 139.7 (C), 147.6 (C), 199.0 (C, C=O).

5-Chloro-2-(2-triphenylenyl)aminophenyl phenyl ketone (3b). It was prepared according to the general procedure by starting from 2-amino-5-chlorobenzophenone (0.23 g) Purification by column chromatography on silica gel (eluent: petroleum ether-AcOEt 90:10; R_f = 0.50) gave **3b** in 91% yield (0.40 g) as an orange powder: mp 160 °C; IR (ATR): 657, 699, 719, 753, 772, 807, 824, 869, 916, 949, 1102, 1118, 1148, 1178, 1236, 1319, 1408, 1444, 1490, 1511, 1571, 1612, 2167, 3057 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 7.33 (dd, 1H, *J* = 9.0 and 2.5 Hz, H4), 7.48 (d, 1H, *J* = 9.1 Hz, H3), 7.51-7.67 (m, 9H), 7.77-7.80 (m, 2H), 8.44 (d, 1H, *J* = 2.1 Hz, H6), 8.48-8.63 (m, 5H), 10.26 (s, 1H, NH); ^{13}C NMR ($CDCl_3$) δ 115.6 (CH), 116.8 (CH), 121.3 (C), 121.7 (C), 122.1 (CH), 123.1 (CH), 123.4 (CH), 123.5 (CH), 123.5 (CH), 125.0 (CH), 126.3 (C), 126.9 (CH), 127.4 (CH), 127.5 (CH), 127.7 (CH), 128.6 (2CH), 129.4 (C), 129.7 (2CH), 129.8 (C), 130.3 (C), 131.3 (C), 132.1 (CH), 133.90 (CH), 134.3 (CH), 139.1 (C), 139.5 (C), 146.5 (C), 198.2 (C, C=O), 1C not seen.

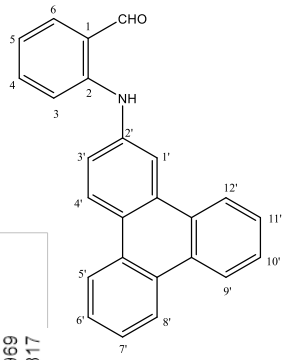
2-(2-Triphenylenyl)aminoacetophenone (3c). It was prepared according to the general procedure by starting from 2-aminoacetophenone (0.14 g). Purification by column chromatography on silica gel (eluent: petroleum ether-AcOEt 90:10; R_f = 0.475) gave **3c** in 66% yield (0.25 g) as a yellow powder: mp 174 °C; IR (ATR): 657, 700, 717, 751, 770, 807, 869, 949, 1119, 1149, 1177, 1236, 1320, 1408, 1430, 1490, 1513, 1571, 1612, 3057 cm^{-1}; ^{1}H

NMR ($CDCl_3$) δ 2.70 (s, 3H, Me), 6.81 (ddd, 1H, *J* = 8.1, 6.9 and 1.2 Hz), 7.37 (ddd, 1H, *J* = 8.5, 6.9 and 1.5 Hz), 7.46 (dd, 1H, *J* = 8.5 and 1.0 Hz), 7.57 (dd, 1H, *J* = 8.8 and 2.2 Hz), 7.60-7.69 (m, 4H), 7.88 (dd, 1H, *J* = 8.1 and 1.4 Hz), 8.48 (d, 1H, *J* = 2.2 Hz), 8.52-8.66 (m, 5H), 10.85 (s, 1H, NH); ^{13}C NMR ($CDCl_3$) δ 28.3 (CH_3), 114.6 (CH), 116.4 (CH), 117.1 (CH), 119.6 (C), 122.8 (CH), 123.1 (CH), 123.4 (CH), 123.5 (CH), 123.5 (CH), 124.7 (CH), 126.2 (C), 126.8 (CH), 127.3 (CH), 127.4 (CH), 127.5 (CH), 129.4 (C), 129.5 (C), 129.8 (C), 130.2 (C), 131.1 (C), 132.7 (CH), 134.8 (CH), 139.7 (C), 147.8 (C), 201.5 (C, C=O).

Ethyl 2-(2-triphenylenyl)aminobenzoate (5). It was prepared under an argon atmosphere by adapting a procedure reported previously.[9] To commercial ethyl anthranilate (ethyl 2-aminobenzoate; 0.17 g, 1.0 mmol) and 2-iodotriphenylene[3] (0.35 g, 1.0 mmol) in degassed Bu_2O (1 mL) were successively added activated Cu[2] (0.20 equiv, 13 mg, 0.20 mmol) and K_2CO_3 (2 equiv, 0.29 g, 2.0 mmol). The mixture was degassed and refluxed under argon for 12 h. During this time, activated Cu[2] (4 x 13 mg, 4 x 0.2 mmol) was added after 2, 4, 6 and 8 h of heating. After cooling to room temperature, the mixture was concentrated. Purification by column chromatography on silica gel (eluent: petroleum ether-AcOEt 98:2; R_f = 0.575) gave **5** in 88% yield (0.34 g) as a yellow solid: mp 135 °C; IR (ATR): 700, 718, 749, 813, 857, 872, 944, 1025, 1050, 1083, 1148, 1162, 1235, 1246, 1316, 1368, 1395, 1442, 1453, 1491, 1513, 1581, 1602, 1617, 1671, 2979, 3313 cm-1; ^{1}H NMR ($CDCl_3$) δ 1.47 (t, 3H, *J* = 7.1 Hz), 4.44 (q, 2H, *J* = 7.1 Hz), 6.84 (t, 1H, *J* = 7.5 Hz), 7.40 (td, 1H, *J* = 7.8 and 1.4 Hz), 7.49 (d, 1H, *J* = 8.4 Hz), 7.56 (dd, 1H, *J* = 8.8 and 2.1 Hz), 7.59-7.67 (m, 4H), 8.09 (dd, 1H, *J* = 8.0 and 1.3 Hz), 8.45-8.64 (m, 6H), 9.87 (br s, 1H, NH); ^{13}C NMR ($CDCl_3$) δ 14.5 (CH_3), 60.9 (CH_2), 112.8 (C), 114.4 (CH), 115.4 (CH), 117.6 (CH), 122.1 (CH), 123.0 (CH), 123.3 (CH), 123.4 (CH), 123.4 (CH), 124.6 (CH), 125.7 (C), 126.6 (CH), 127.2 (CH), 127.3 (CH), 127.4 (CH), 129.2 (C), 129.4 (C), 129.8 (C), 130.2 (C), 131.1 (C), 131.9 (CH), 134.2 (CH), 140.1 (C), 147.7 (C), 168.7 (C).

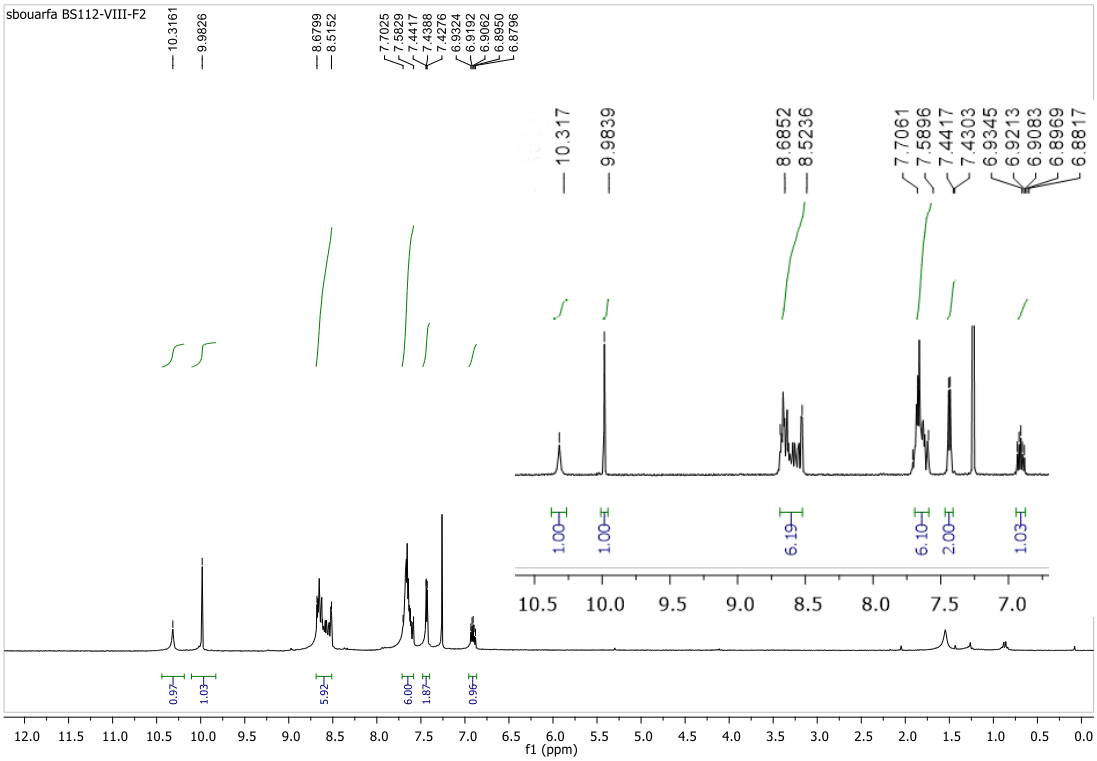
2-(2-Triphenylenyl)aminobenzoic acid (6) was prepared by adapting a procedure reported previously.[10] Ethyl 2-(2-triphenylenyl)aminobenzoate (**5**; 0.39 g, 1.0 mmol) was suspended in acetone (10 mL) and treated by 10 mL of a 5% aqueous solution of sodium hydroxide (12 mmol). The reaction mixture was refluxed for 16 h and cooled to room temperature. The solvent was removed under reduced pressure. CH_2Cl_2 (30 mL) and water (20 mL) were added to the residue. The aqueous phase was collected and acidified until pH = 1 by addition at 0 °C of concentrated hydrochloric acid. The obtained precipitate was dried under vacuum at 100 °C for 2 h and used in the next step without further purification. Compound **6** was obtained in a quantitative yield (0.36 g) as a beige solid: mp > 260 °C; IR (ATR): 719, 745, 760, 882, 919, 1043, 1162, 1252, 1319, 1338, 1434, 1450, 1491, 1509, 1570, 1617, 1664, 2567, 2839, 3342 cm-1; ^{1}H NMR ($(CD_3)_2SO$) δ 6.85-6.90 (m, 1H), 7.47 (d, 2H, *J* = 3.7 Hz), 7.62-7.74 (m, 5H), 7.98 (d, 1H, *J* = 8.2 Hz), 8.59 (d, 1H, *J* = 1.8 Hz, H1'), 8.71-8.81 (m, 5H), 9.96 (br s, 1H, NH), 13.17 (br s, 1H, CO_2H); ^{13}C NMR ($(CD_3)_2SO$) δ 113.5 (C), 114.2 (CH), 114.4 (CH), 118.0 (CH), 121.2 (CH), 123.1 (CH), 123.5 (CH), 123.5 (CH), 123.7 (CH), 124.6 (C), 125.0 (CH), 126.8 (CH), 127.5 (CH), 127.6 (CH), 127.7 (CH), 128.4 (C), 128.8 (C), 129.2 (C), 129.5 (C), 130.5 (C), 131.9 (CH), 134.2 (CH), 140.3 (C), 146.4 (C), 169.8 (C, C=O).

NMR spectra

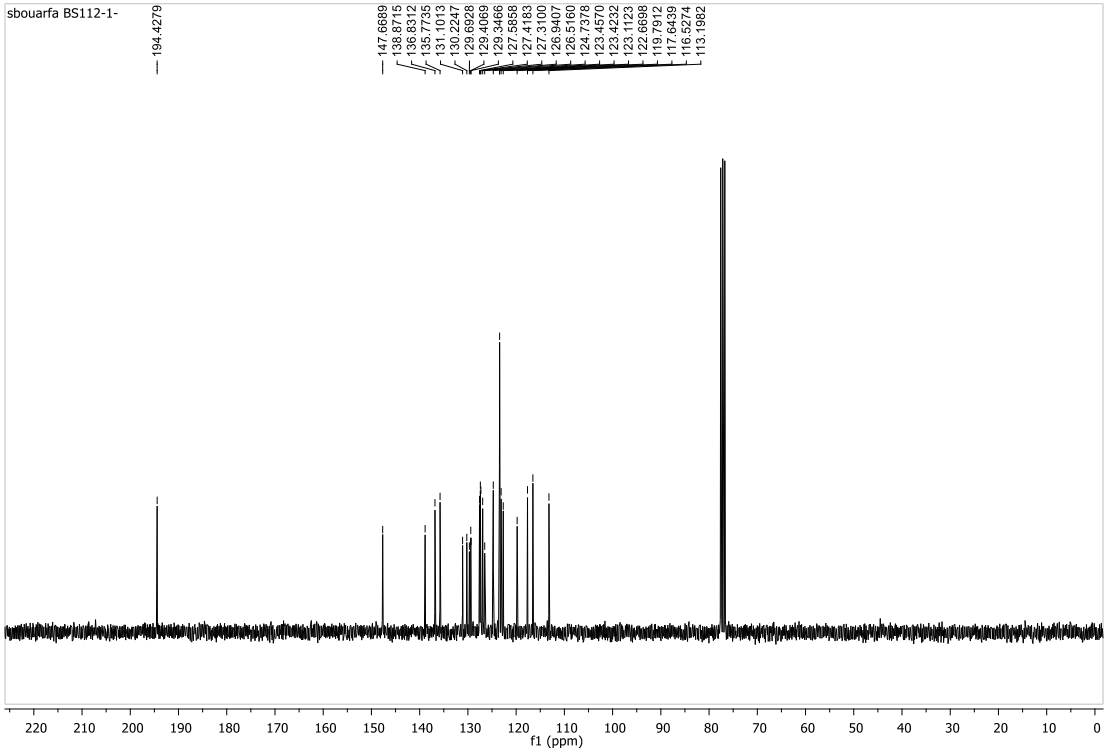


2-(2-Triphenylenyl)aminobenzaldehyde (1)

^{1}H NMR (300 MHz, $CDCl_3$)

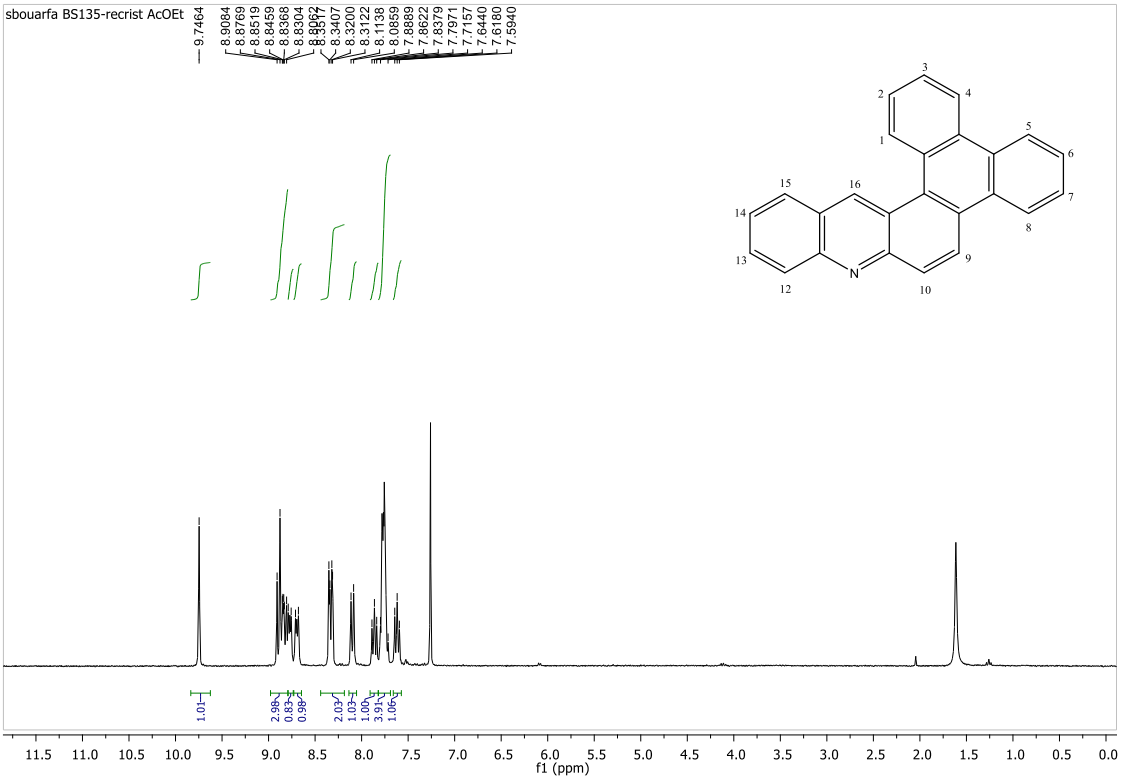


^{13}C NMR (75 MHz, $CDCl_3$)

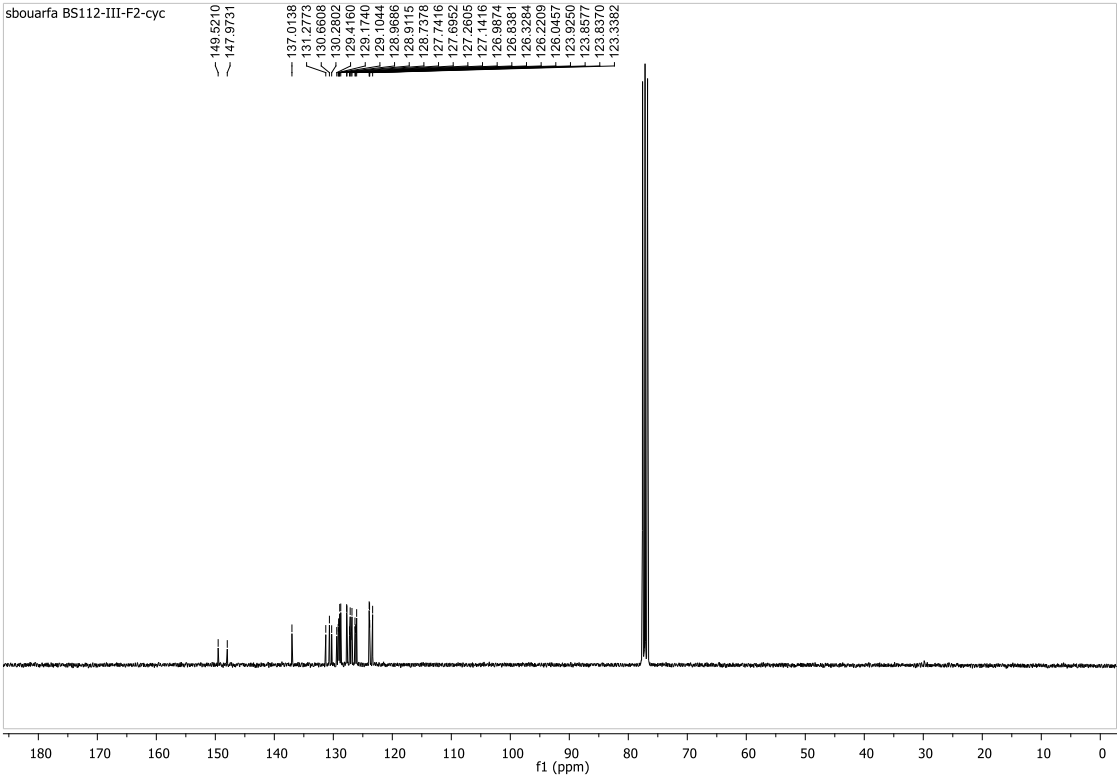


Phenanthro[9,10-*a*]acridine (2)

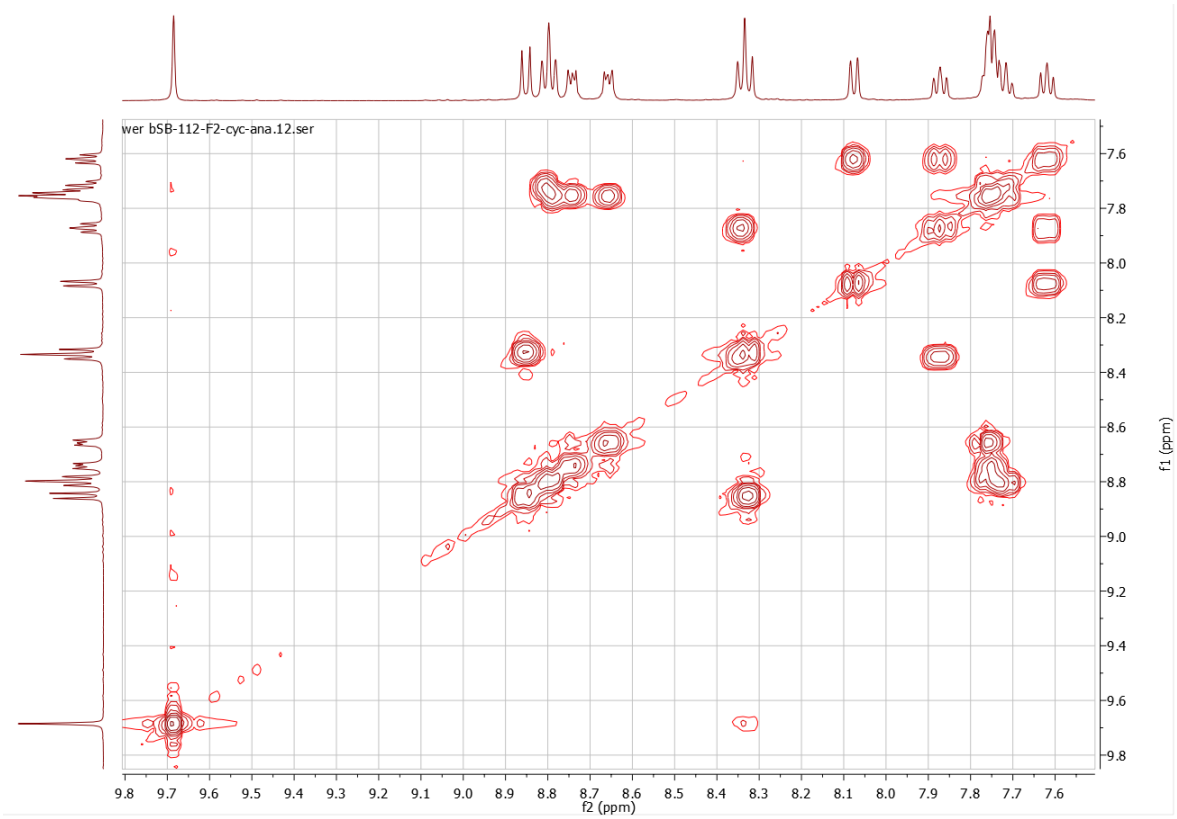
^{1}H NMR (500 MHz, $CDCl_3$)



