Electronic Supplementary Information

DBU-mediated [4 + 2] Annulations of Donor-Acceptor Cyclopropanes with 3-Aryl-2-cyanoacrylates for Synthesis of Fully Substituted Anilines

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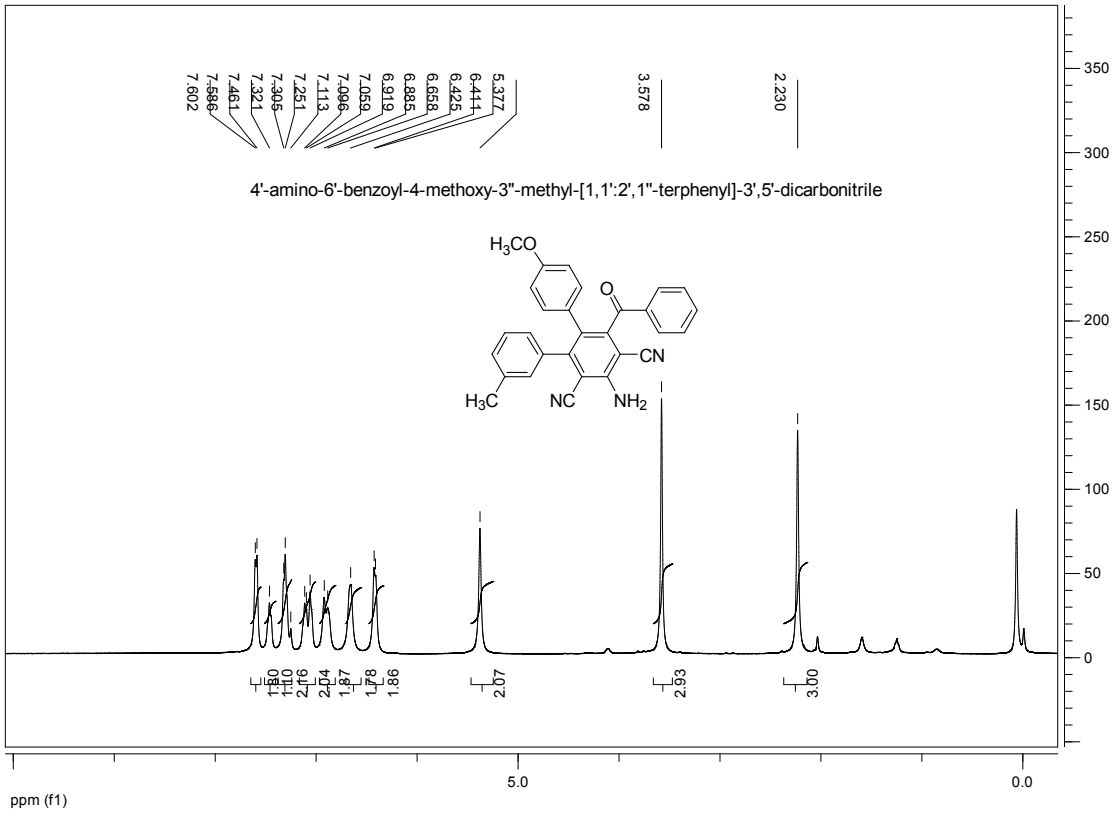
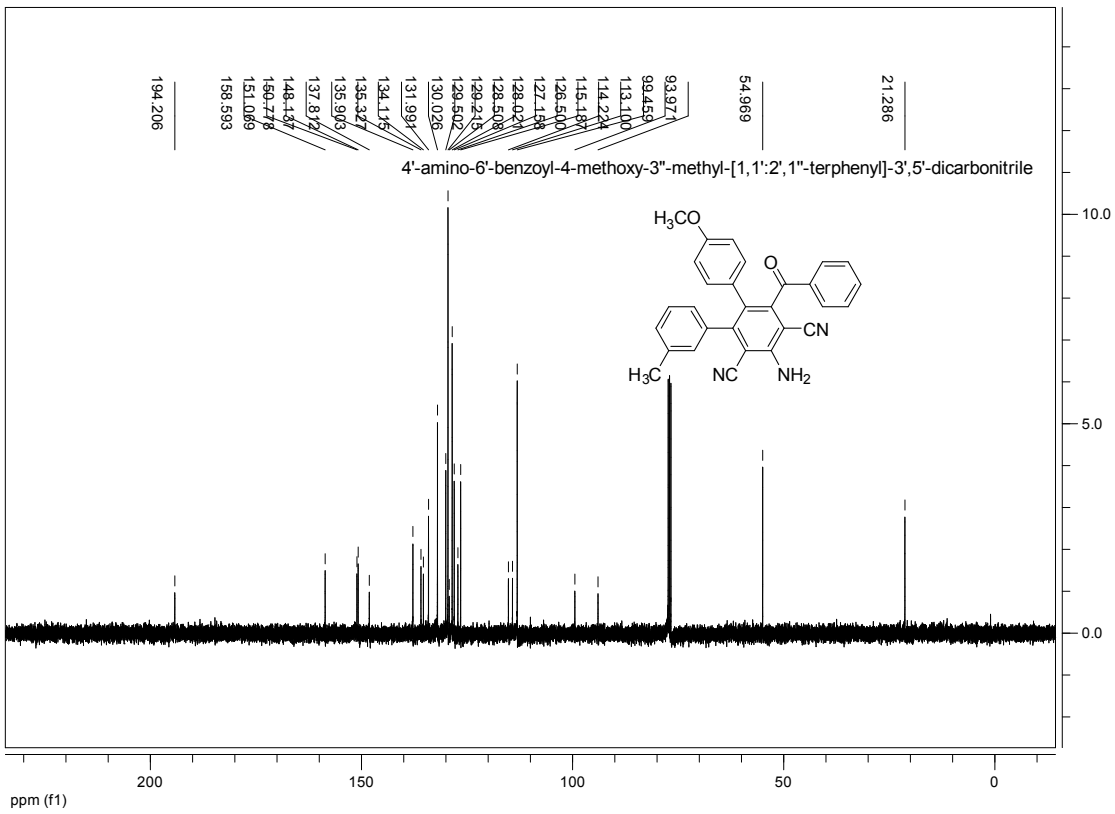
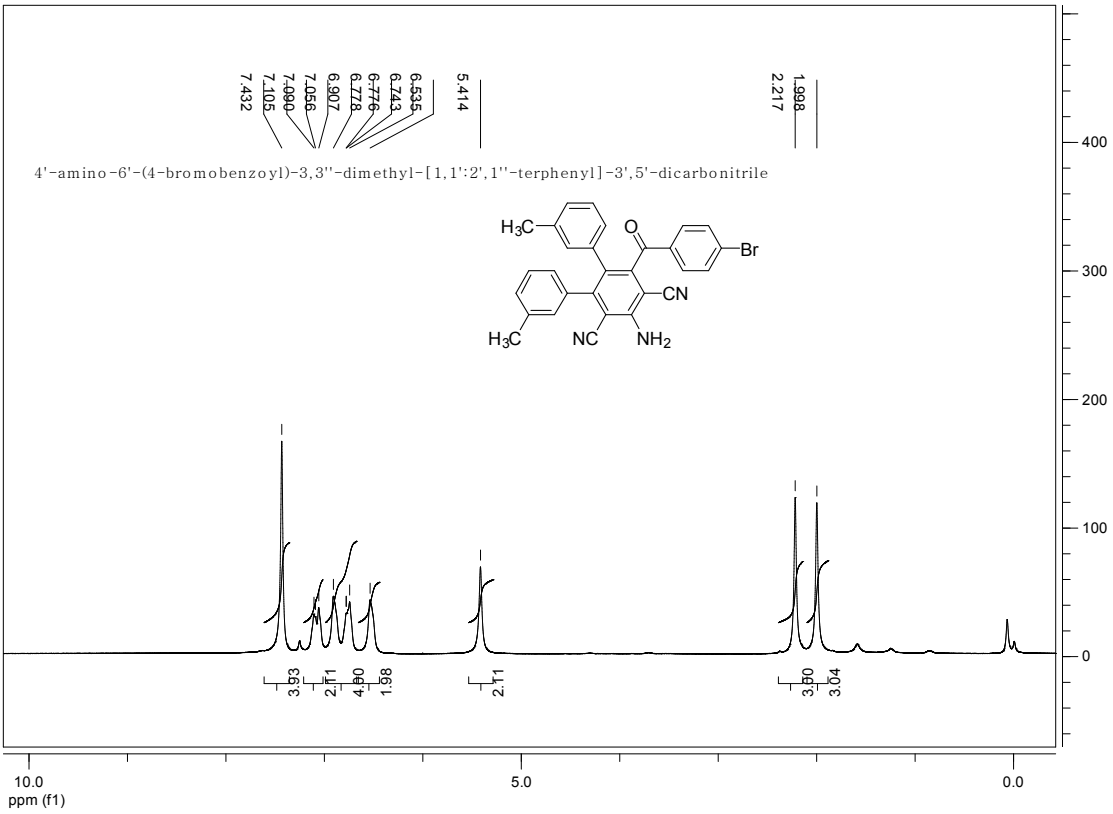