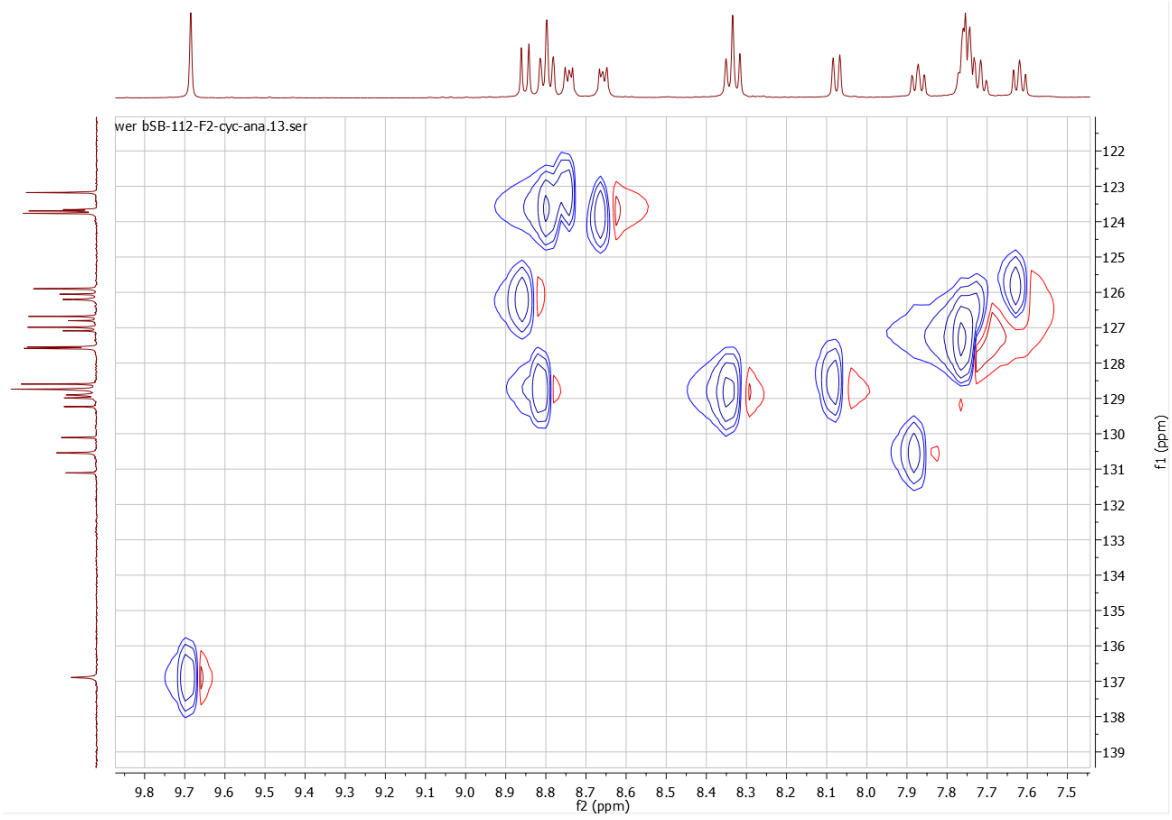
^{13}C NMR (75 MHz, $CDCl_3$)



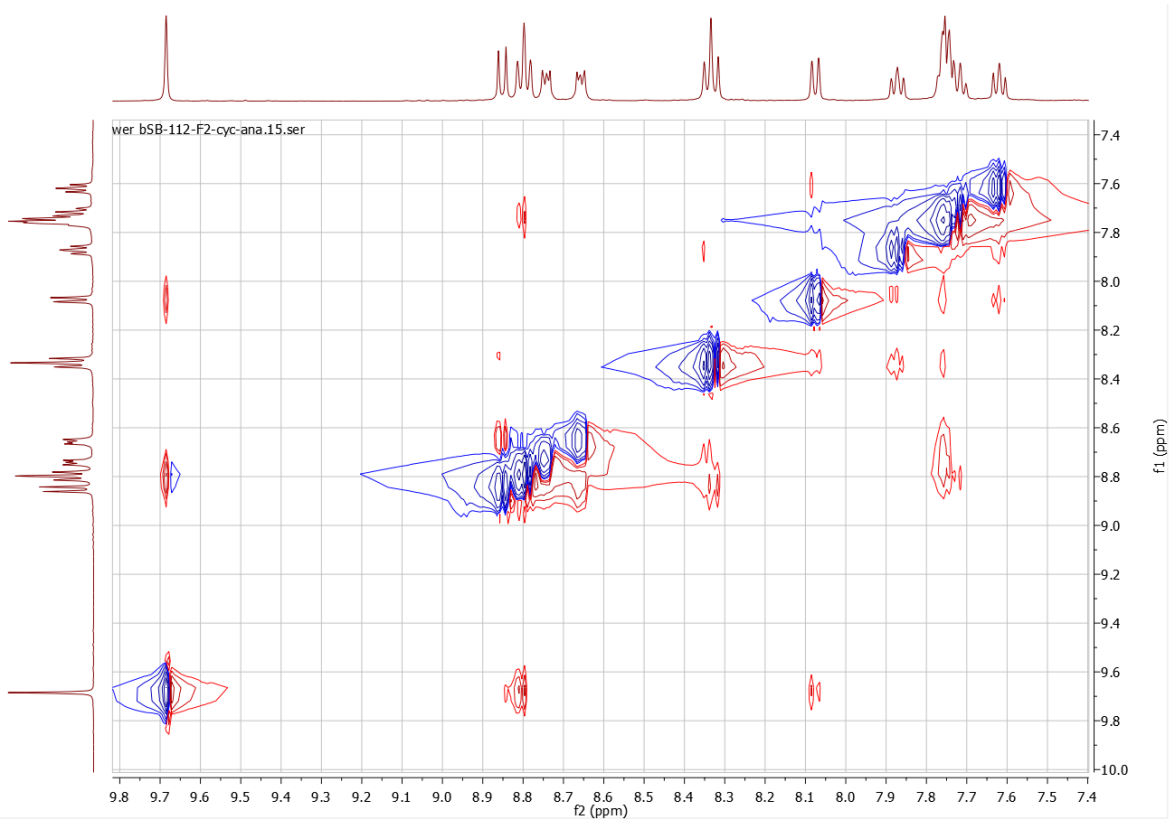
COSY (500 MHz, $CDCl_3$)



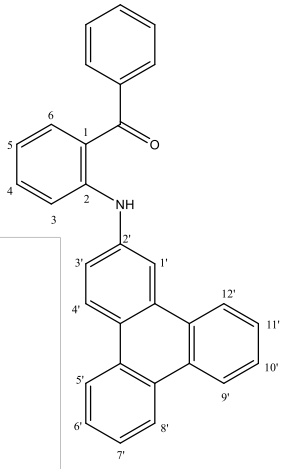
HSQC (500 MHz, $CDCl_3$)



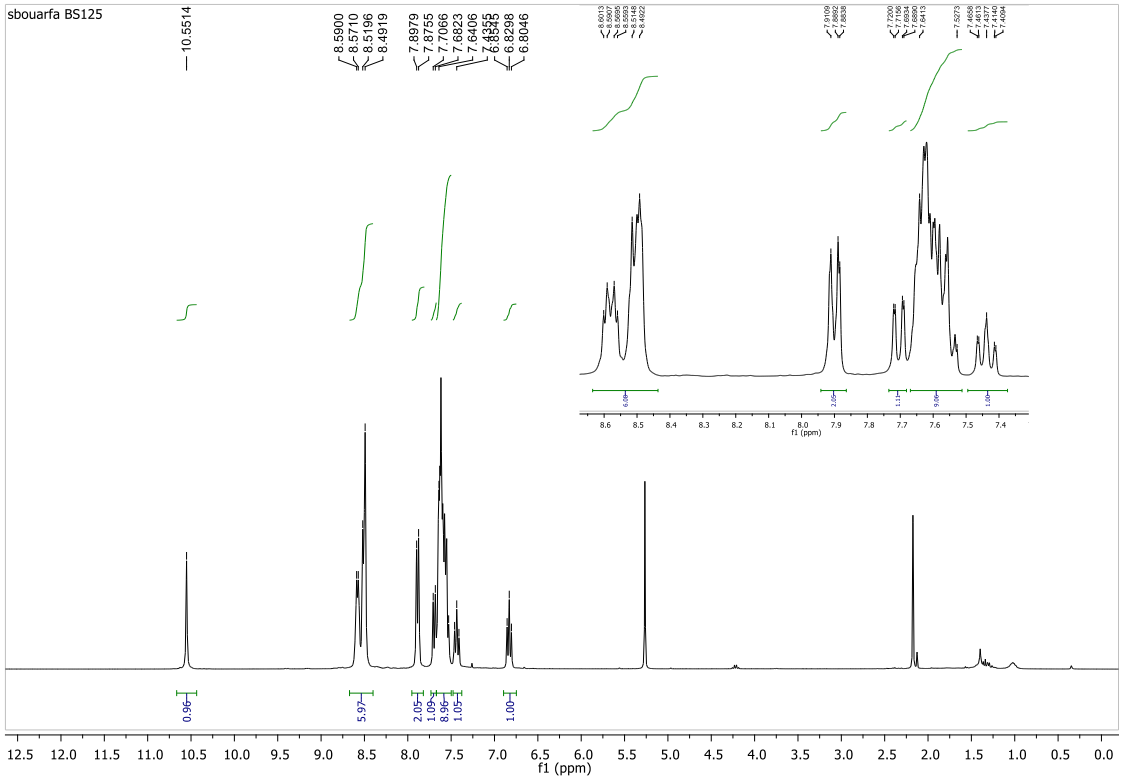
NOESY (500 MHz, $CDCl_3$)



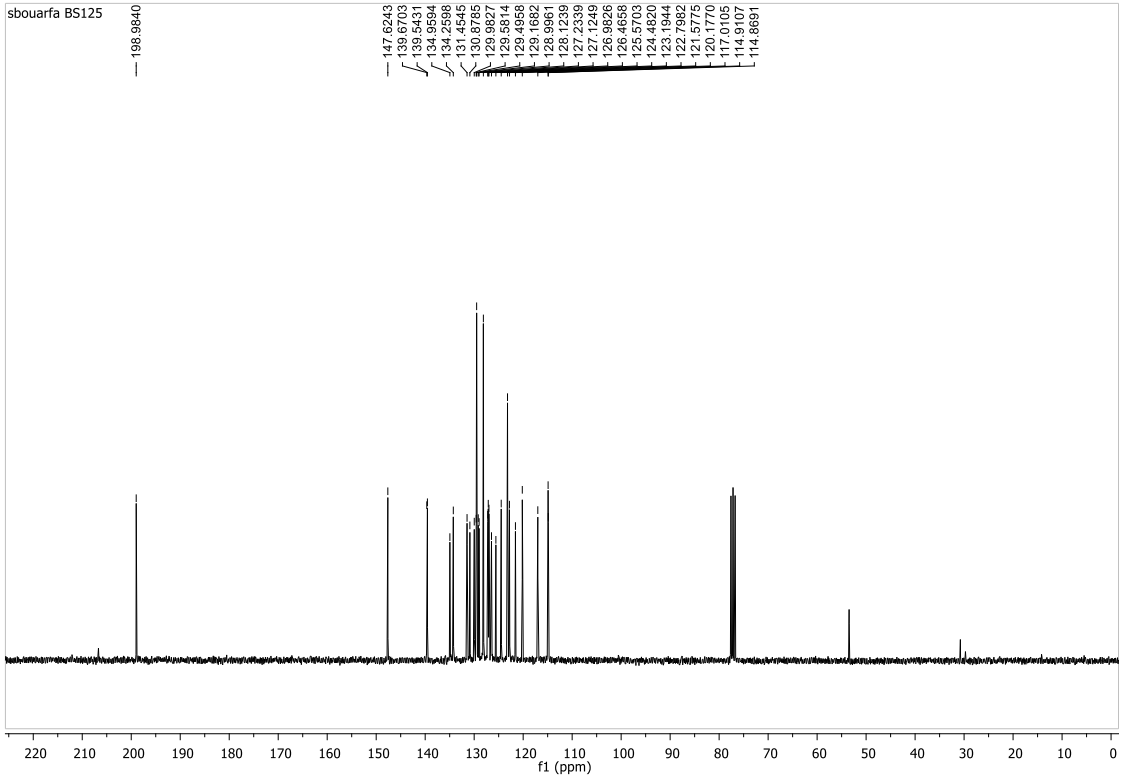
Phenyl 2-(2-triphenylenyl)aminophenyl ketone (3a)



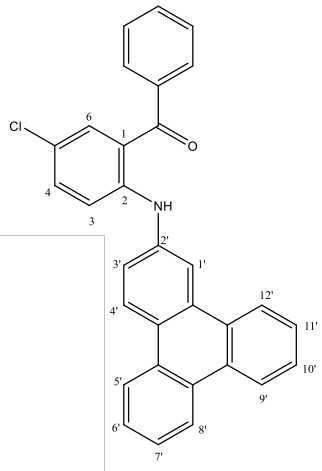
^{1}H NMR (300 MHz, $CDCl_3$)



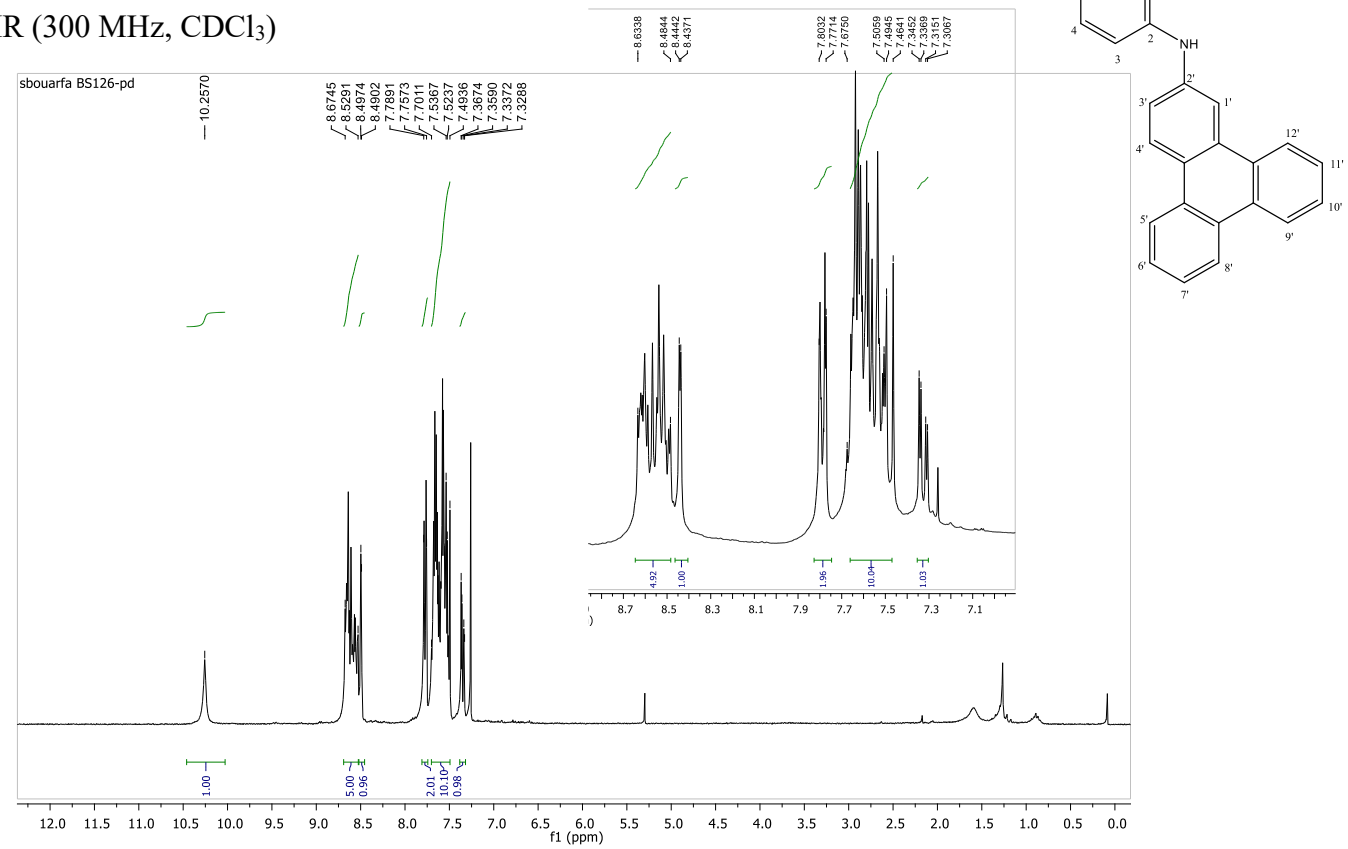
^{13}C NMR (75 MHz, $CDCl_3$)



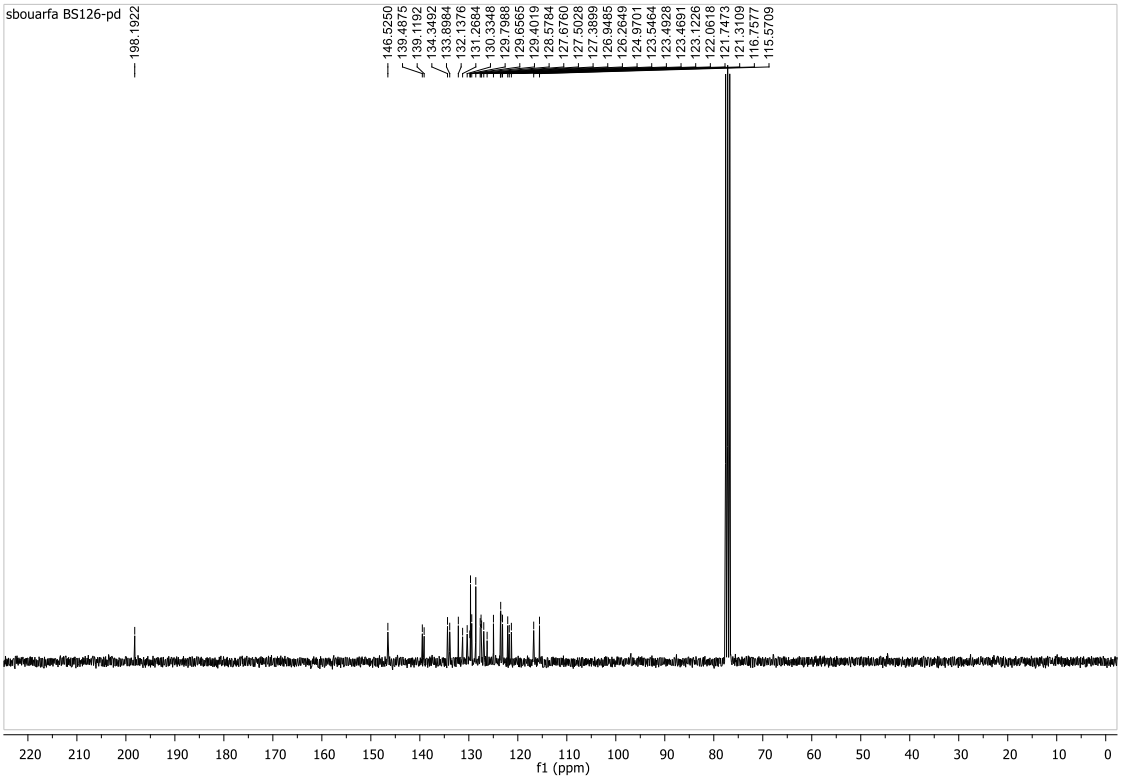
5-Chloro-2-(2-triphenylenyl)aminophenyl phenyl ketone (3b)



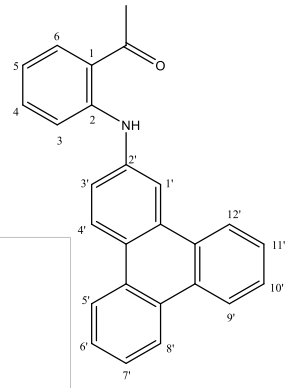
^{1}H NMR (300 MHz, $CDCl_3$)



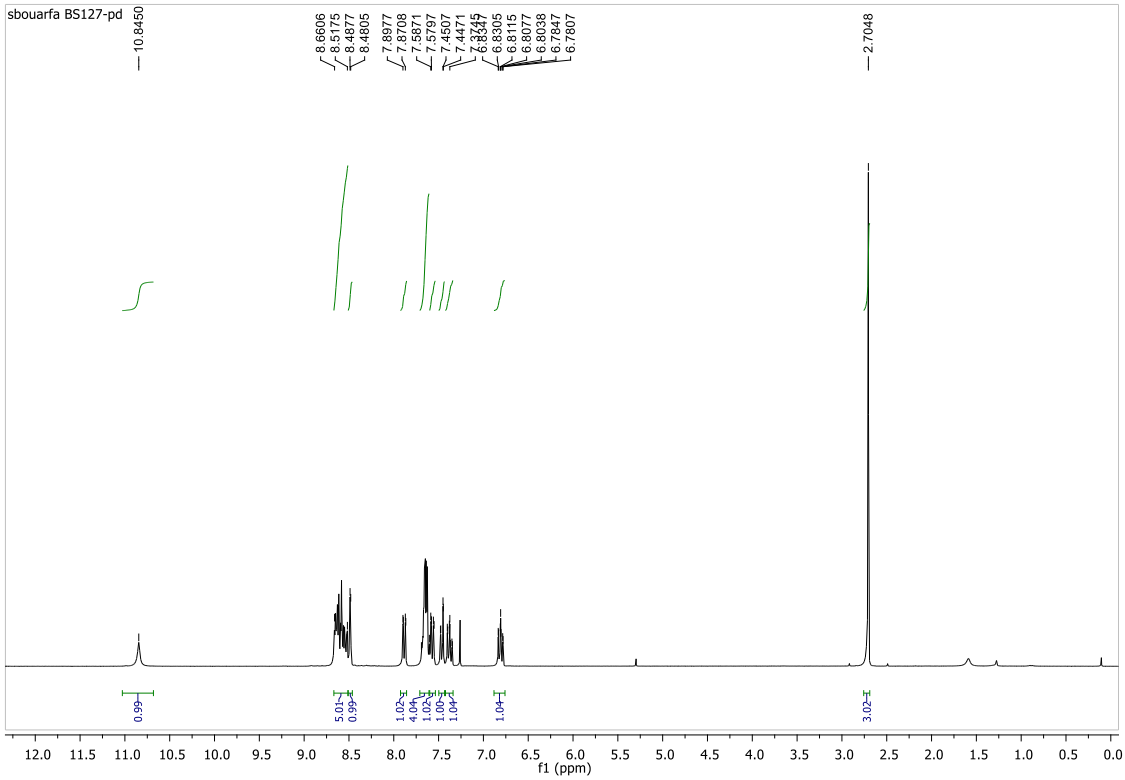
^{13}C NMR (75 MHz, $CDCl_3$)



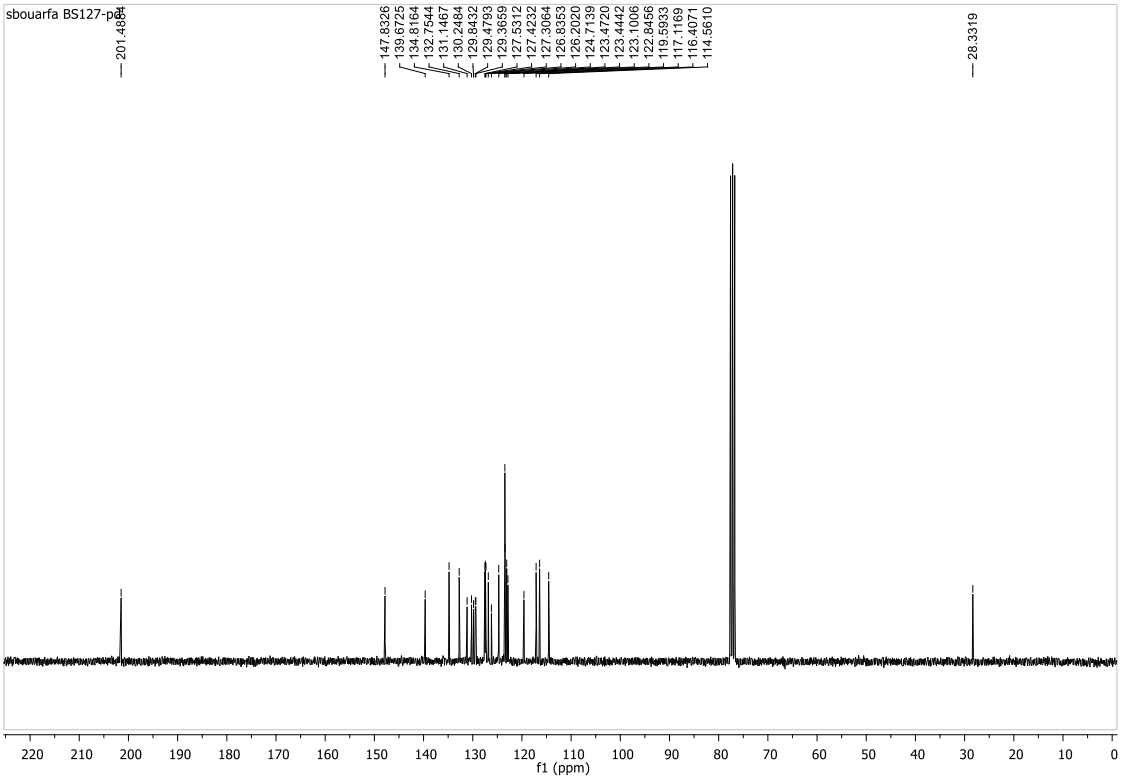
2-(2-Triphenylenyl)aminoacetophenone (3c)



^{1}H NMR (300 MHz, $CDCl_3$)

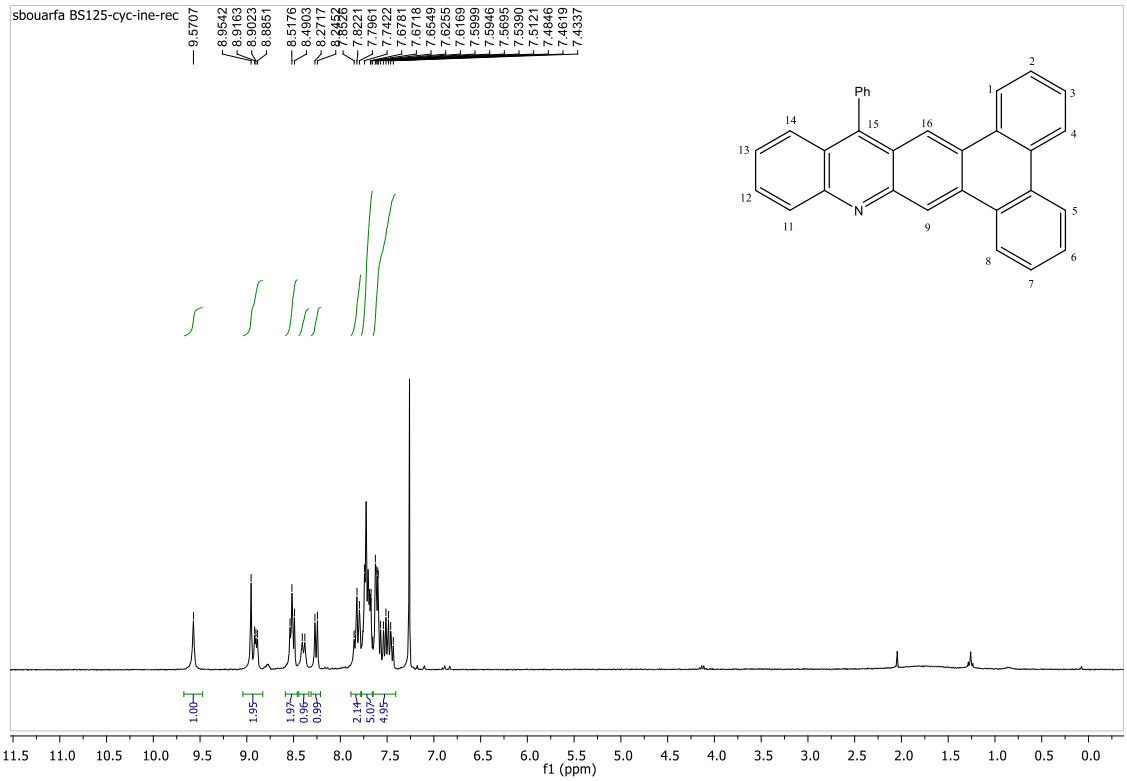


^{13}C NMR (75 MHz, $CDCl_3$)

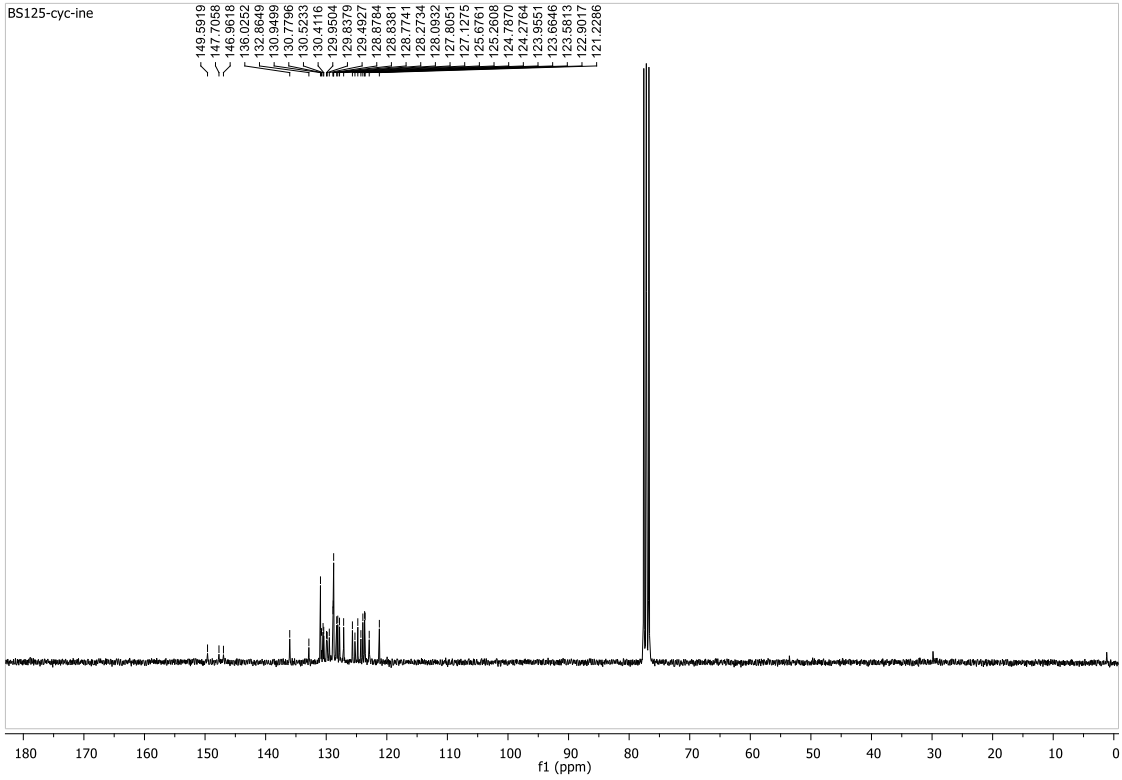


15-Phenylphenanthro[9,10-*b*]acridine (4a)

^{1}H NMR (300 MHz, $CDCl_3$)

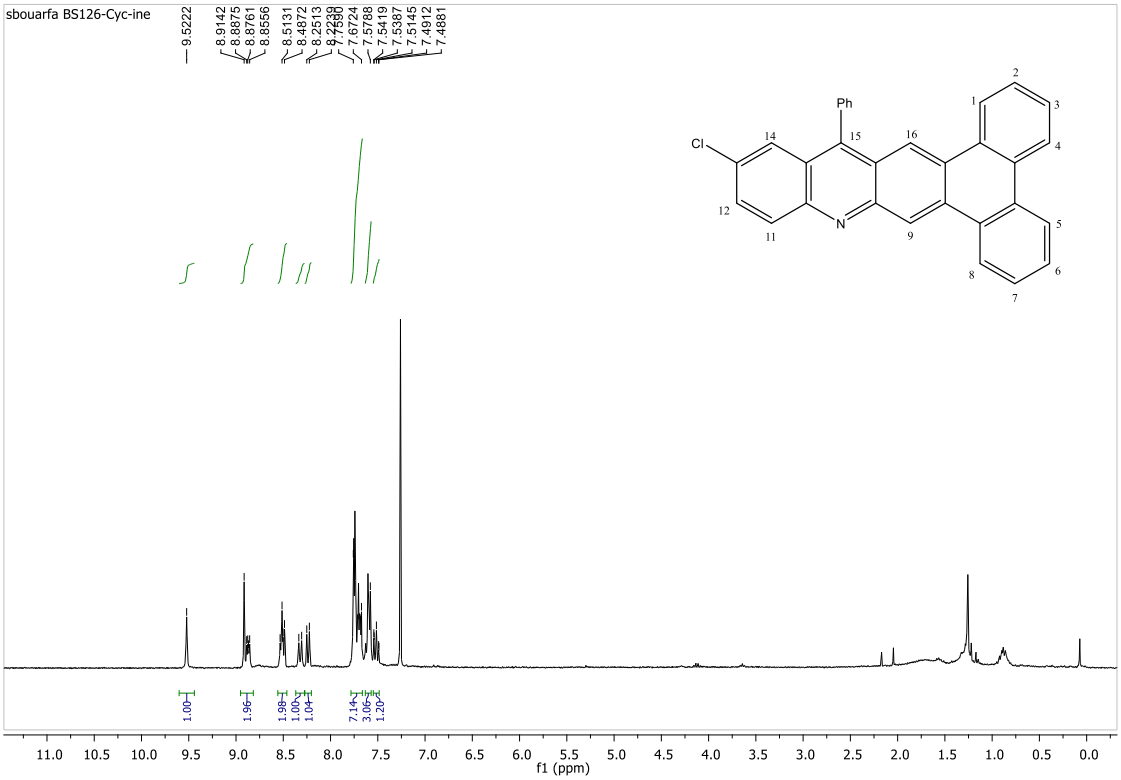


^{13}C NMR (75 MHz, $CDCl_3$)

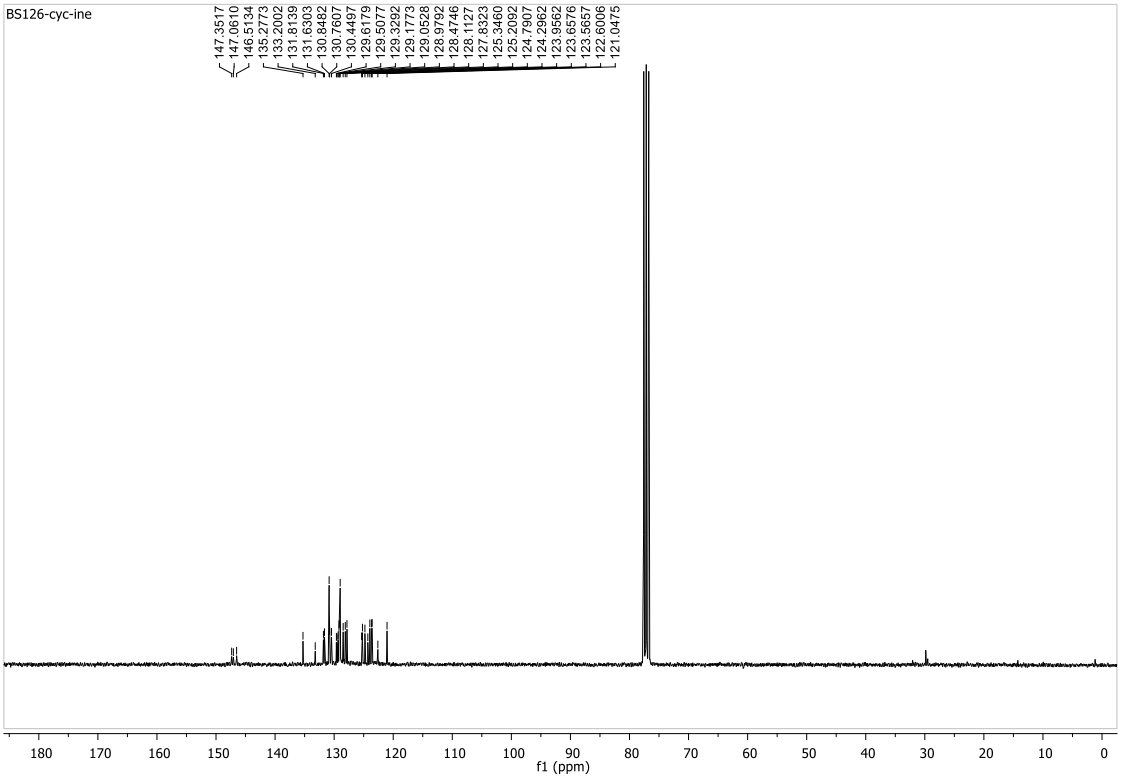


13-Chloro-15-phenylphenanthro[9,10-*b*]acridine (4b)

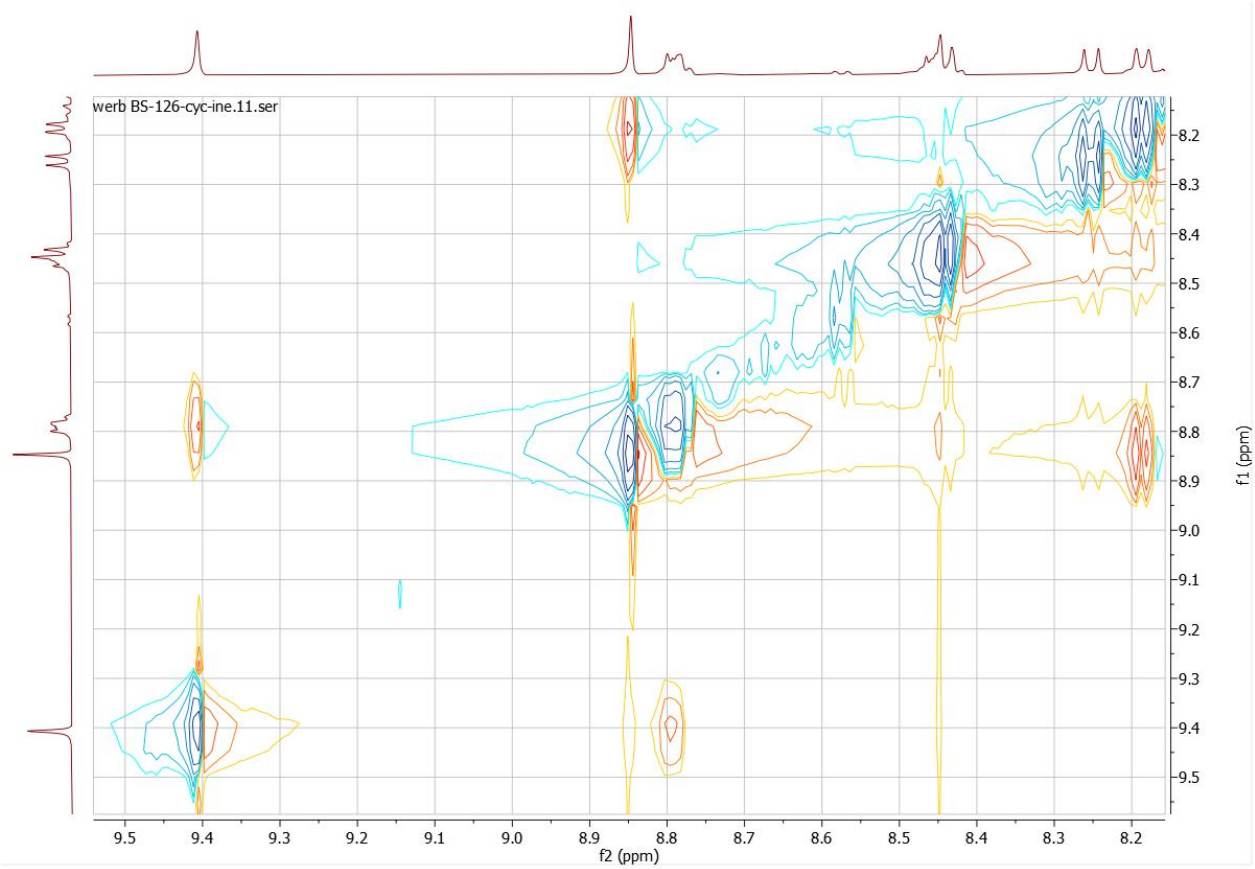
^{1}H NMR (500 MHz, $CDCl_3$)



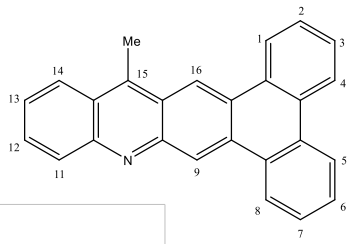
^{13}C NMR (75 MHz, $CDCl_3$)



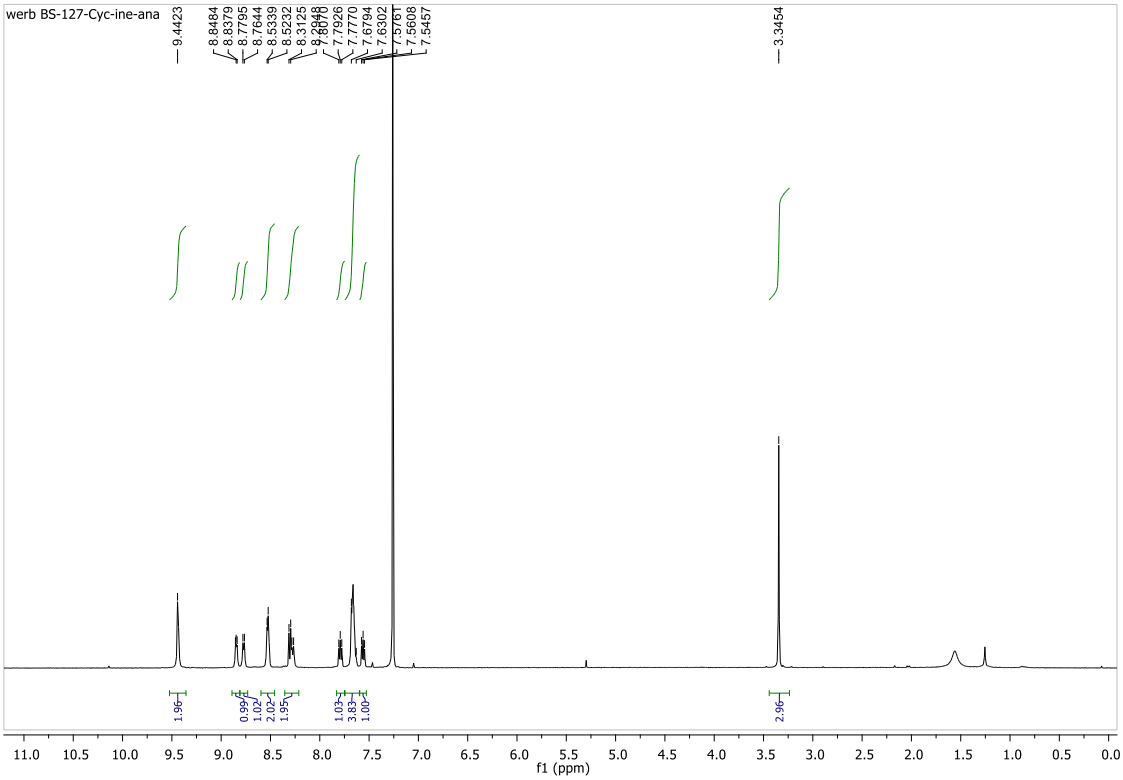
NOESY (500 MHz, $CDCl_3$)



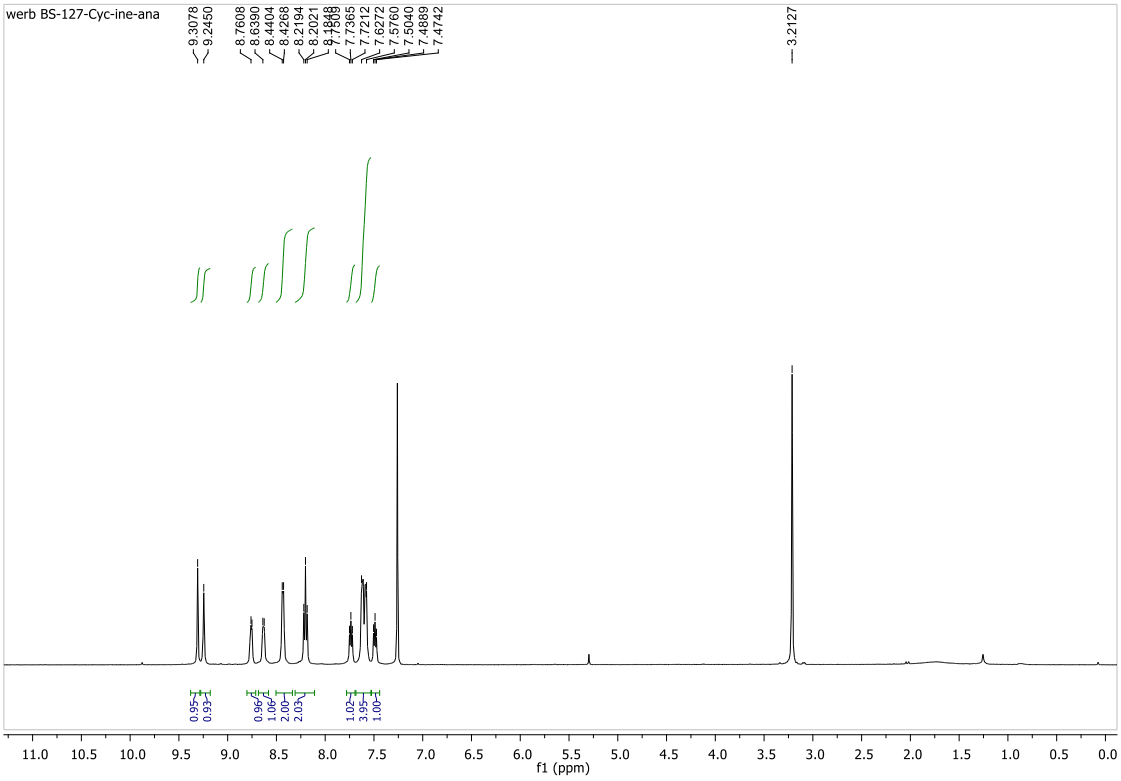
15-Methylphenanthro[9,10-*b*]acridine (4c)