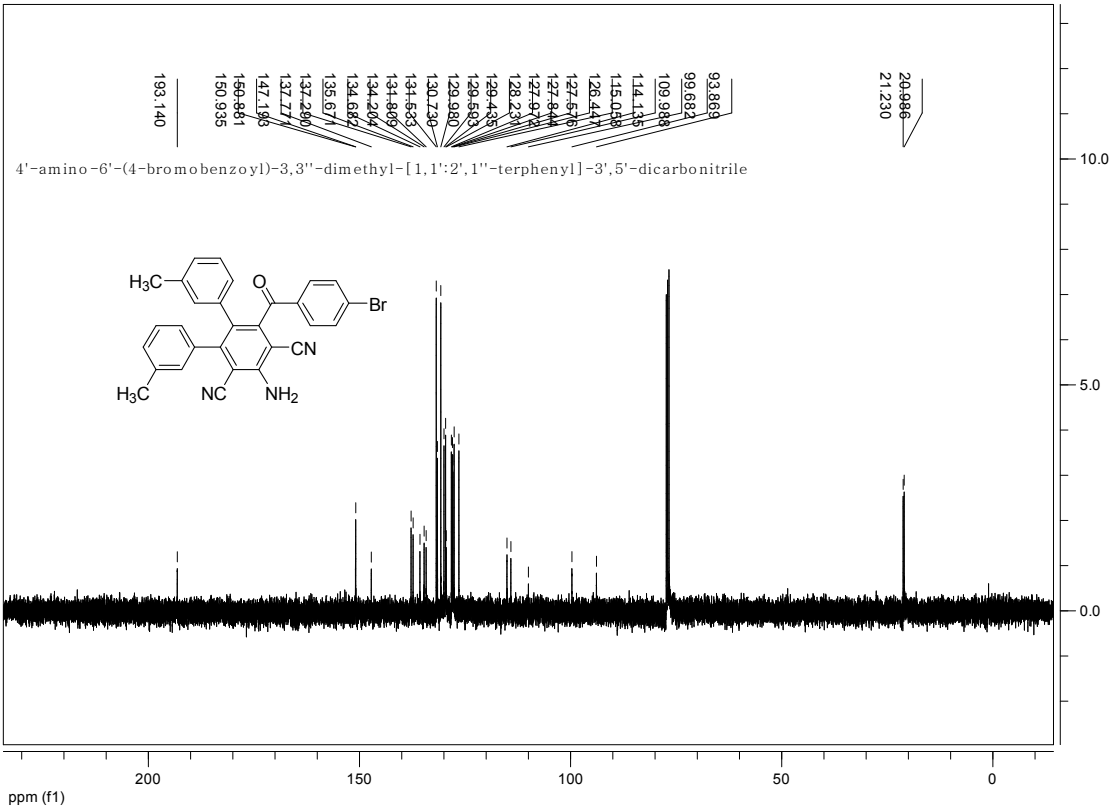


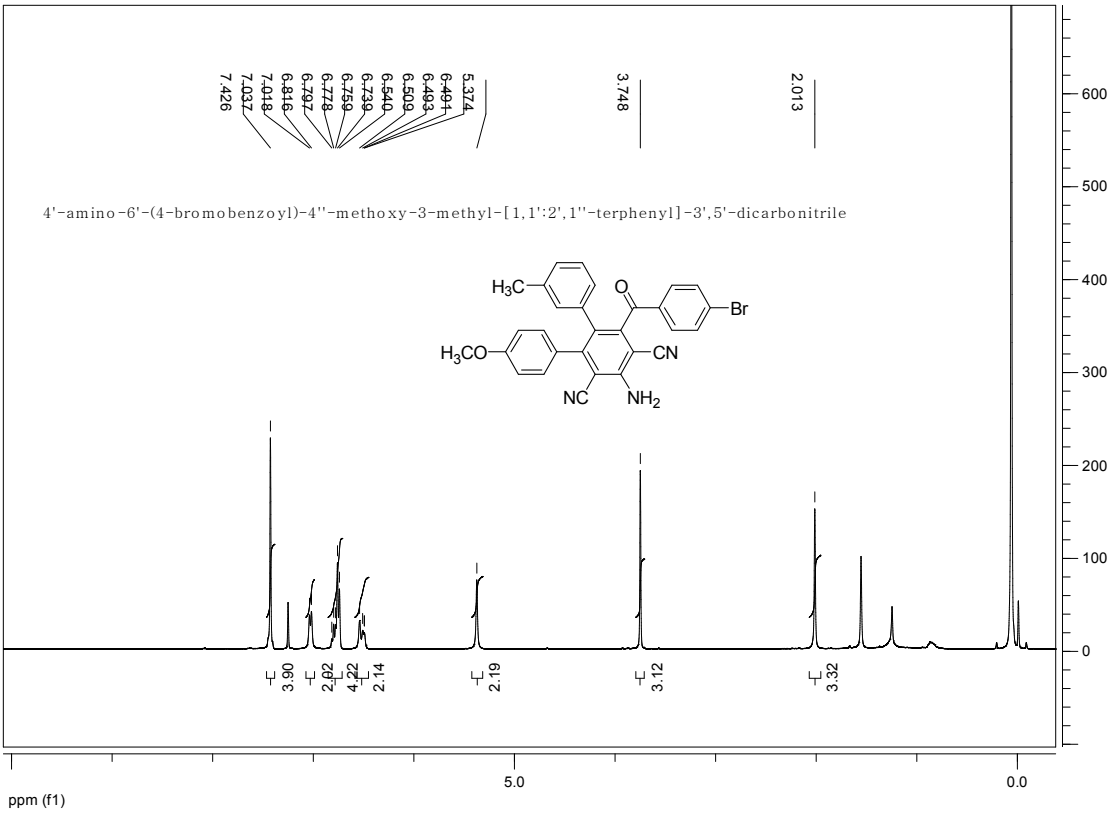


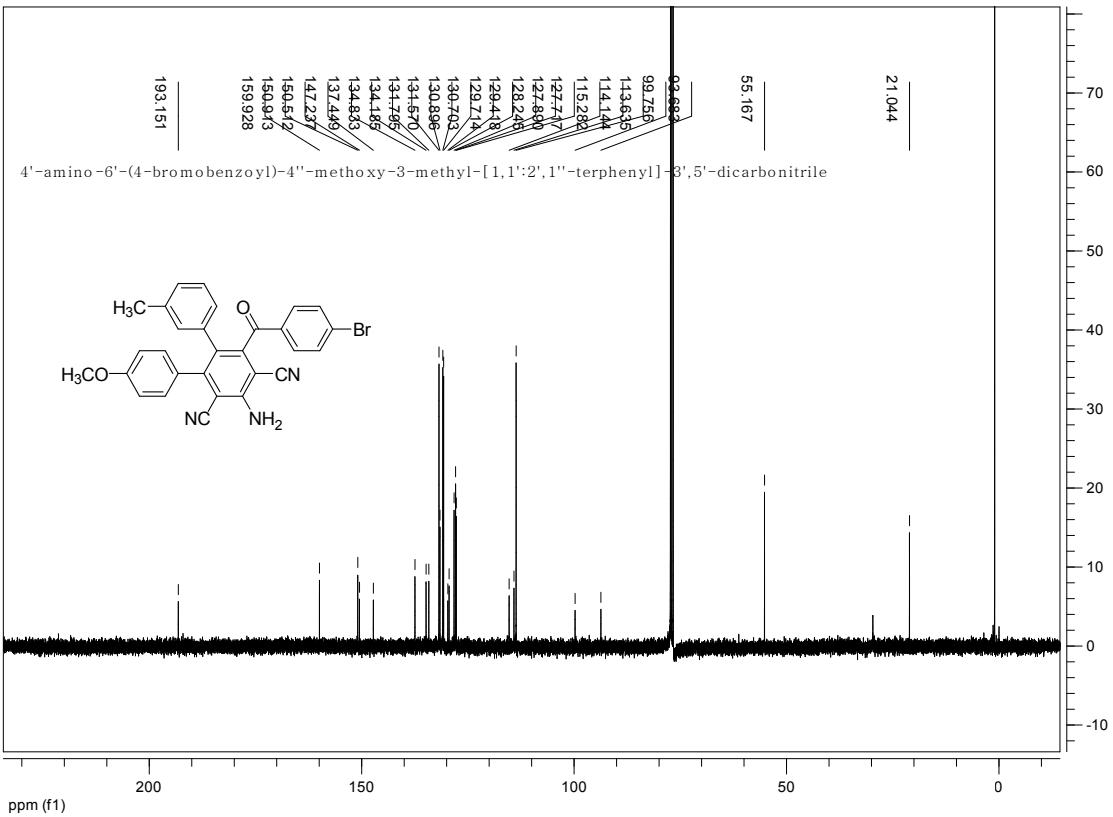
4'-amino-6'-(4-bromobenzoyl)