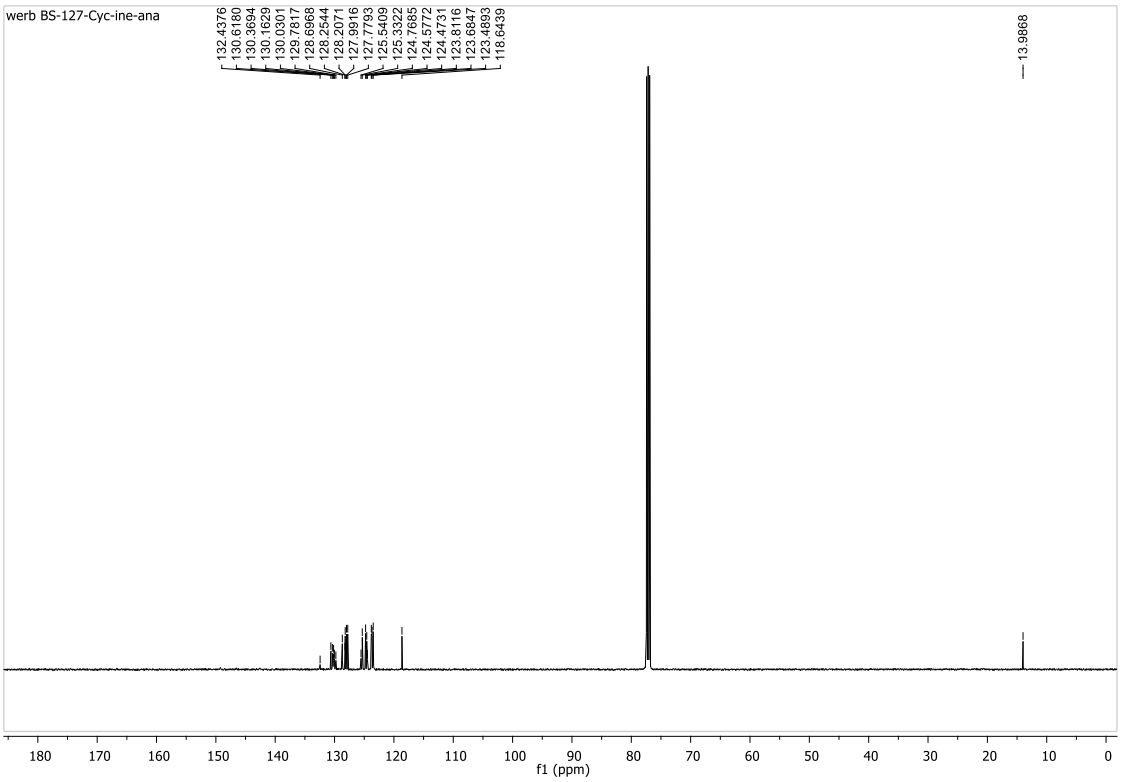
^{1}H NMR (500 MHz, $CDCl_3$) – lower concentration (about 1 mg in 0.5 mL)

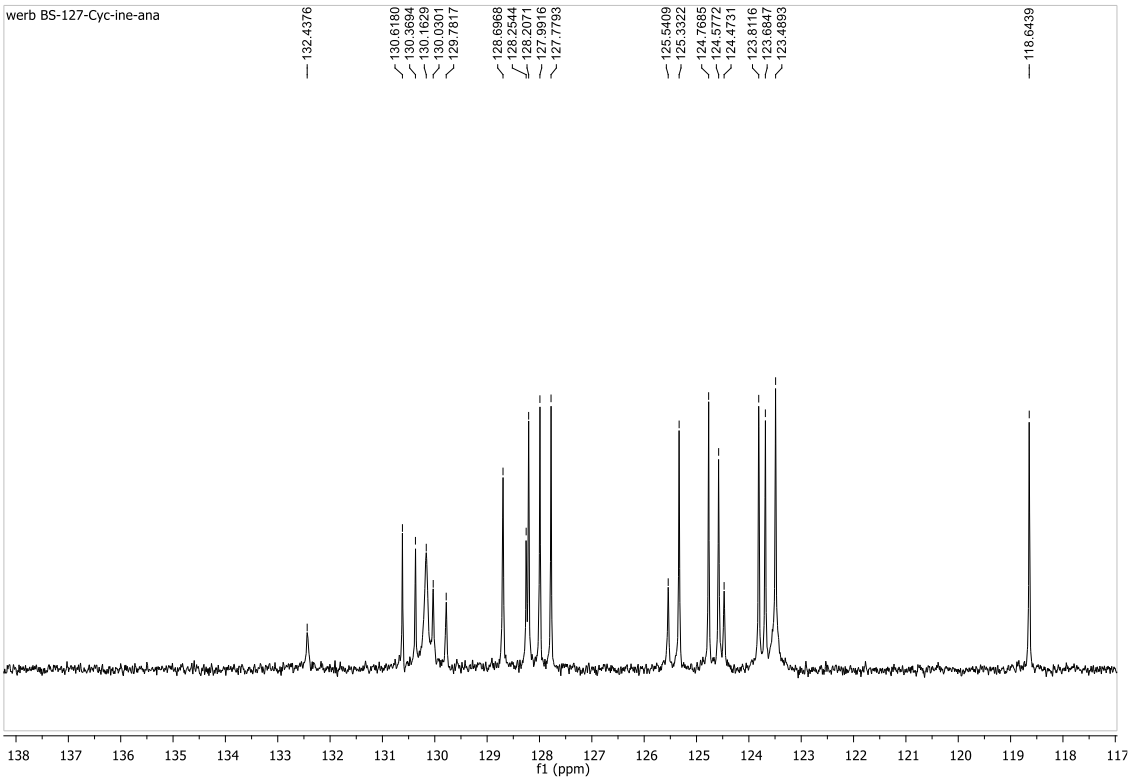


^{1}H NMR (500 MHz, $CDCl_3$) – higher concentration (about 2 mg in 0.5 mL)



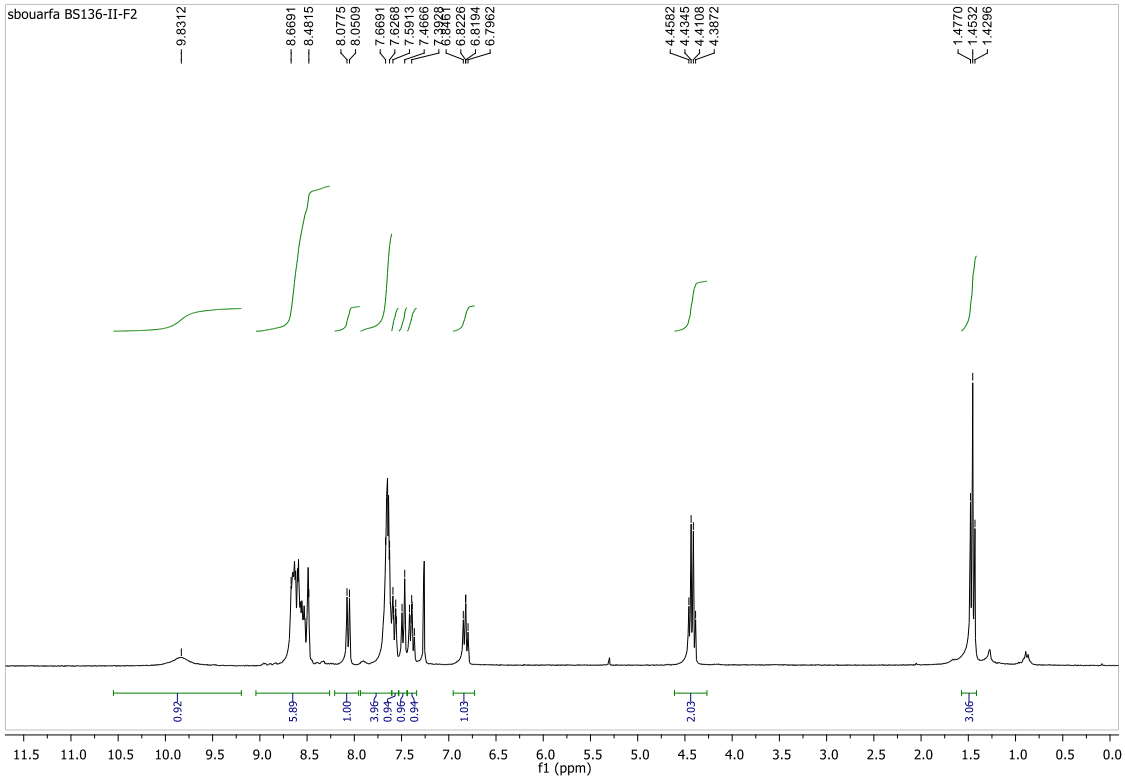
^{13}C NMR (126 MHz, $CDCl_3$)

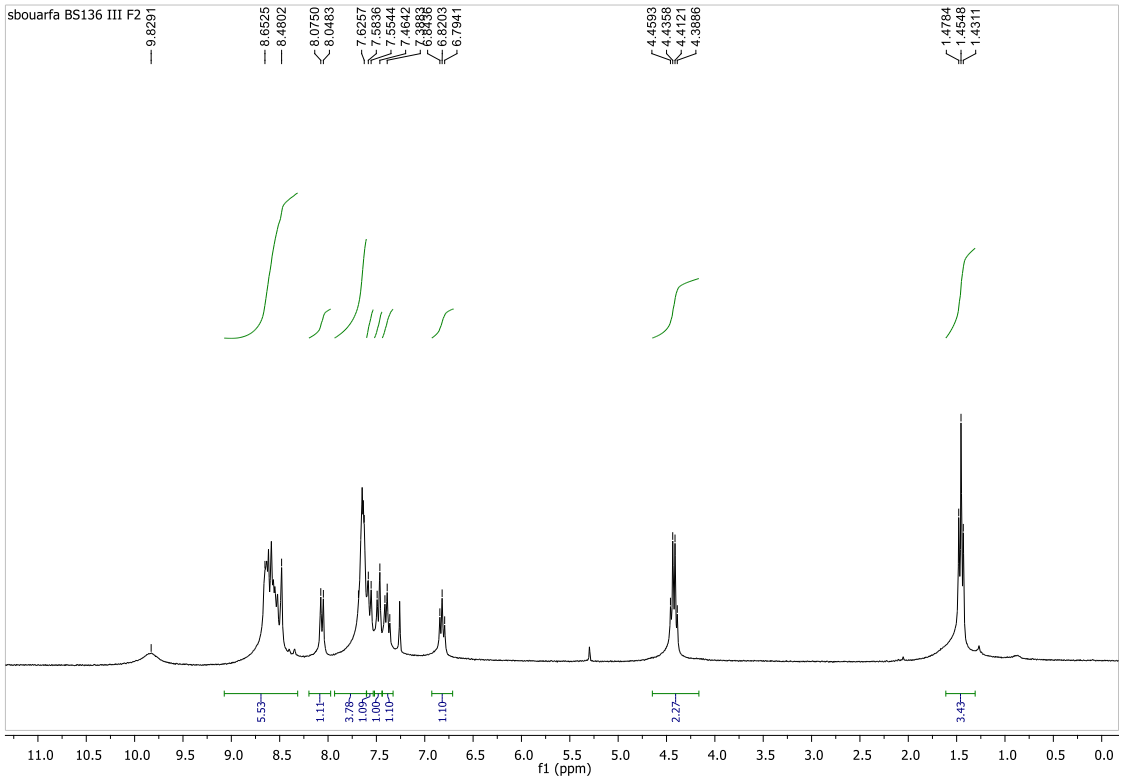




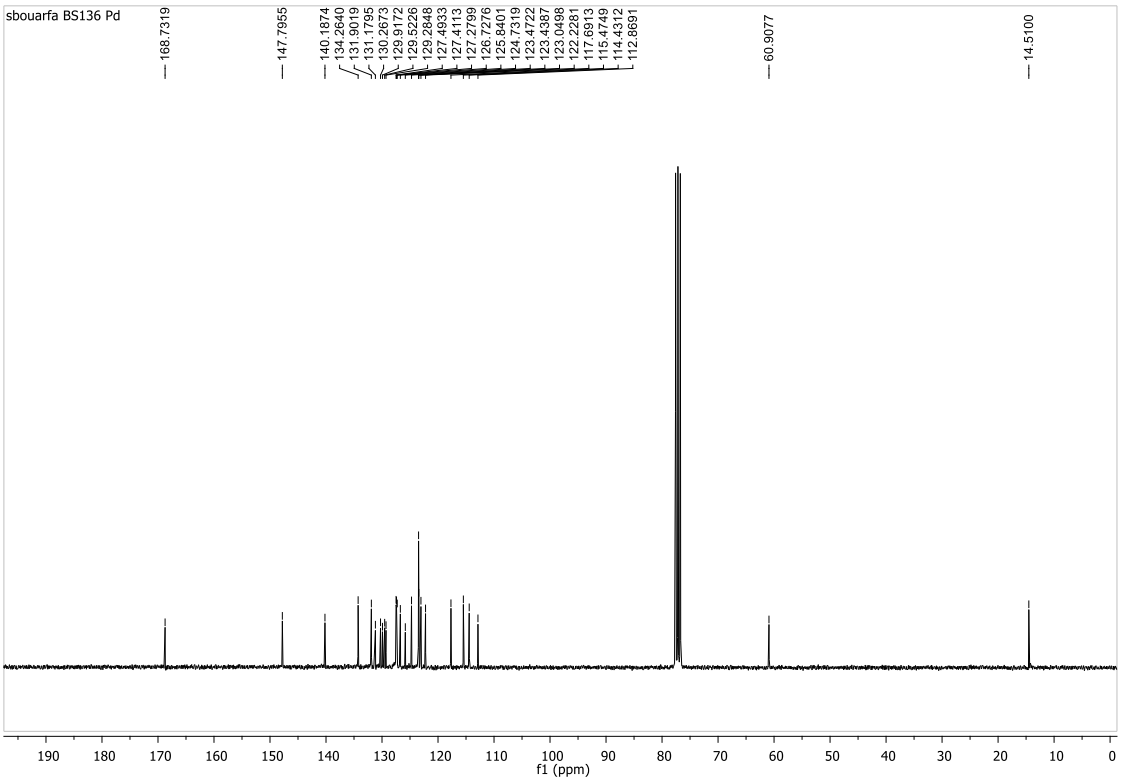
Ethyl 2-(2-triphenylenyl)aminobenzoate (5)

^{1}H NMR (300 MHz, $CDCl_3$)

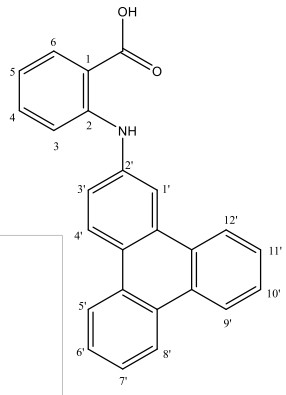




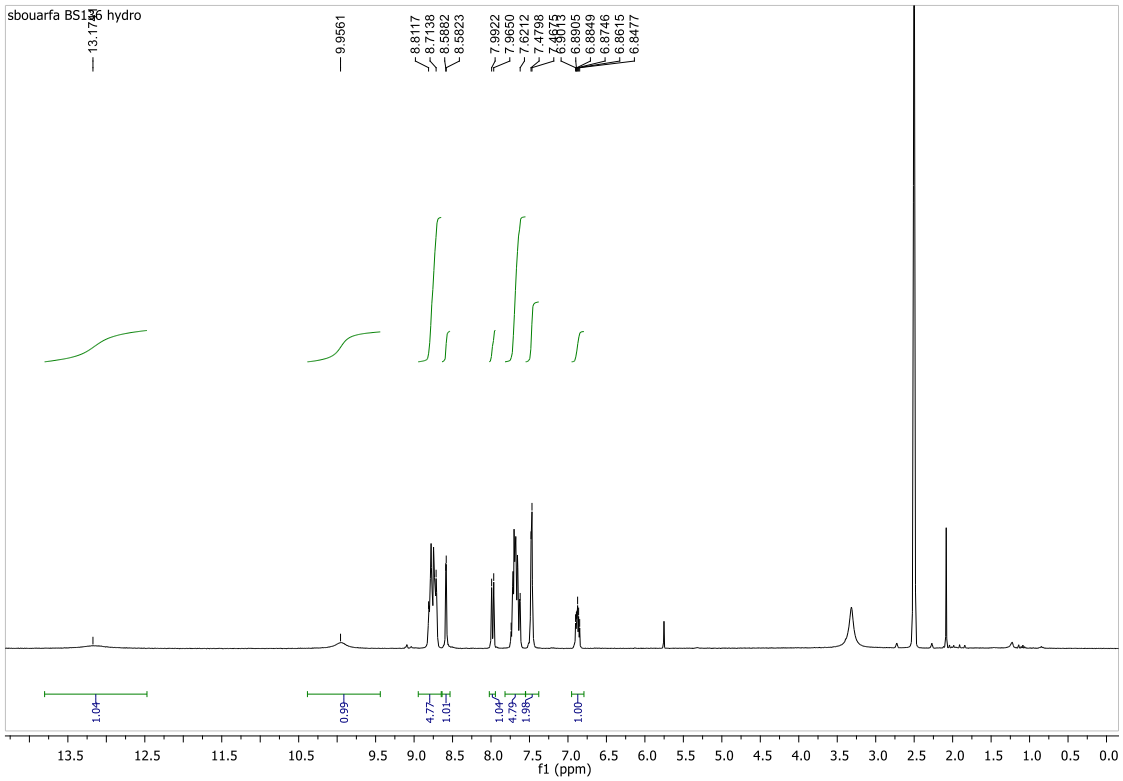
^{13}C NMR (75 MHz, $CDCl_3$)



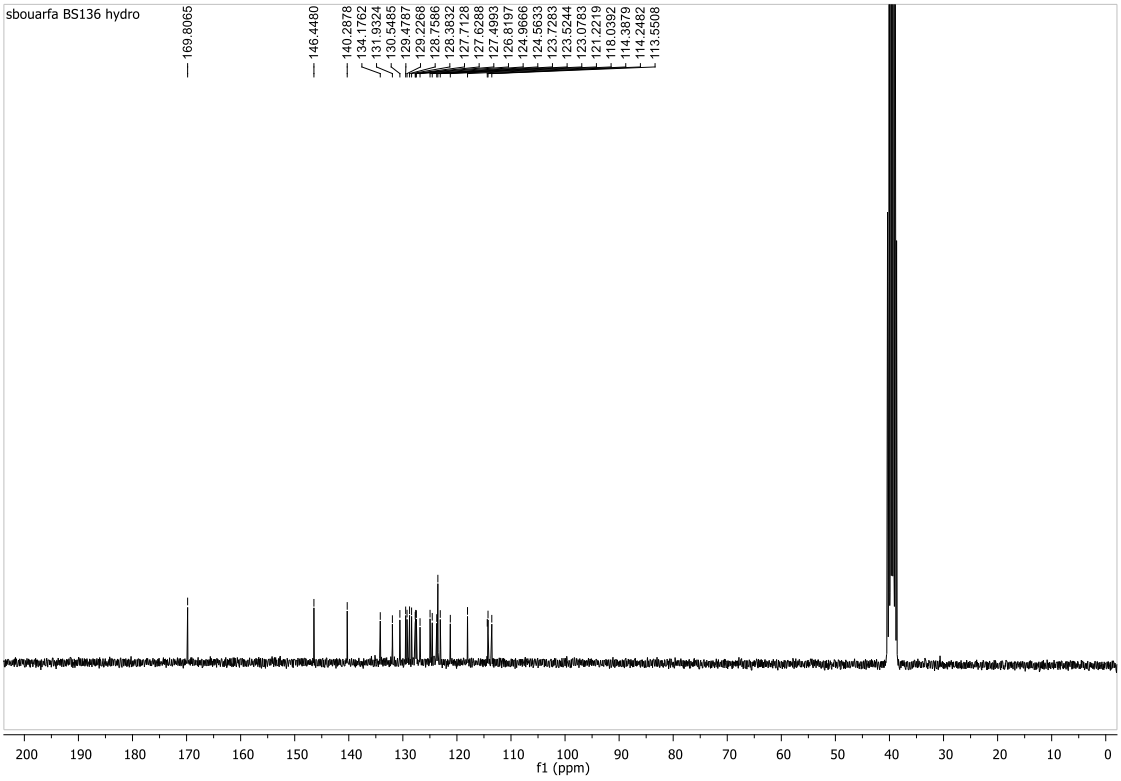
2-(2-Triphenylenyl)aminobenzoic acid (6)



^{1}H NMR (300 MHz, $(CD_3)_2SO$)

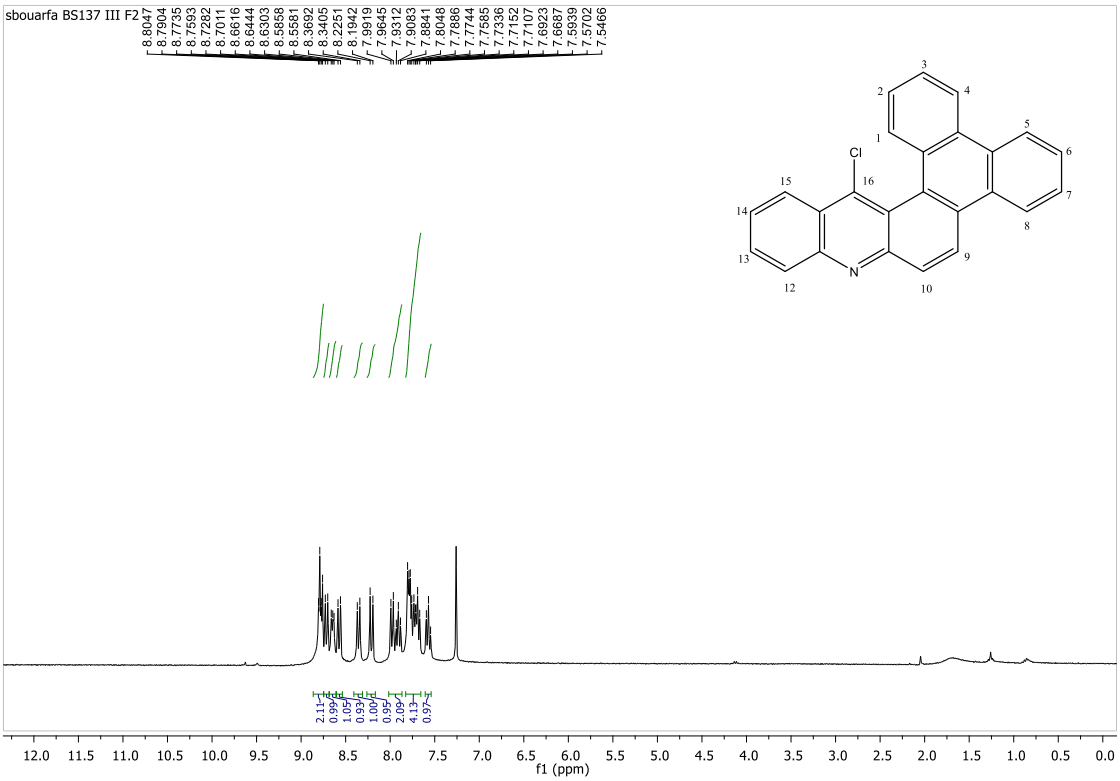


^{13}C NMR (75 MHz, $(CD_3)_2SO$)

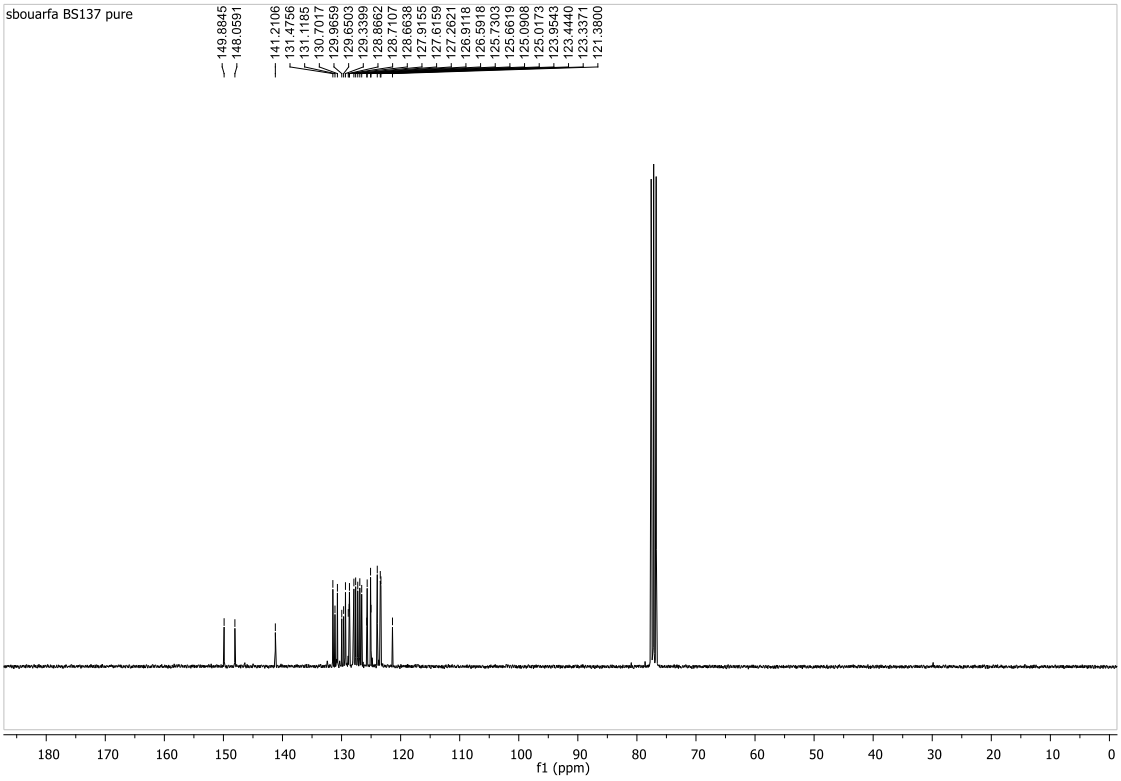


16-Chlorophenanthro[9,10-*a*]acridine (7)

^{1}H NMR (300 MHz, $CDCl_3$)

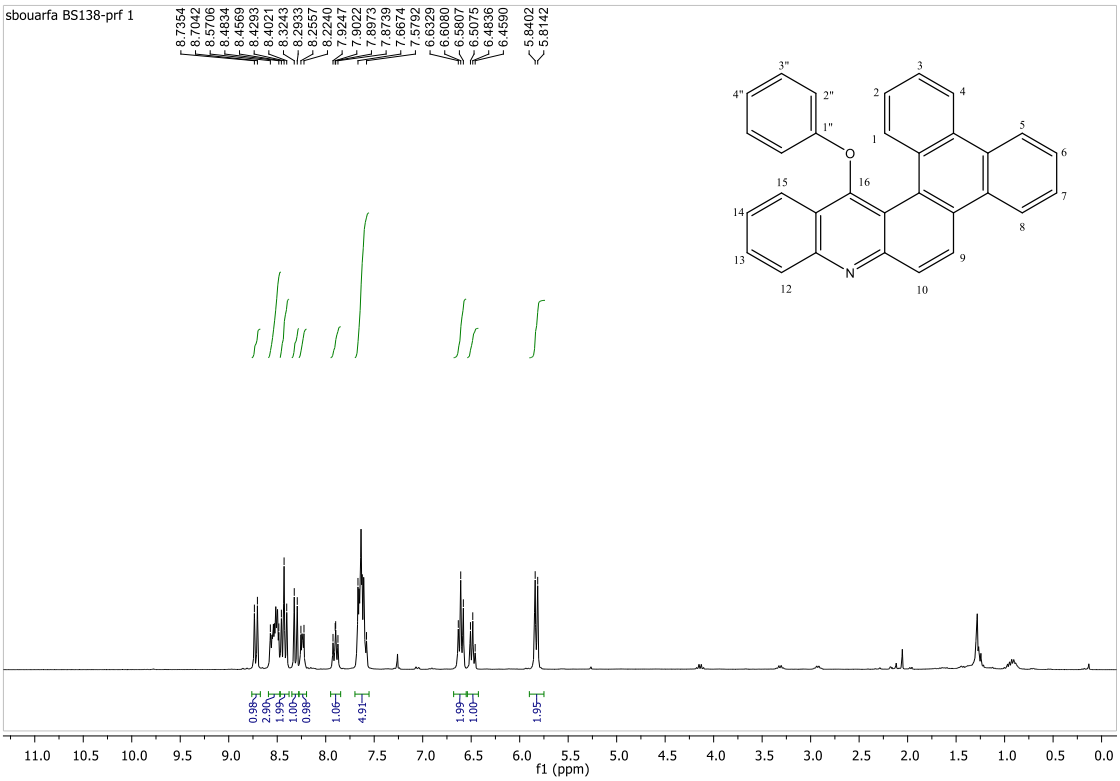


^{13}C NMR (75 MHz, $CDCl_3$)

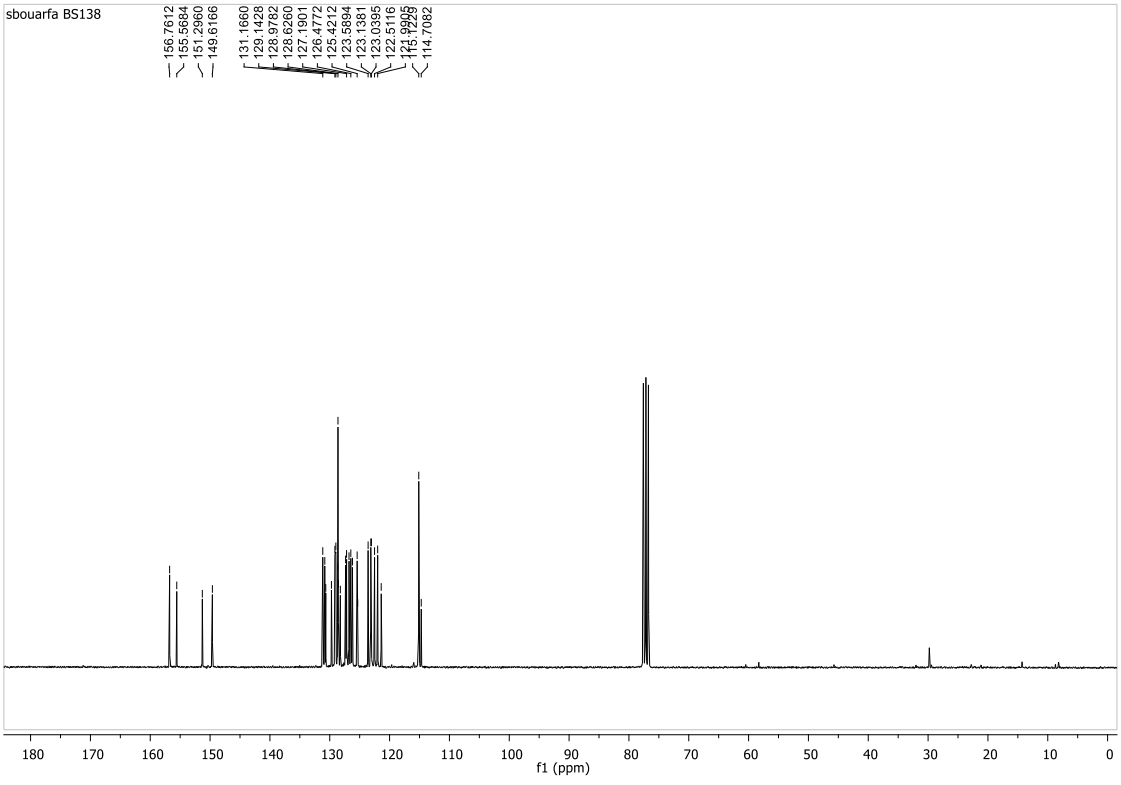


16-Phenoxyphenanthro[9,10-*a*]acridine (8)

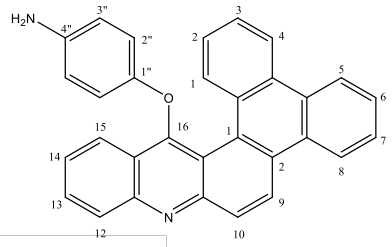
^{1}H NMR (300 MHz, $CDCl_3$)



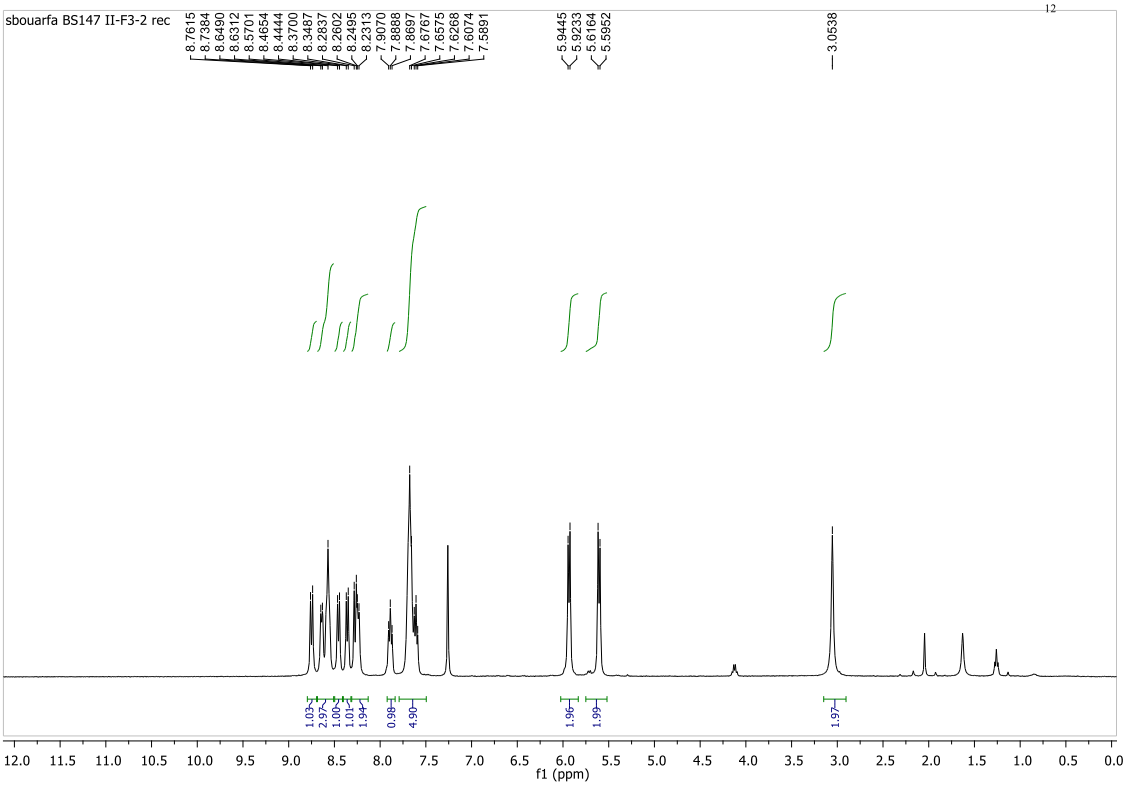
^{13}C NMR (75 MHz, $CDCl_3$)



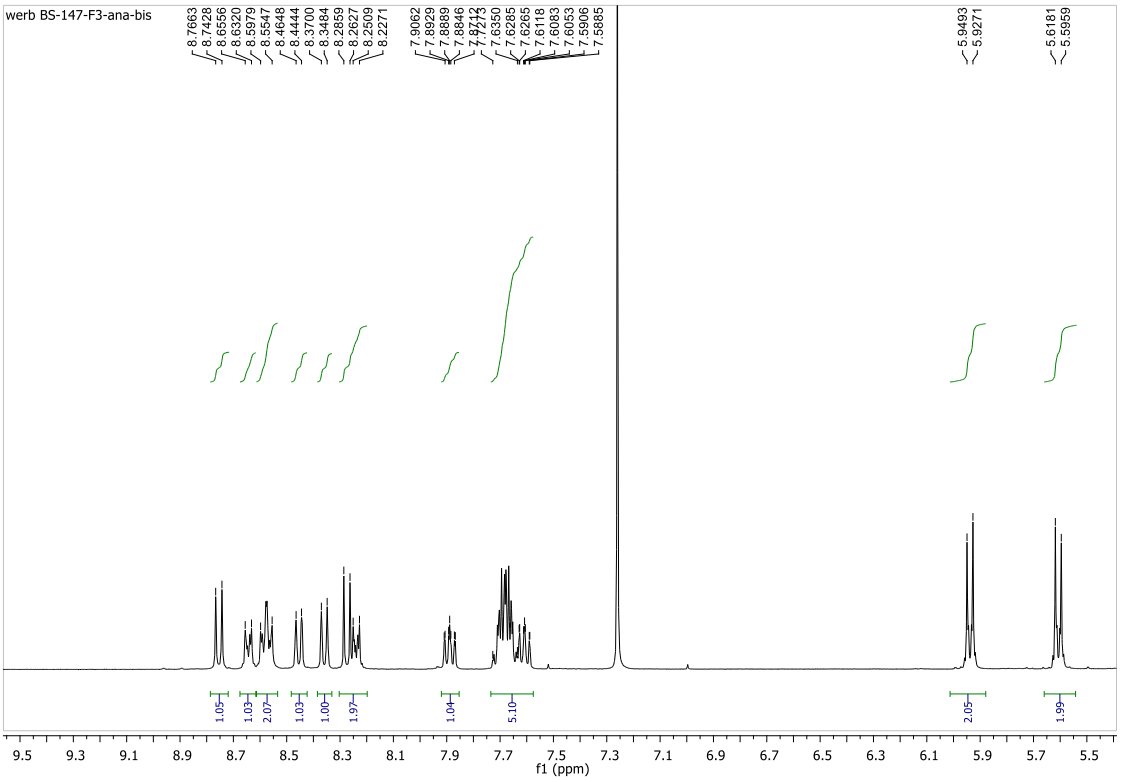
16-(4-Aminophenoxy)phenanthro[9,10-*a*]acridine (9)



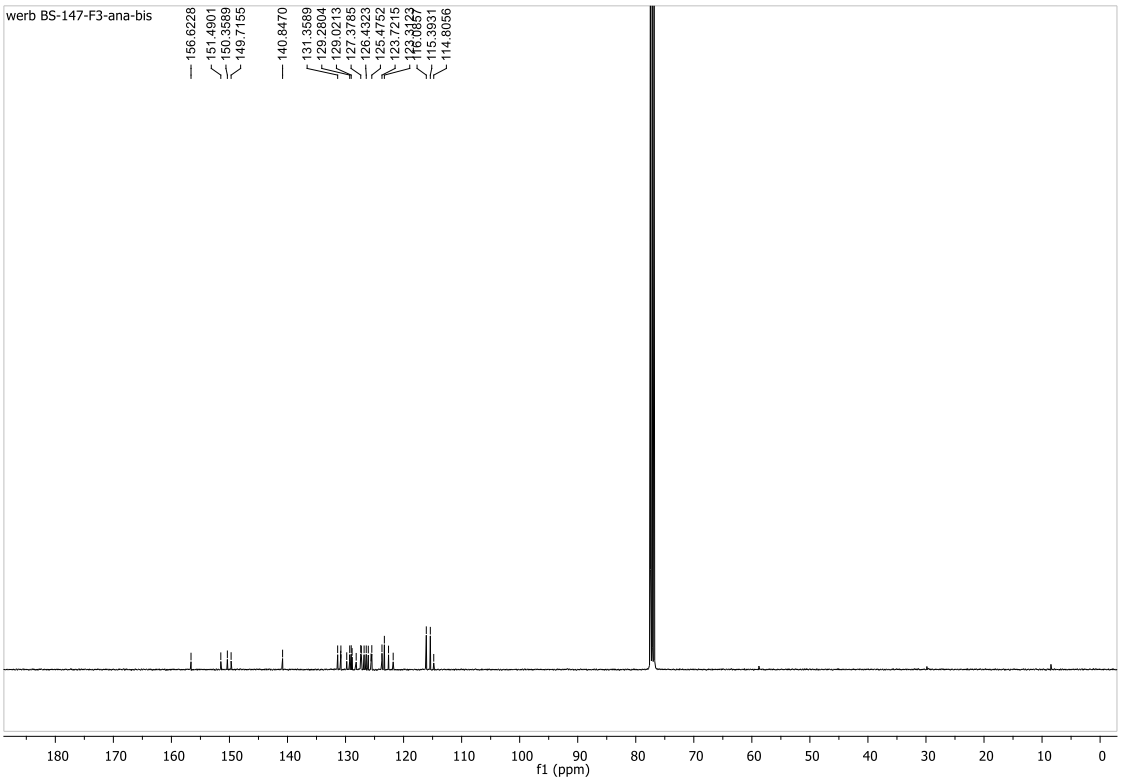
^{1}H NMR (400 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)

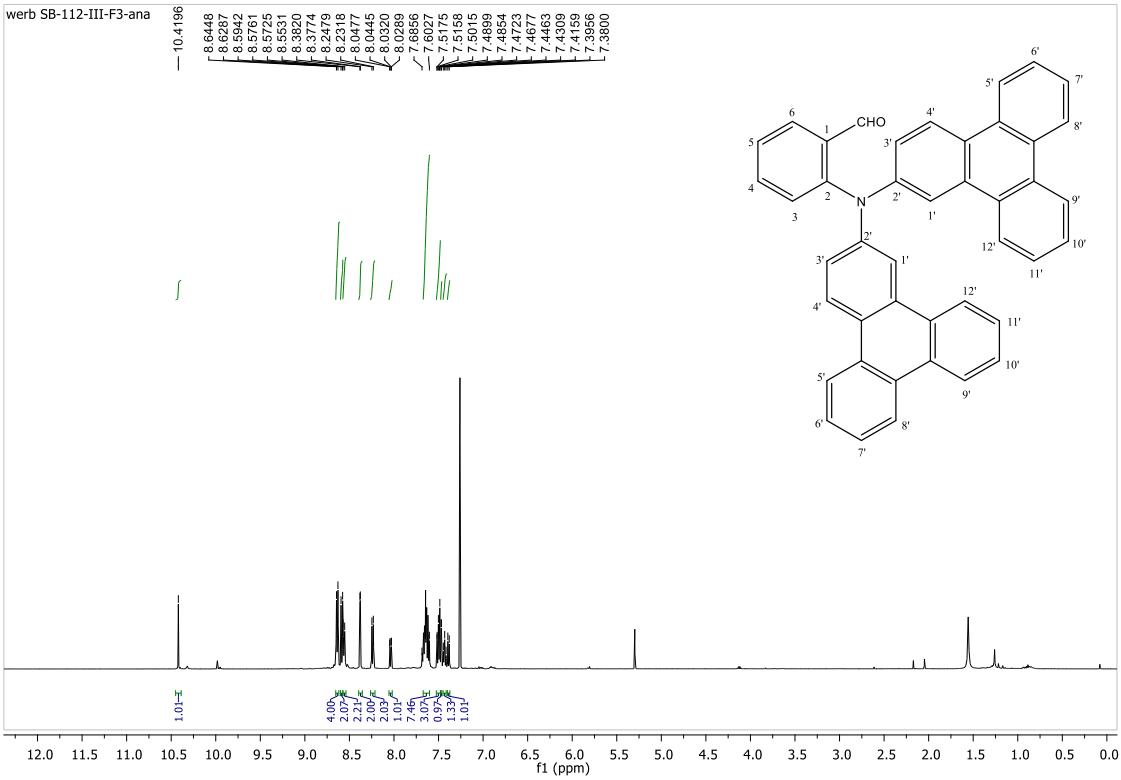


^{13}C NMR (101 MHz, $CDCl_3$)

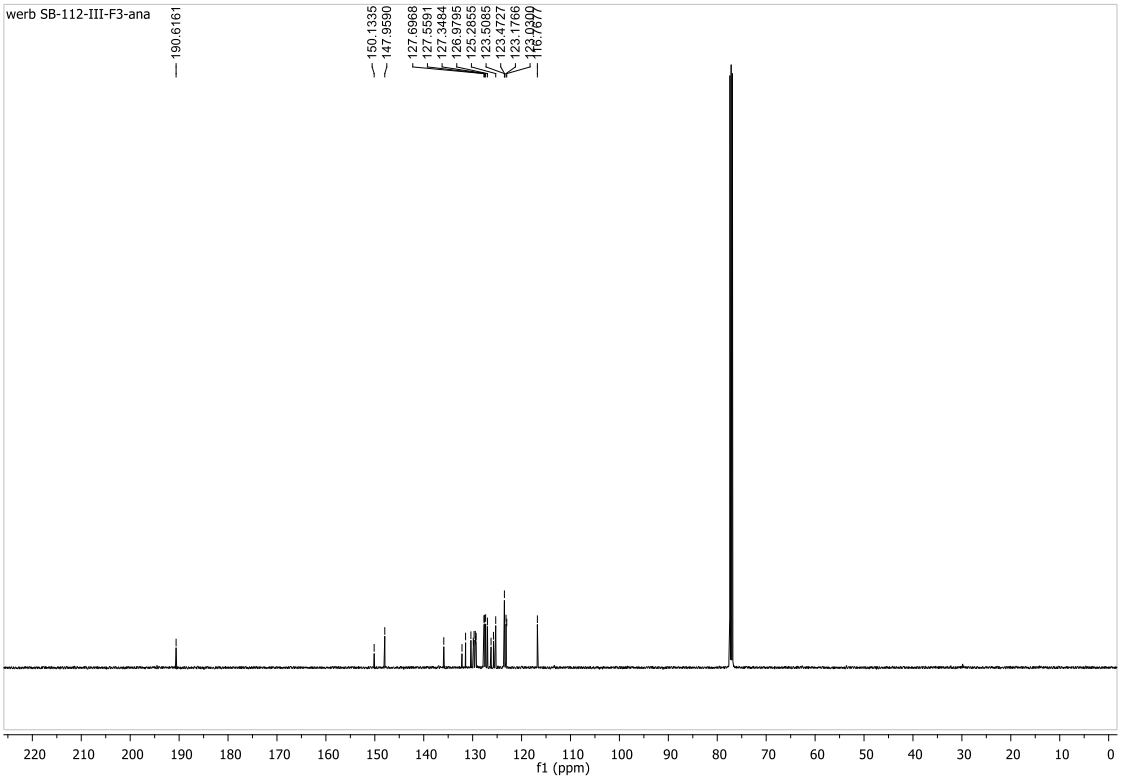


N,*N*-Bis(2-triphenylenyl)-2-aminobenzaldehyde (10)

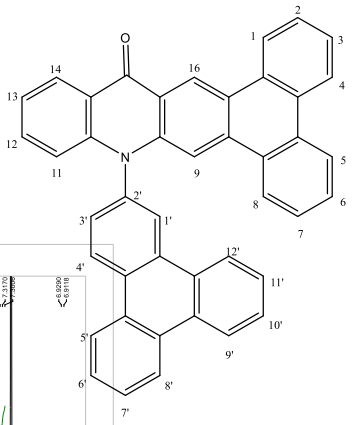
^{1}H NMR (500 MHz, $CDCl_3$)