-3,3''-dimethyl-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3b**)



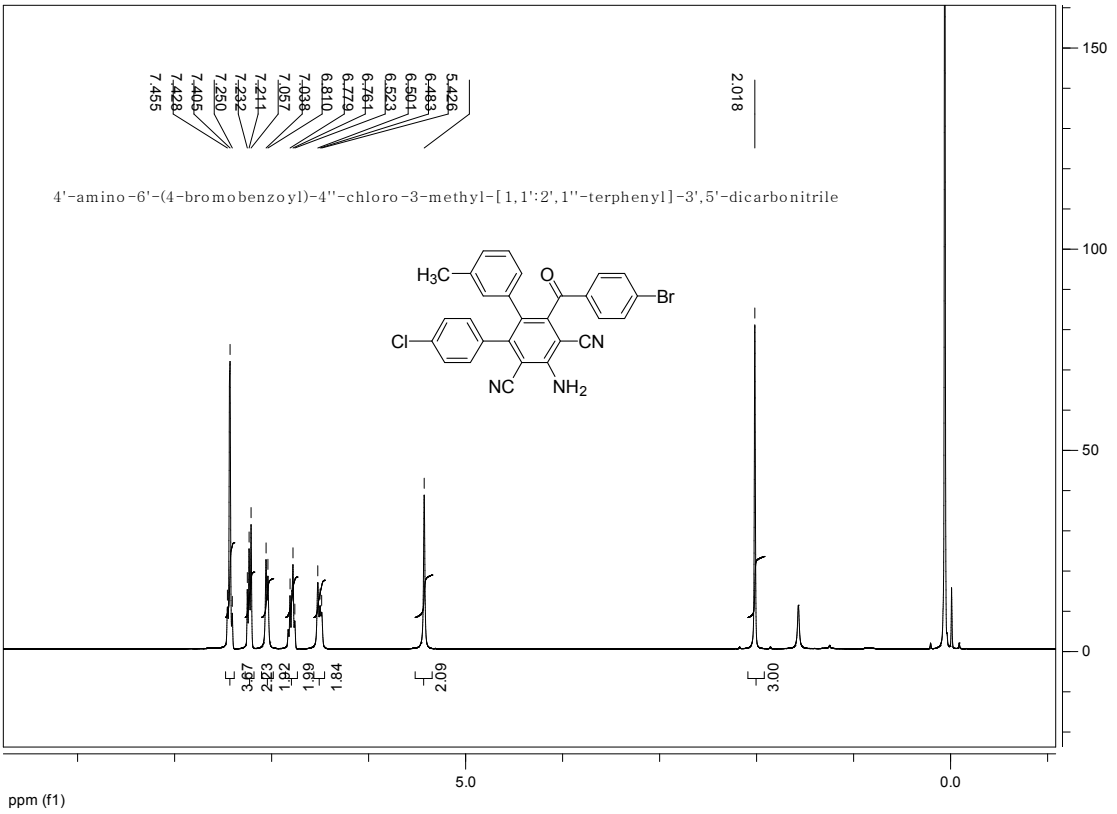


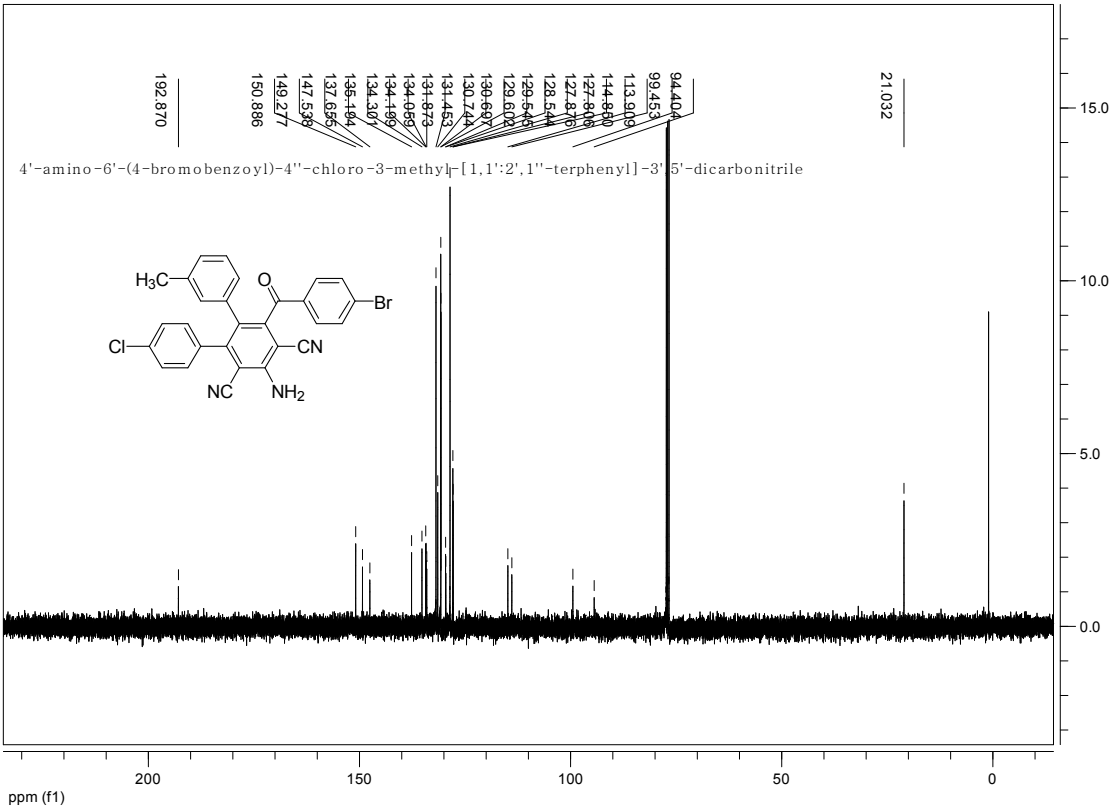