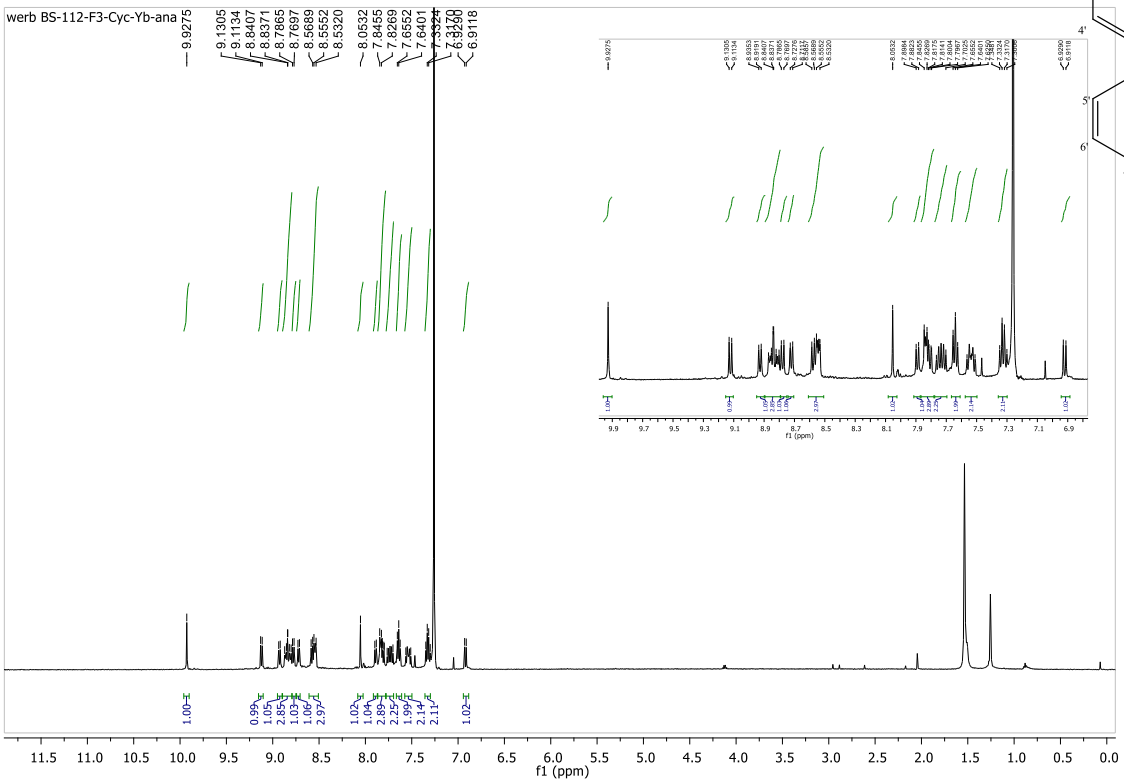
^{13}C NMR (125 MHz, $CDCl_3$)



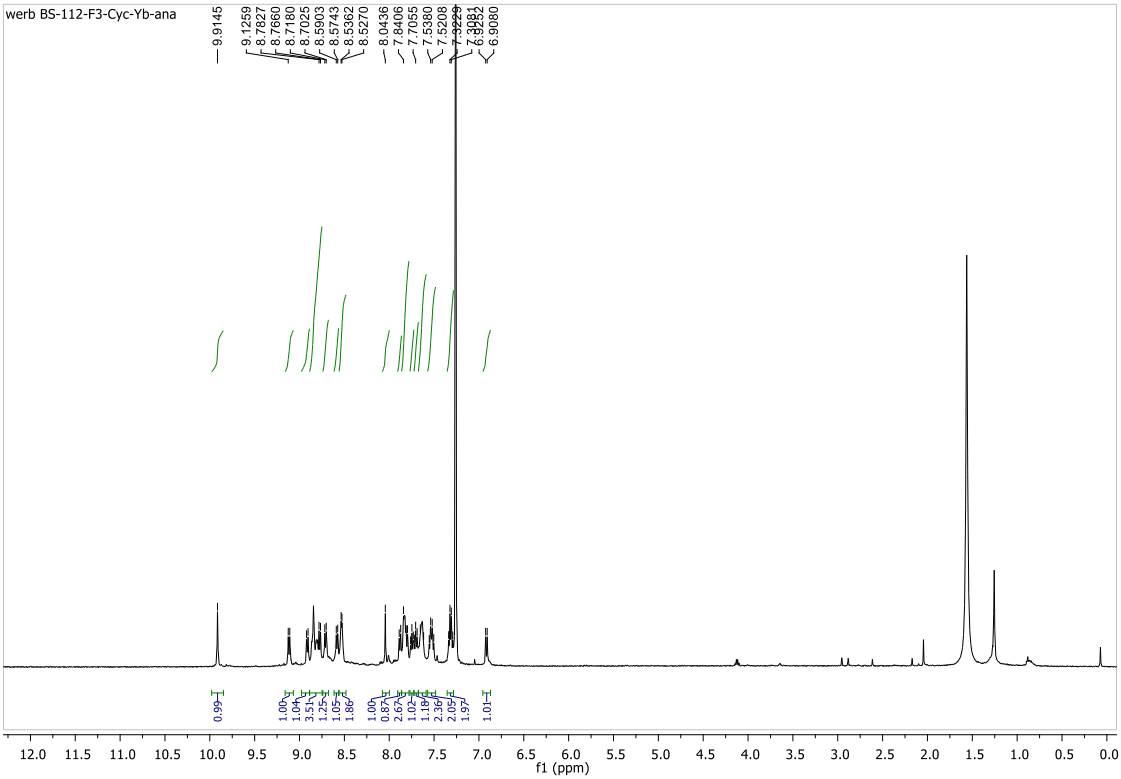
N-(2-Triphenylenyl)phenanthro[9,10-*b*]-15-acridone (11)



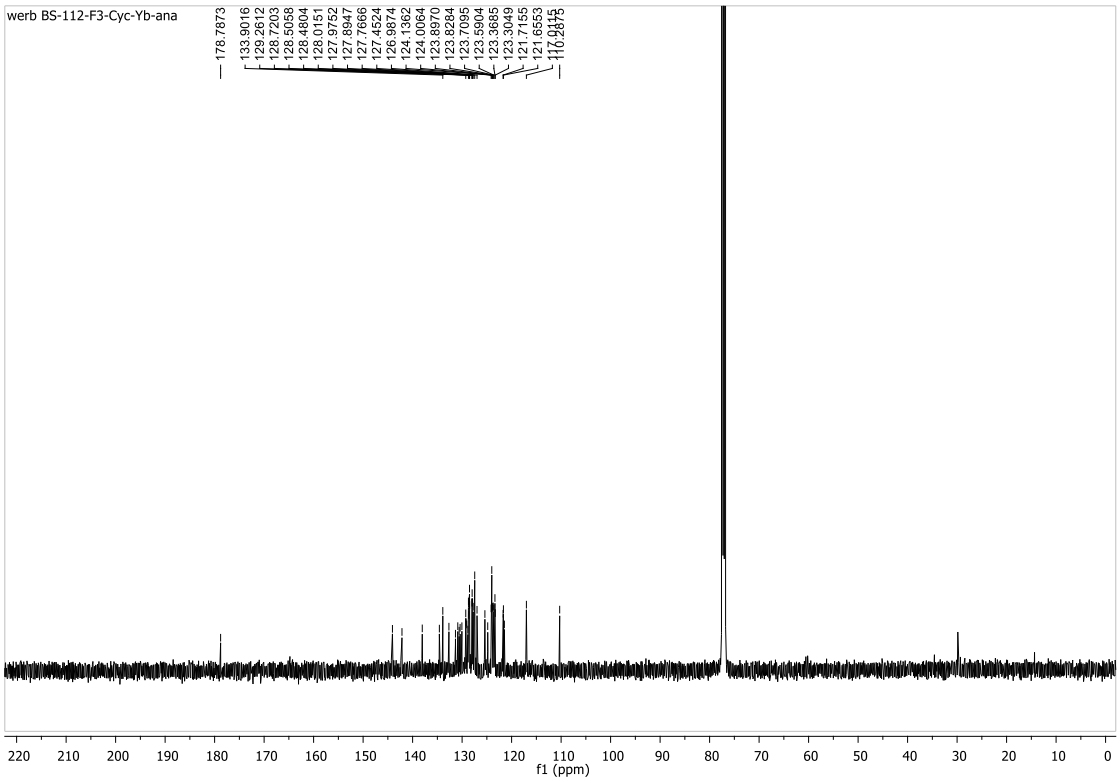
^{1}H NMR (500 MHz, $CDCl_3$) – lower concentration (about 0.5 mg in 0.5 mL)



^{1}H NMR (500 MHz, $CDCl_3$) – lower concentration (about 0.5 mg in 0.5 mL)

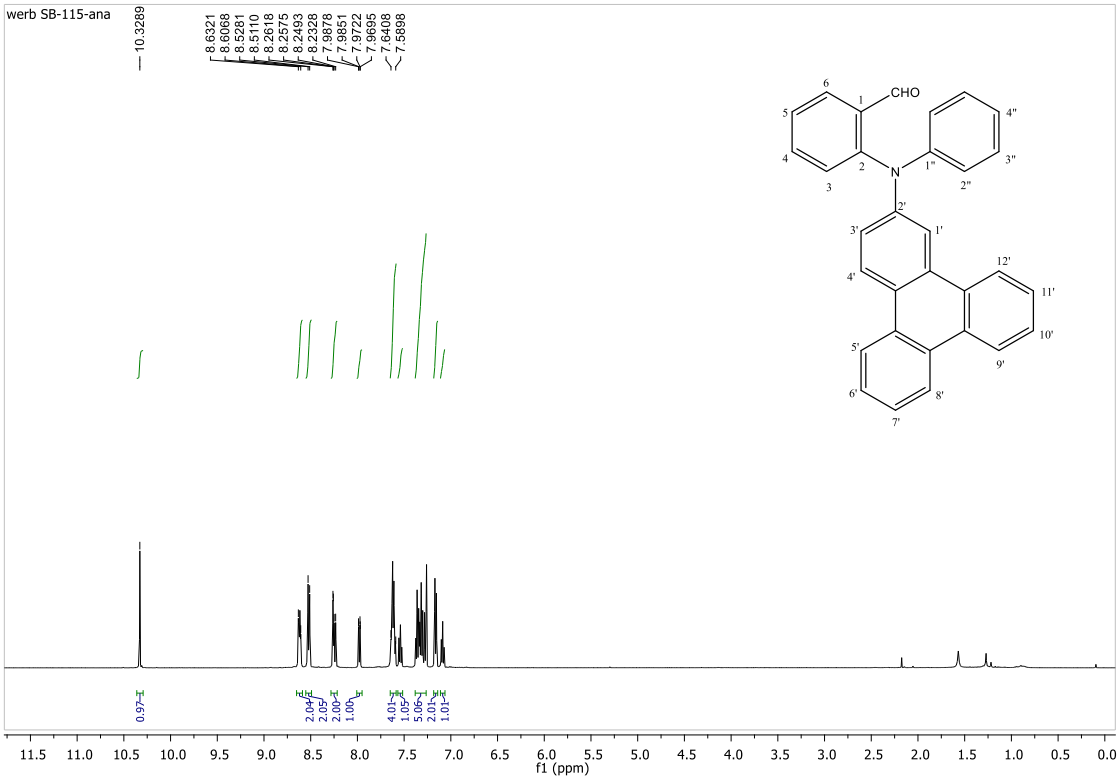


^{13}C NMR (126 MHz, $CDCl_3$)

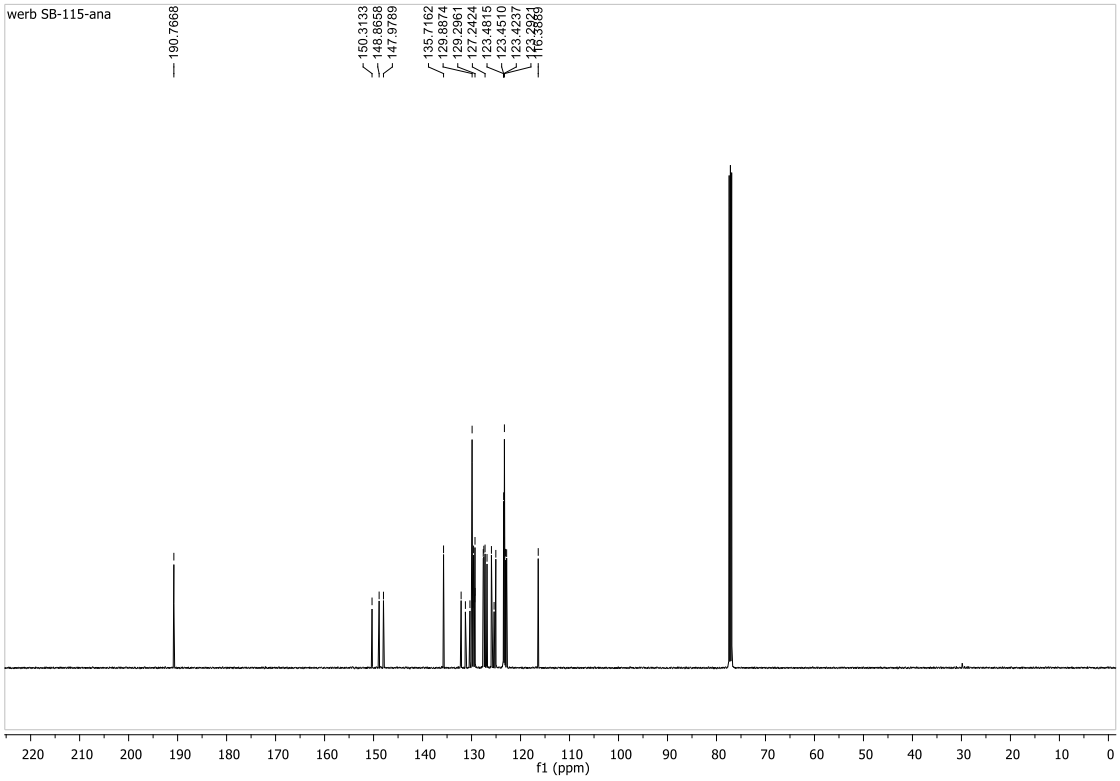


N-Phenyl-*N*-(2-triphenylenyl)-2-aminobenzaldehyde (12)

^{1}H NMR (500 MHz, $CDCl_3$)

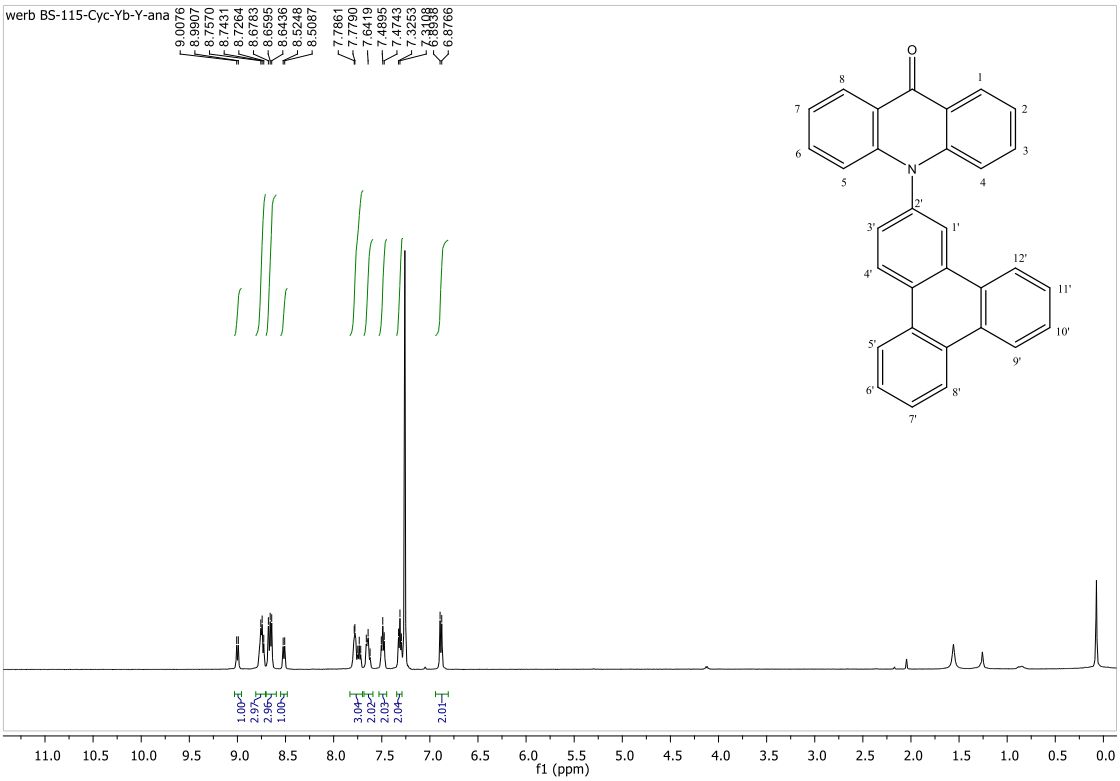


^{13}C NMR (126 MHz, $CDCl_3$)

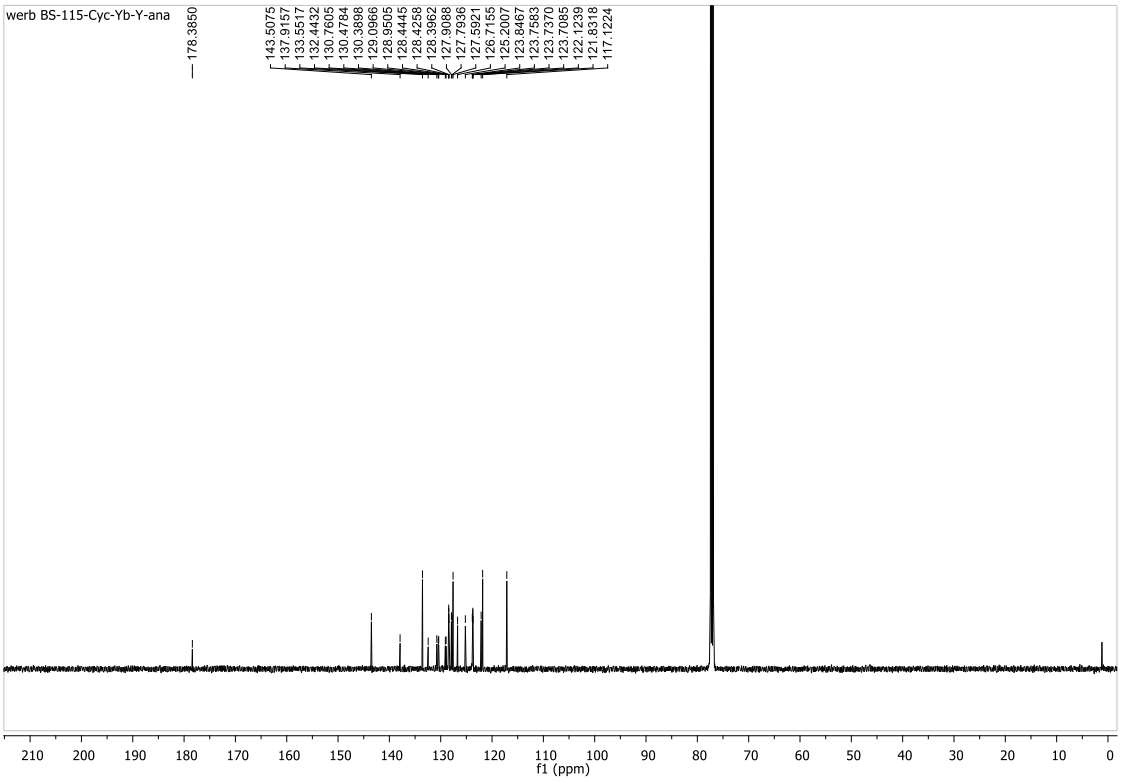


N-(2-Triphenylenyl)-9-acridone (13)

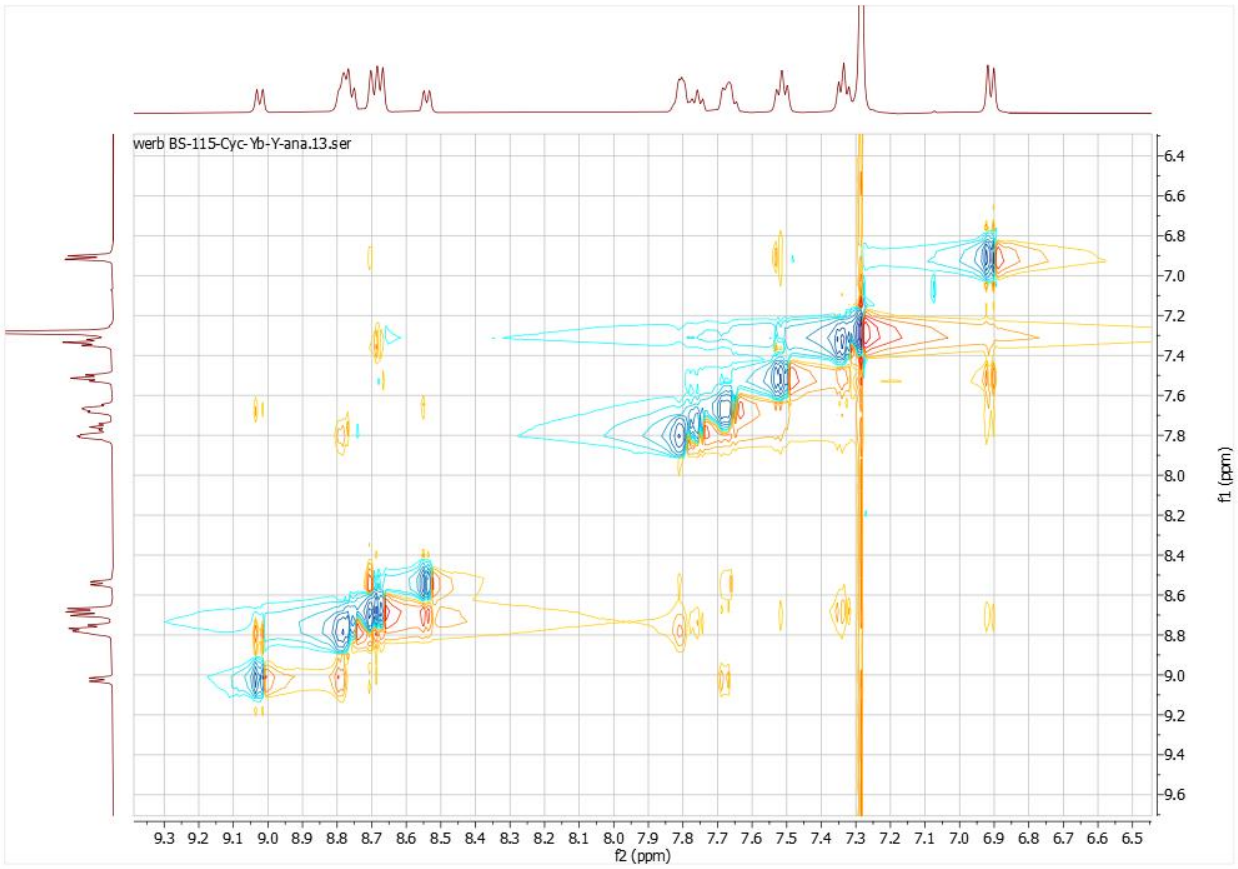
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)