4'-amino-6'-(4-bromobenzoyl)-4''-methoxy-3-methyl-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3c**)





4'-amino-6'-(4-bromobenzoyl)-4''-chloro-3-methyl-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile(**3d**)





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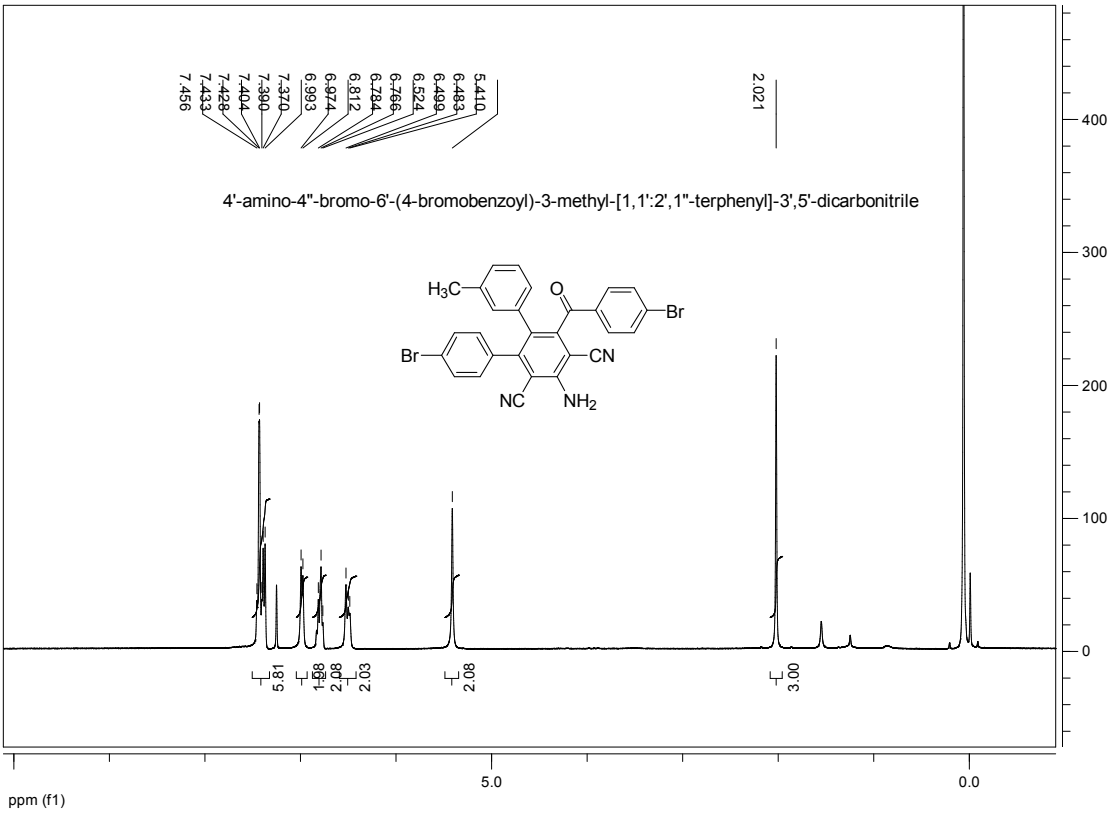
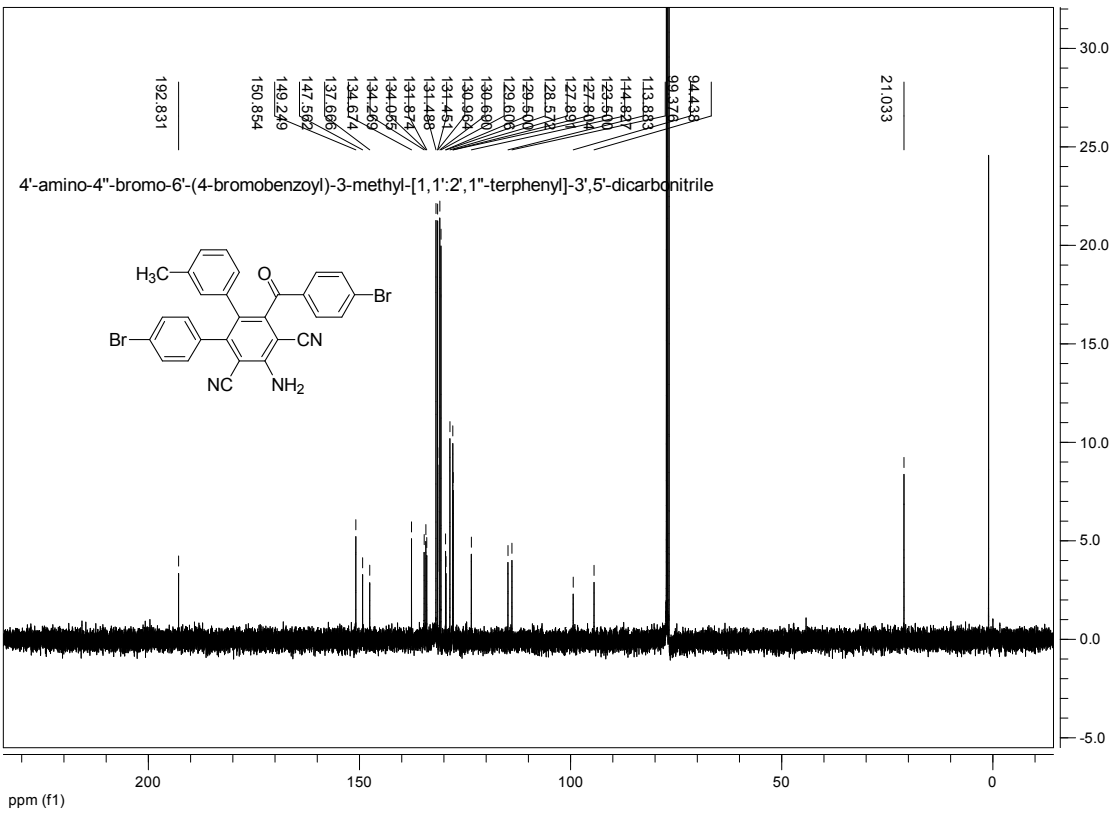
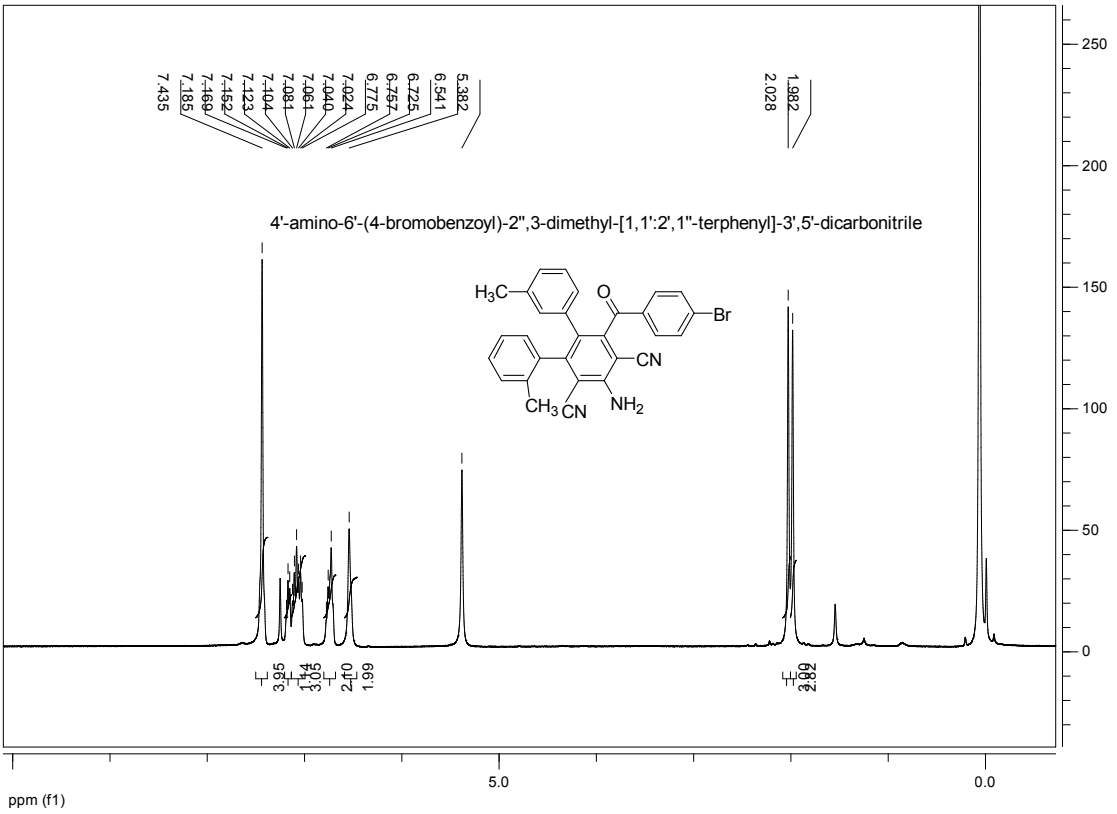
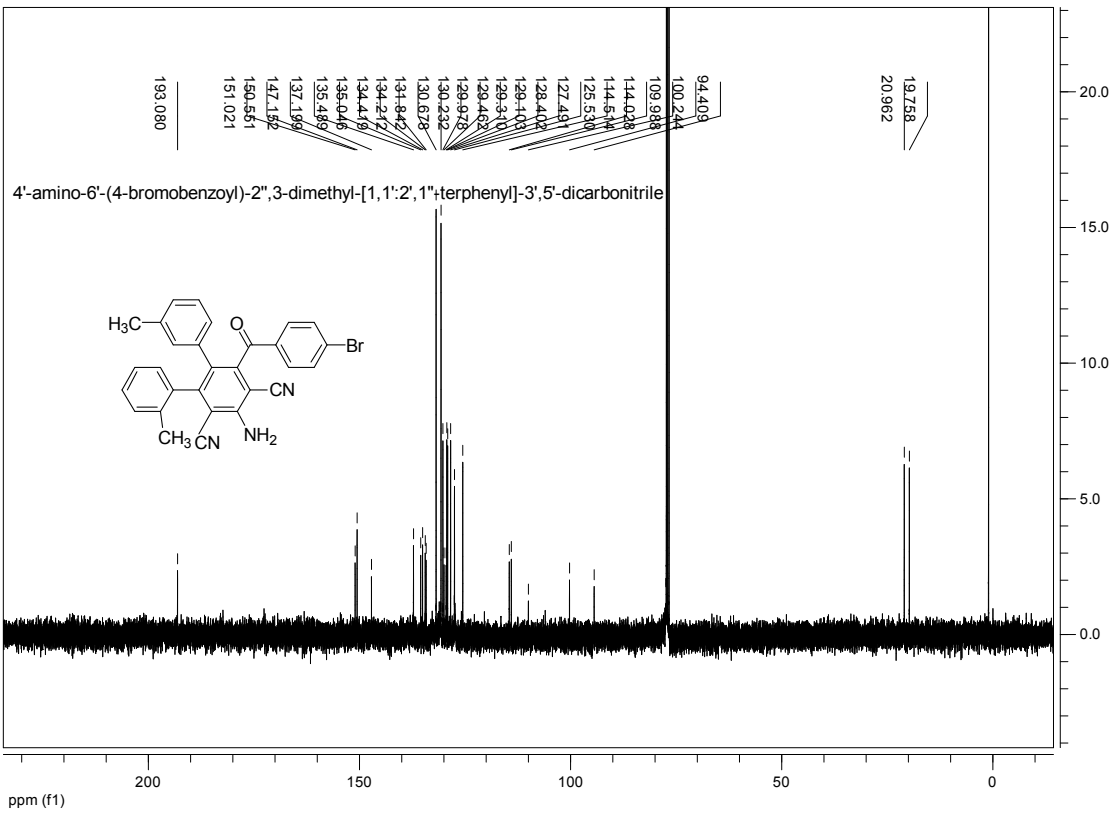


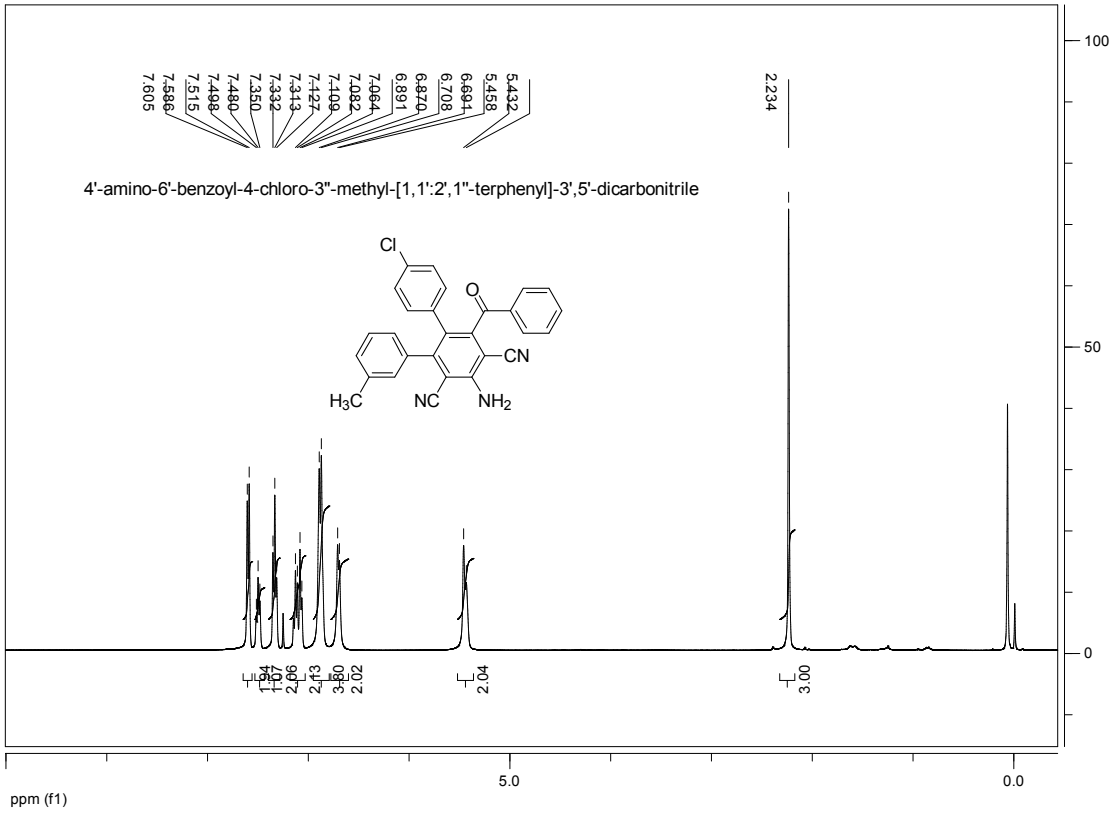


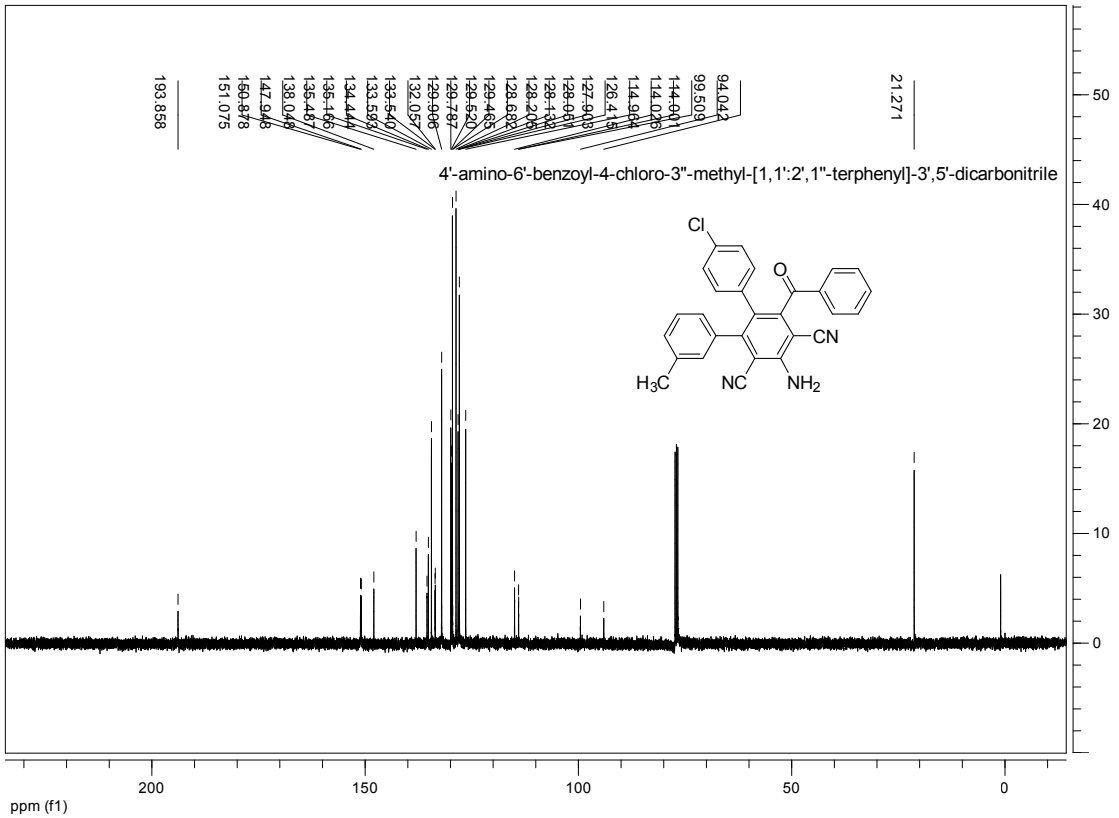