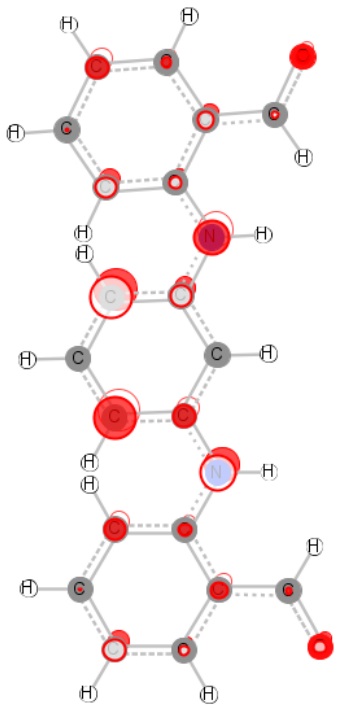


NOESY (500 MHz, $CDCl_3$)

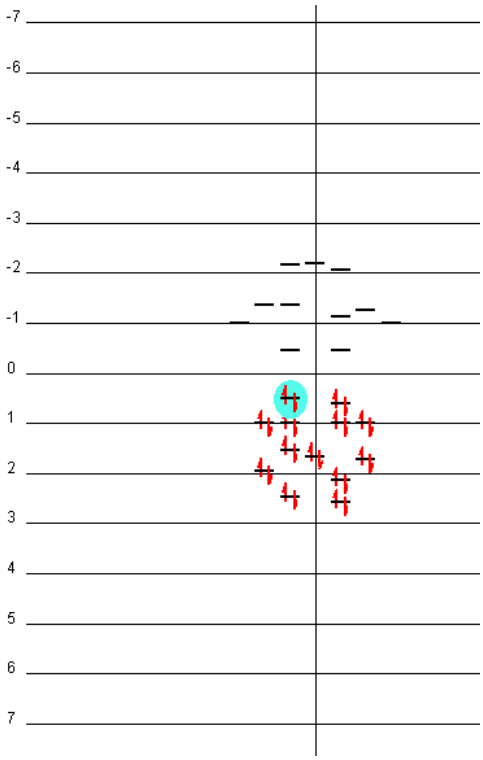


Highest occupied Hückel molecular orbitals (HOMO)

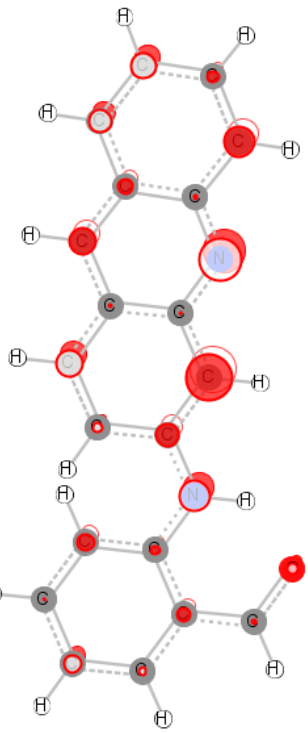
A



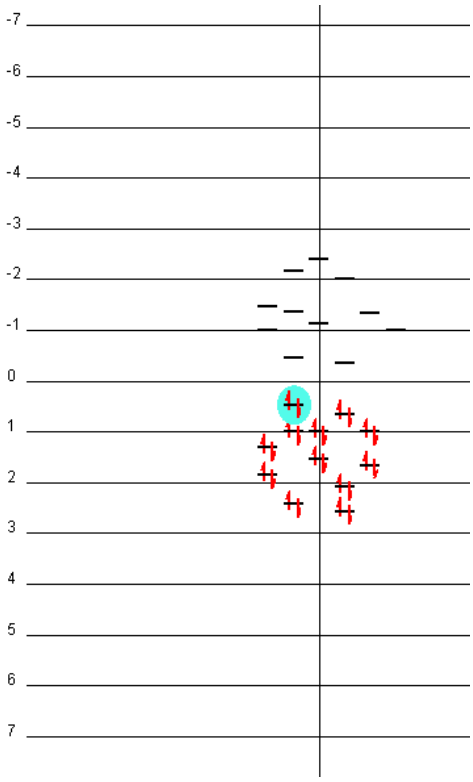
ε = α + 0,51β



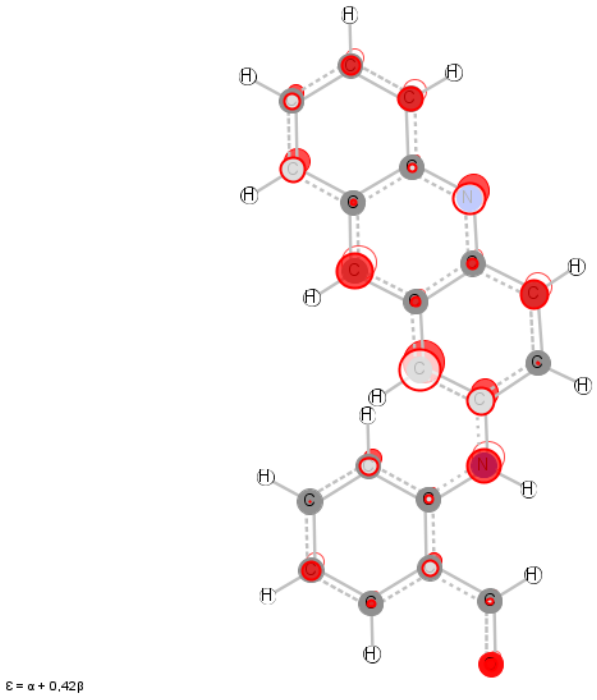
B

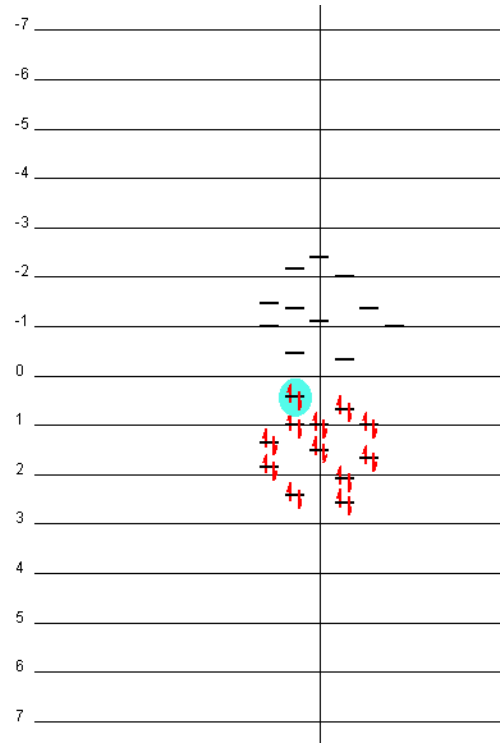


ε = α + 0,46β

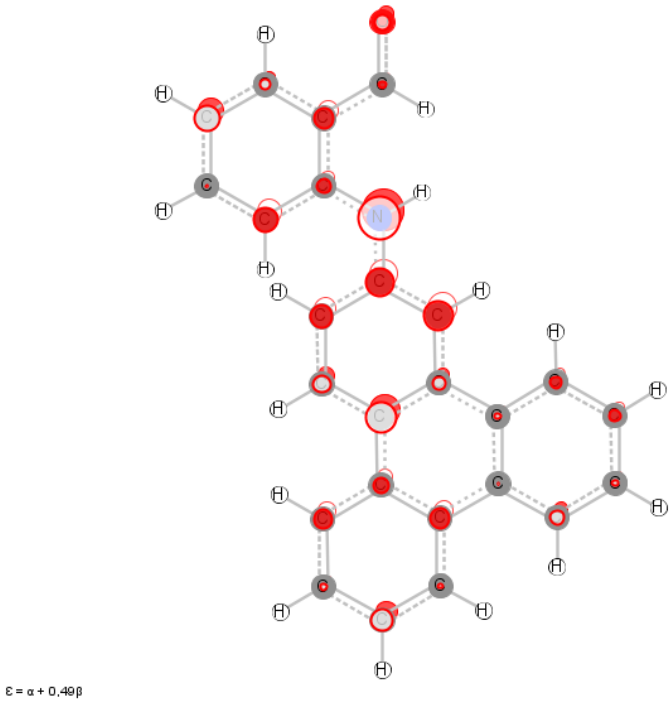


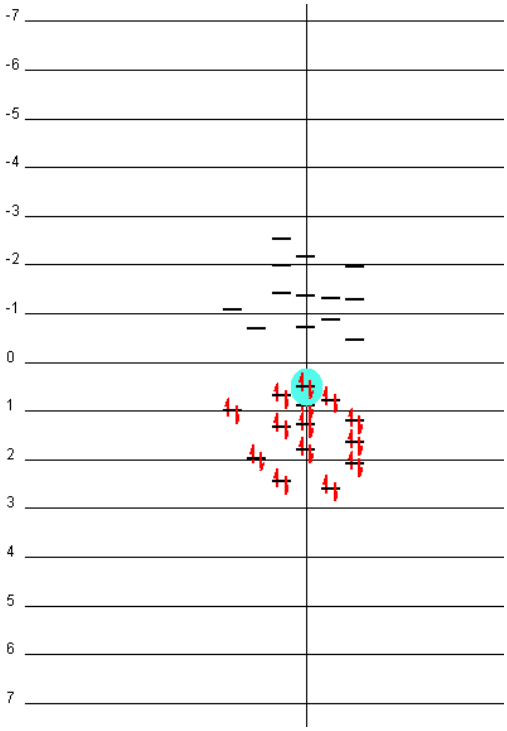
C



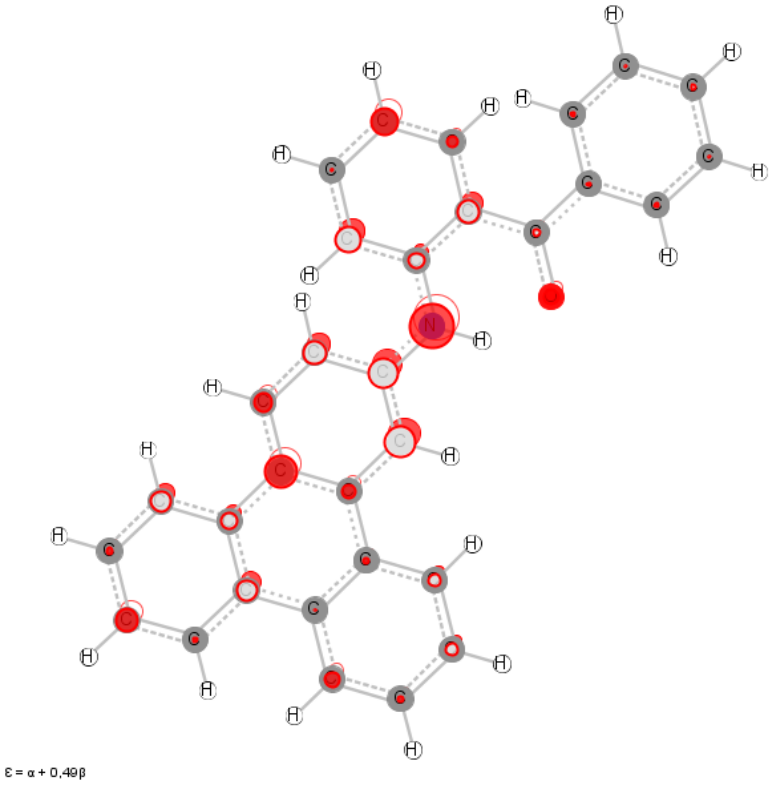


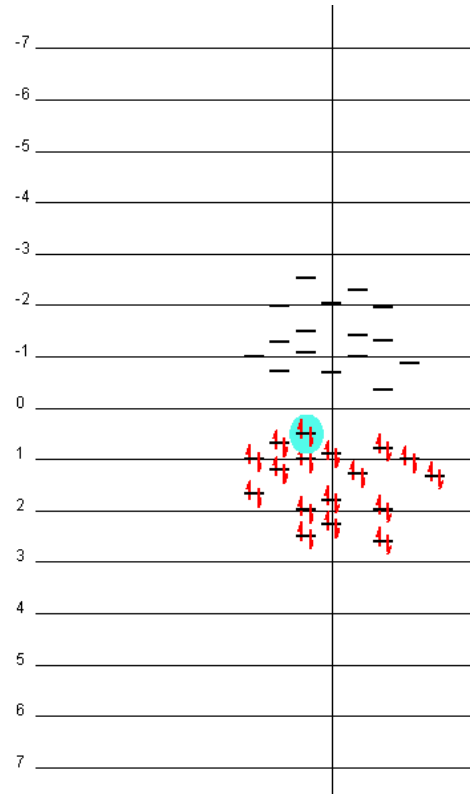
1



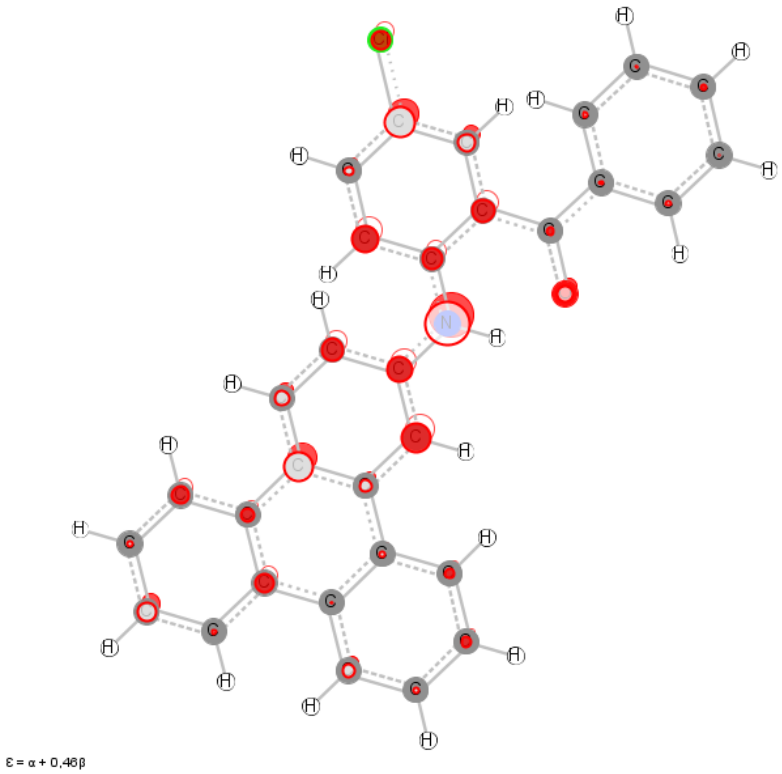


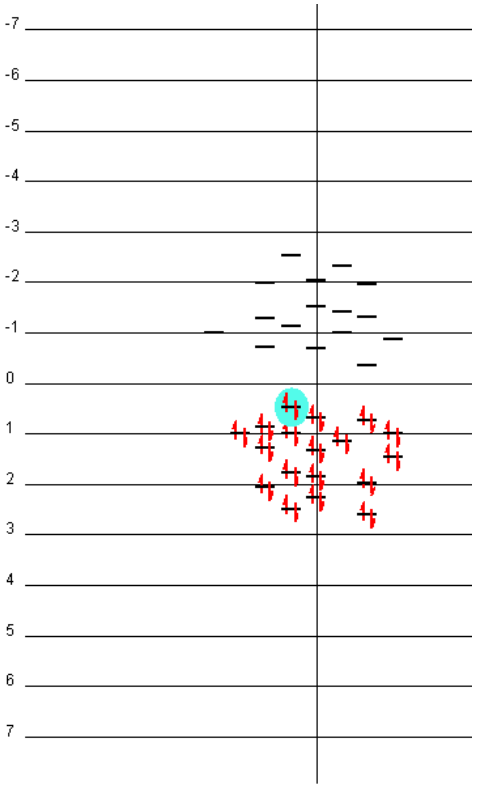
3a



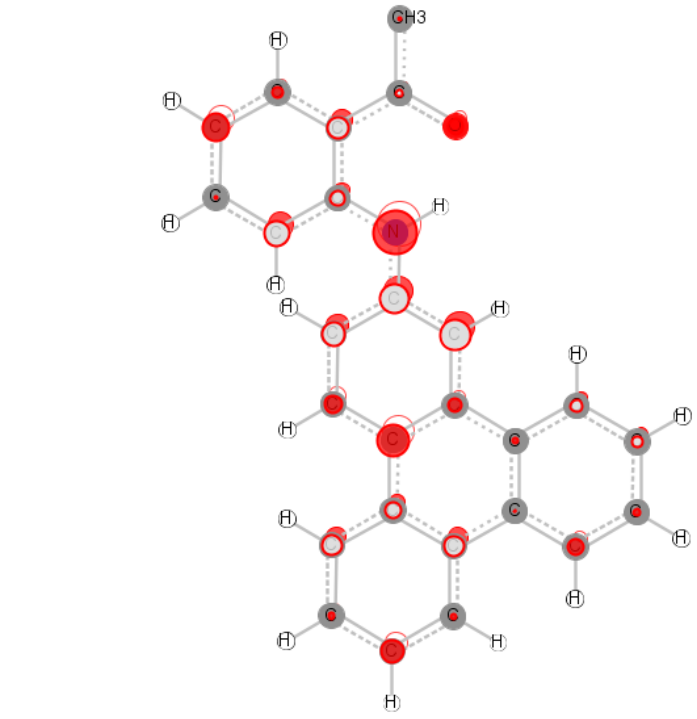


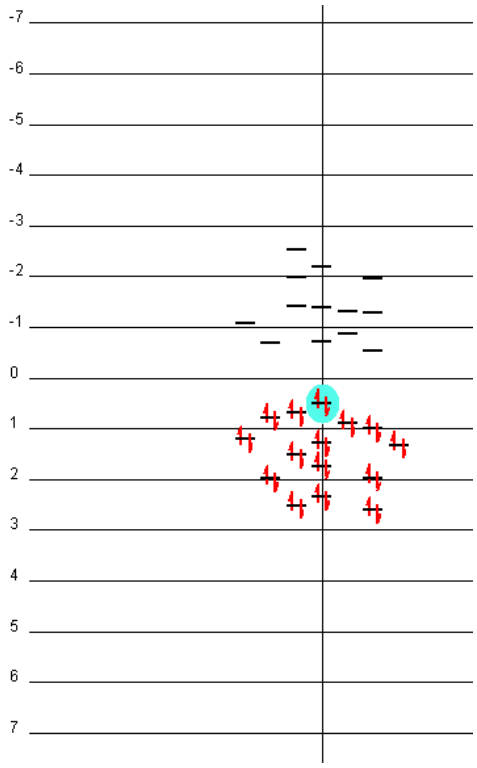
3b



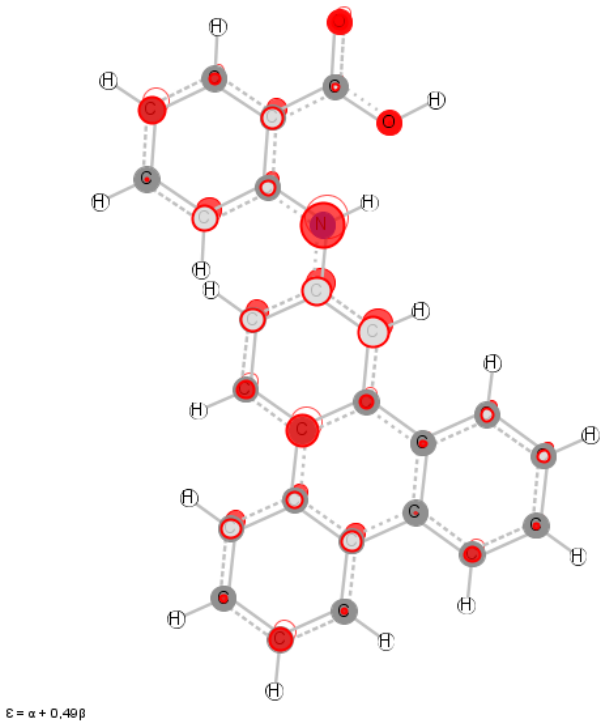


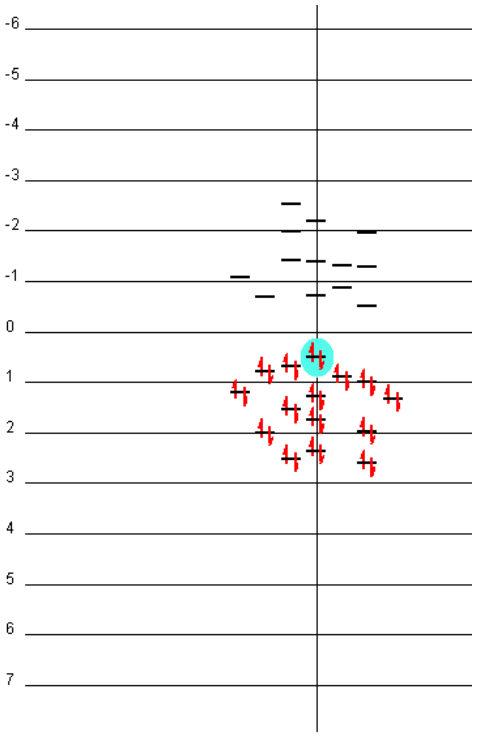
3c





5





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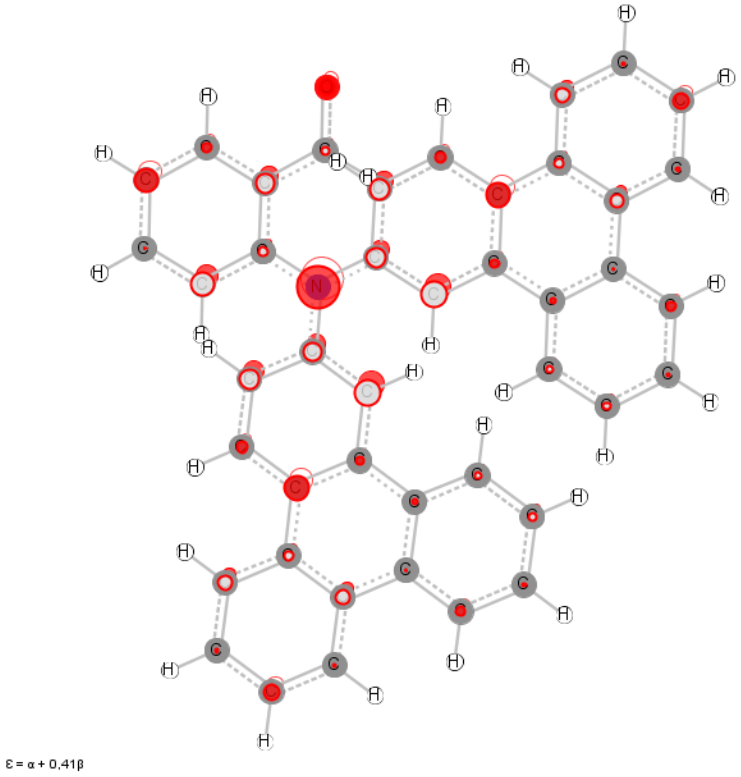
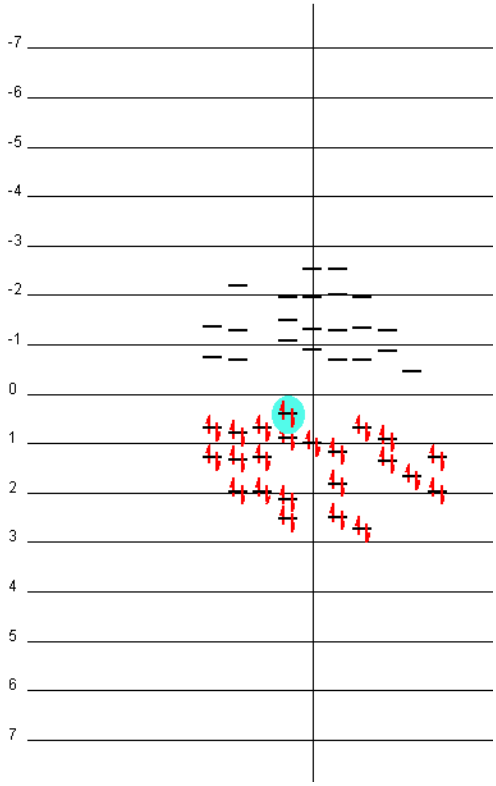
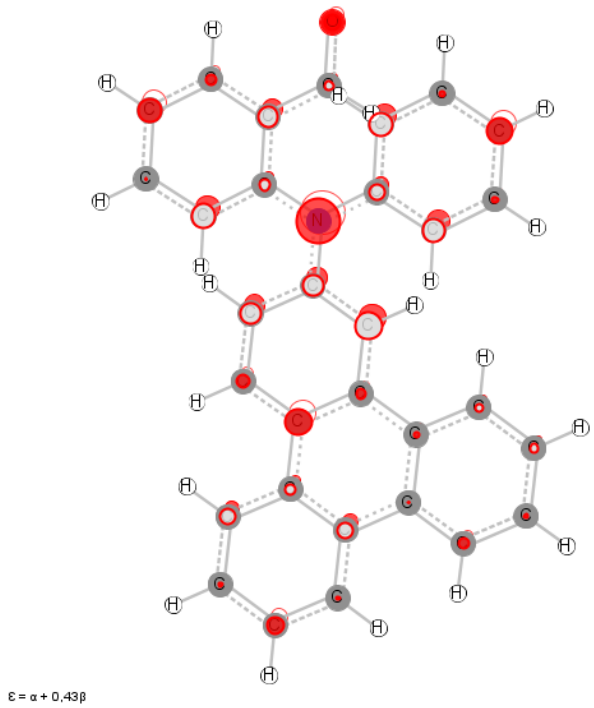
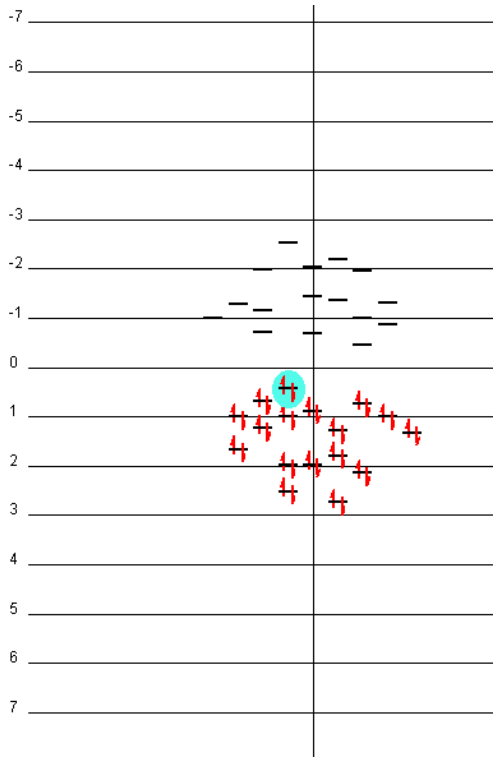




12

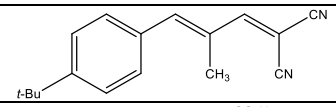
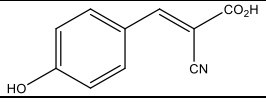
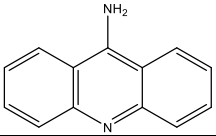
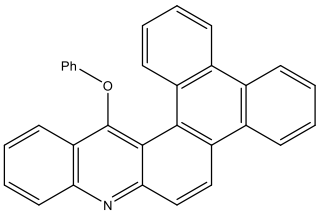
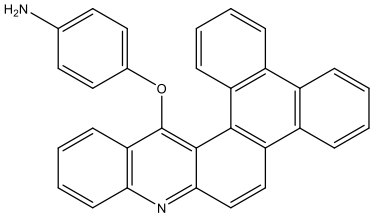




Qualitative evaluation of 8 and 9 as matrices for MALDI-MS

Matrices

DCTB, HCCA, 9-AA, **8** and **9** were used as matrices.

Name	Structure	Formula	$[M-H]^-$	$[M+H]^+$	$[M+Na]^+$
DCTB		$C_{17}H_{18}N_2$	249.14	251.15	273.14
HCCA		$C_{10}H_7NO_3$	188.04	190.05	212.03
9-AA		$C_{13}H_{10}N_2$	193.08	195.09	217.07
8		$C_{31}H_{19}NO$	420.14	422.15	444.14
9		$C_{31}H_{20}N_2O$	435.15	437.16	459.15

Target compounds

#	Dénomination	Formula	$[M-H]^-/A^-$	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$	$[M-H+2Na]^+$
1	Aspirin	$C_9H_8O_4$	179.03	181.05	203.03	219.01	225.01
2	Captopril	$C_9H_{15}NO_3S$	216.07	218.08	240.07	256.05	262.05
3	Metolachlor ESA	$C_{15}H_{23}NO_5S$	328.12	330.14	352.12	368.09	374.10
4	Paracetamol	$C_8H_9NO_2$	150.06	152.07	174.05	190.03	196.03
5	Phenytoin	$C_{15}H_{12}N_2O_2$	251.08	253.10	275.08	291.05	297.06
6	Penicilin V	$C_{16}H_{18}N_2O_5S$	349.09	351.10	373.08	389.06	395.06
7	Penicillin V (K)	(A^-: $C_{16}H_{17}N_2O_5S$; K^+)	349.09	389.06	411.04	427.01	433.02
8	SDS	(A^-: $C_{12}H_{25}O_4S$;Na^+)	265.15	289.14	311.13	327.10	333.11
9	Sodium taurocholate	(A^-: $C_{26}H_{44}NO_7S$;Na^+)	514.28	538.28	560.26	576.24	582.24

Qualitative detection

The experiments were performed in both positive and negative modes, with five matrices (DCTB, HCCA, 9-AA, **8** and **9**), with two solvents for a two-layer spotting (90 spots and 180 experiments).

Matrices were dissolved at 10 mg/mL in methanol or dichloromethane. Target compounds were dissolved at 1 mg/mL in the same solvent. The solutions were dispensed onto an MTP AnchorChip 384 TF target (Bruker Daltonics, P/N 209514) with a GELoader pipette tip. A first layer of target compounds mixture was twice spotted (2*0.25 µL) and dried at room temperature. A second layer of matrix mixture was twice spotted (2*0.25 µL) and dried at room temperature. The 90 spots were analyzed with an Ultraflex III MALDI-TOF/TOF mass spectrometer (Bruker Daltonics) operating under Flex Control^{TM} software (Version 3.4, Build 119, Bruker Daltonics). MALDI-TOF spectra were observed in positive and negative ion reflector mode recording ions between 100 to 2000 Da. The laser power was adjusted to a point slightly above the fluence of the base peak and fired to accumulate 500 counts on the base peak with 200 laser shots. Analysis and annotations of MS spectra were performed manually.

Qualitative information and evaluation factors

For the qualitative information, evaluation factors were chosen and scaled from 0 to 6.

Laser power is better with a small value.

Laser Power	<15%	15-24%	25-34%	35-44%	45-55%	56-65%	>66%
Laser (+ or -)	6	5	4	3	2	1	0

The presence of the target compounds is represented by the factor target.in in correlation with the relative intensity in mass spectrum.

Relative Intensity	Base peak (100%)	Intense (50-99%)	Present (10-49%)	Weak (1-10%)	Traces (1%)	Not seen
Target.in (+ or -)	5	4	3	2	1	0

A factor [Product.LT] representing both the laser power applied and the presence of target compounds was calculated by summing the multiplications of Target.in(+) by Laser(+) and Target.in(-) by Laser(-).

The number of target compounds obtained as a base peak, in positive, negative or in both, without redundancy is specified with the factor Target.BP:

	Target.BP(-)	Target.BP(+)	Target.BP
DCTB	3	3	5
HCCA	0	1	1
9-AA	3	0	3
8	3	1	3
9	3	0	3

Experiments overview tables

For the matrix DCTB

#+	#-	Product	Matrix	Solvent	Laser(+)	Laser(-)	Target.in(+)	Target.in(-)	Product.LT
1	91	1	DCTB	CH_2Cl_2	5	5	0	0	0
6	96	1	DCTB	MeOH	5	5	0	0	0
11	101	2	DCTB	CH_2Cl_2	6	5	3	1	23
16	106	2	DCTB	MeOH	5	5	0	2	10
21	111	3	DCTB	CH_2Cl_2	5	4	5	5	45
26	116	3	DCTB	MeOH	5	5	4	5	45
31	121	4	DCTB	CH_2Cl_2	6	4	2	0	12
36	126	4	DCTB	MeOH	5	4	4	0	20
41	131	5	DCTB	CH_2Cl_2	6	4	3	1	22
46	136	5	DCTB	MeOH	5	4	0	0	0
51	141	6	DCTB	CH_2Cl_2	5	4	5	0	25
56	146	6	DCTB	MeOH	5	4	4	0	20
61	151	7	DCTB	CH_2Cl_2	5	5	5	2	35
66	156	7	DCTB	MeOH	5	5	4	2	30
71	161	8	DCTB	CH_2Cl_2	6	5	0	5	25
76	166	8	DCTB	MeOH	5	5	1	5	30
81	171	9	DCTB	CH_2Cl_2	5	5	0	2	10
86	176	9	DCTB	MeOH	5	5	0	5	25
				Average values	5,22	4,61	2,22	1,94	20,94

For the matrix HCCA

#+	#-	Product	Matrix	Solvent	Laser(+)	Laser(-)	Target.in(+)	Target.in(-)	Product.LT
2	92	1	HCCA	CH_2Cl_2	3	2	0	0	0
7	97	1	HCCA	MeOH	3	4	0	0	0
12	102	2	HCCA	CH_2Cl_2	3	3	4	0	12
17	107	2	HCCA	MeOH	5	4	3	0	15
22	112	3	HCCA	CH_2Cl_2	2	0	2	0	4
27	117	3	HCCA	MeOH	4	5	2	1	13
32	122	4	HCCA	CH_2Cl_2	5	1	2	0	10
37	127	4	HCCA	MeOH	5	4	1	0	5
42	132	5	HCCA	CH_2Cl_2	3	1	0	0	0
47	137	5	HCCA	MeOH	5	4	0	0	0
52	142	6	HCCA	CH_2Cl_2	4	2	0	0	0
57	147	6	HCCA	MeOH	5	3	5	0	25
62	152	7	HCCA	CH_2Cl_2	4	0	0	0	0
67	157	7	HCCA	MeOH	4	4	0	0	0
72	162	8	HCCA	CH_2Cl_2	2	0	0	0	0
77	167	8	HCCA	MeOH	5	3	2	4	22
82	172	9	HCCA	CH_2Cl_2	5	4	0	0	0
87	177	9	HCCA	MeOH	5	4	0	2	8
				Average values	4,00	2,67	1,17	0,39	6,33

For the matrix 9-AA

#+	#-	Product	Matrix	Solvent	Laser(+)	Laser(-)	Target.in(+)	Target.in(-)	Product.LT
3	93	1	9-AA	CH_2Cl_2	3	3	0	1	3
8	98	1	9-AA	MeOH	3	2	0	1	2
13	103	2	9-AA	CH_2Cl_2	4	1	0	0	0
18	108	2	9-AA	MeOH	3	2	0	2	4
23	113	3	9-AA	CH_2Cl_2	4	3	2	5	23
28	118	3	9-AA	MeOH	3	2	1	5	13
33	123	4	9-AA	CH_2Cl_2	3	1	0	1	1
38	128	4	9-AA	MeOH	4	1	0	0	0
43	133	5	9-AA	CH_2Cl_2	3	2	0	4	8
48	138	5	9-AA	MeOH	3	2	0	2	4
53	143	6	9-AA	CH_2Cl_2	3	1	0	0	0
58	148	6	9-AA	MeOH	2	1	0	0	0
63	153	7	9-AA	CH_2Cl_2	3	2	0	0	0
68	158	7	9-AA	MeOH	3	2	3	0	9
73	163	8	9-AA	CH_2Cl_2	4	1	0	2	2
78	168	8	9-AA	MeOH	4	1	0	5	5
83	173	9	9-AA	CH_2Cl_2	4	2	0	5	10
88	178	9	9-AA	MeOH	4	3	0	5	15
				Average values	3,33	1,78	0,33	2,11	5,50

For the matrix **8**

#+	#-	Product	Matrix	Solvent	Laser(+)	Laser(-)	Target.in(+)	Target.in(-)	Product.LT
4	94	1	**8**	CH_2Cl_2	4	2	0	0	0
9	99	1	**8**	MeOH	3	2	0	0	0
14	104	2	**8**	CH_2Cl_2	2	2	0	0	0
19	109	2	**8**	MeOH	3	3	0	0	0
24	114	3	**8**	CH_2Cl_2	3	1	5	3	18
29	119	3	**8**	MeOH	3	2	1	5	13
34	124	4	**8**	CH_2Cl_2	3	1	0	0	0
39	129	4	**8**	MeOH	4	2	0	0	0
44	134	5	**8**	CH_2Cl_2	3	3	0	4	12
49	139	5	**8**	MeOH	3	2	0	2	4
54	144	6	**8**	CH_2Cl_2	3	2	0	0	0
59	149	6	**8**	MeOH	3	1	0	0	0
64	154	7	**8**	CH_2Cl_2	3	2	0	0	0
69	159	7	**8**	MeOH	3	1	0	0	0
74	164	8	**8**	CH_2Cl_2	4	1	0	5	5
79	169	8	**8**	MeOH	3	1	0	4	4
84	174	9	**8**	CH_2Cl_2	3	2	0	5	10
89	179	9	**8**	MeOH	3	2	0	4	8
				Average values	3,11	1,78	0,33	1,78	4,11

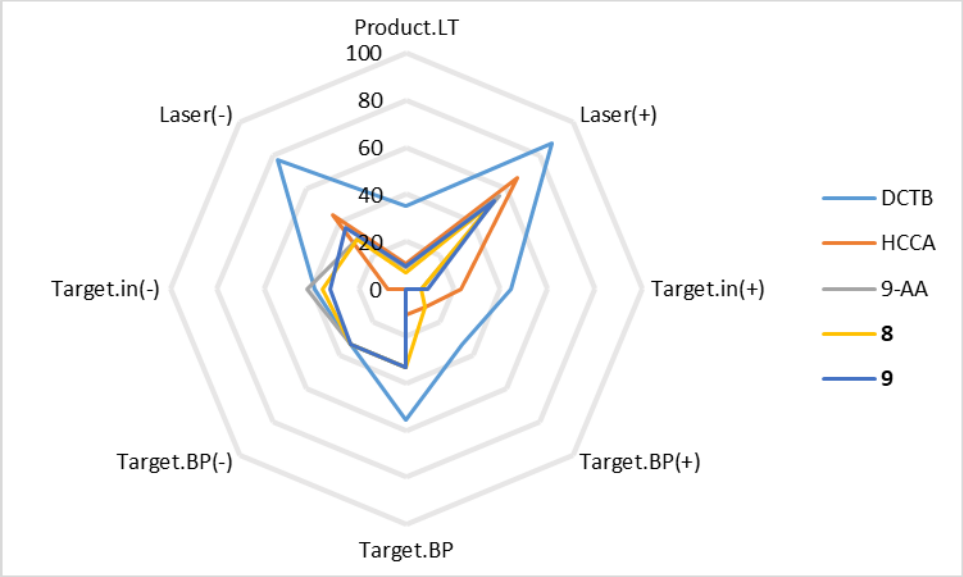
For the matrix **9**

#+	#-	Product	Matrix	Solvent	Laser(+)	Laser(-)	Target.in(+)	Target.in(-)	Product.LT
5	95	1	**9**	CH_2Cl_2	3	3	0	1	3
10	100	1	**9**	MeOH	3	1	0	1	1
15	105	2	**9**	CH_2Cl_2	3	2	0	0	0
20	110	2	**9**	MeOH	3	3	0	0	0
25	115	3	**9**	CH_2Cl_2	3	2	4	5	22
30	120	3	**9**	MeOH	3	2	4	5	22
35	125	4	**9**	CH_2Cl_2	3	2	0	0	0
40	130	4	**9**	MeOH	4	2	0	0	0
45	135	5	**9**	CH_2Cl_2	3	2	0	0	0
50	140	5	**9**	MeOH	3	2	0	2	4
55	145	6	**9**	CH_2Cl_2	3	2	0	0	0
60	150	6	**9**	MeOH	3	1	0	0	0
65	155	7	**9**	CH_2Cl_2	3	2	0	0	0
70	160	7	**9**	MeOH	3	2	0	0	0
75	165	8	**9**	CH_2Cl_2	4	1	0	0	0
80	170	8	**9**	MeOH	3	3	0	5	15
85	175	9	**9**	CH_2Cl_2	4	3	0	5	15
90	180	9	**9**	MeOH	3	4	0	5	20
				Average values	3,17	2,17	0,44	1,61	5,67

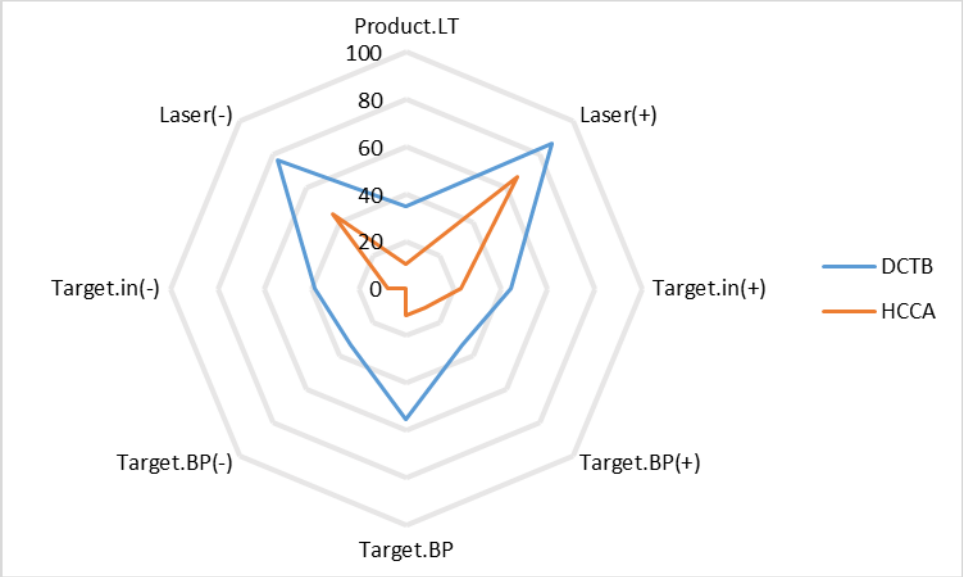
The average values as a percentage are summarized in order to generate the Kiviat's diagram.

	Product.LT	Laser(+)	Target.in(+)	Target.BP(+)	Target.BP	Target.BP(-)	Target.in(-)
DCTB	34,9	87,0	44,4	33,3	55,6	33,3	38,8
HCCA	10,6	66,7	23,2	11,1	11,1	0,0	7,8
9-AA	9,2	55,5	6,6	0,0	33,3	33,3	42,2
8	6,9	51,8	6,6	11,1	33,3	33,3	35,6
9	9,5	52,8	8,8	0,0	33,3	33,3	32,2

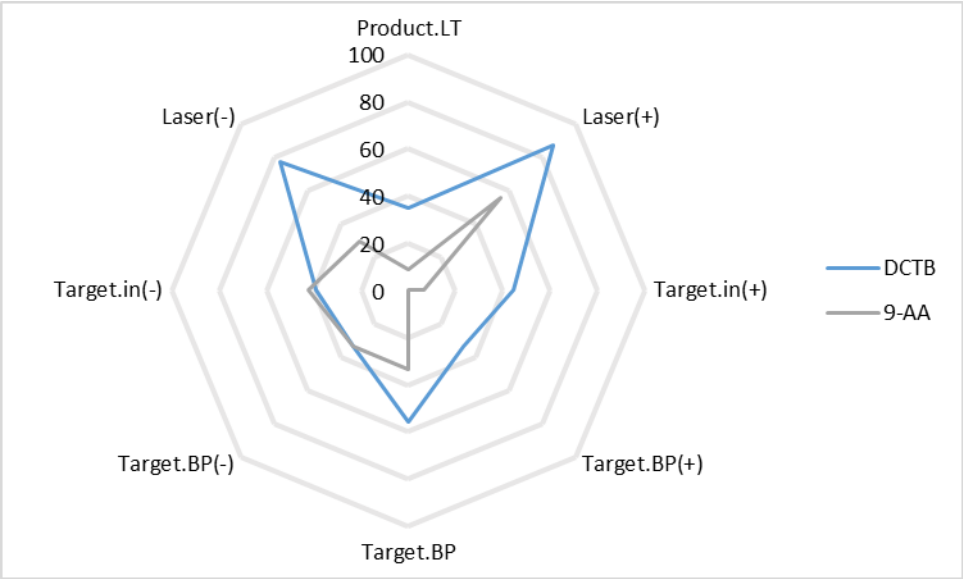
Qualitative analysis of the five matrices



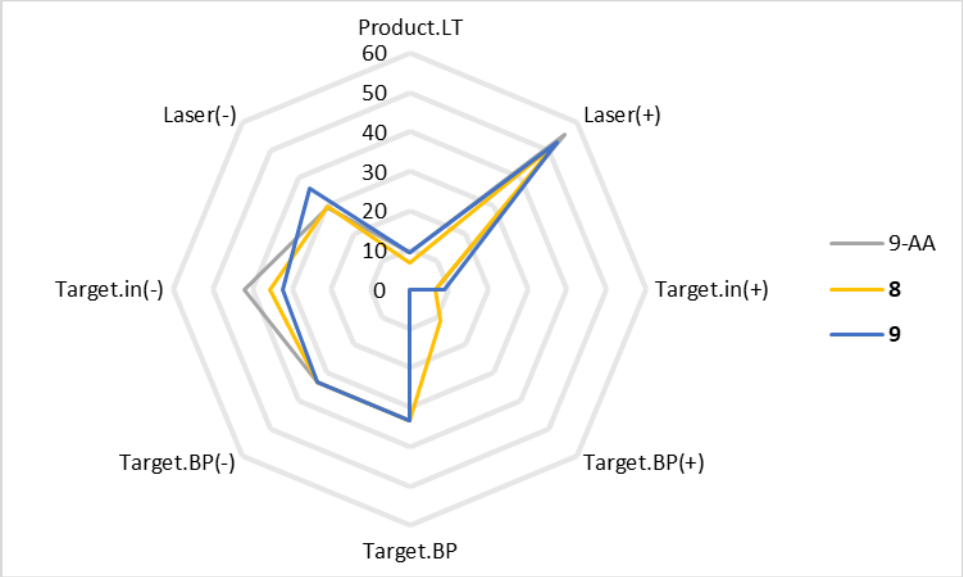
Qualitative analysis of DCTB *vs.* HCCA



Qualitative analysis of DCTB *vs.* 9-AA



Qualitative analysis of 9-AA, **8** and **9**



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