4'-amino-6'-(4-bromobenzoyl)-2'',3-dimethyl-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3f**)



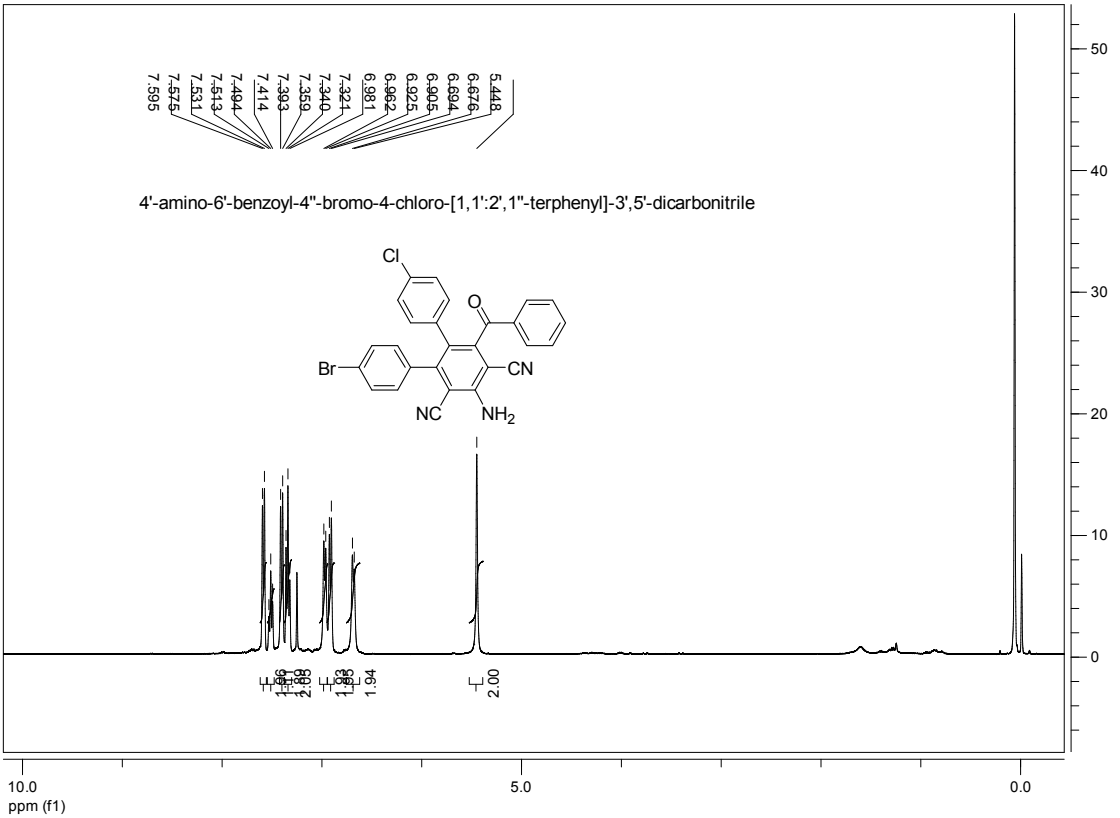


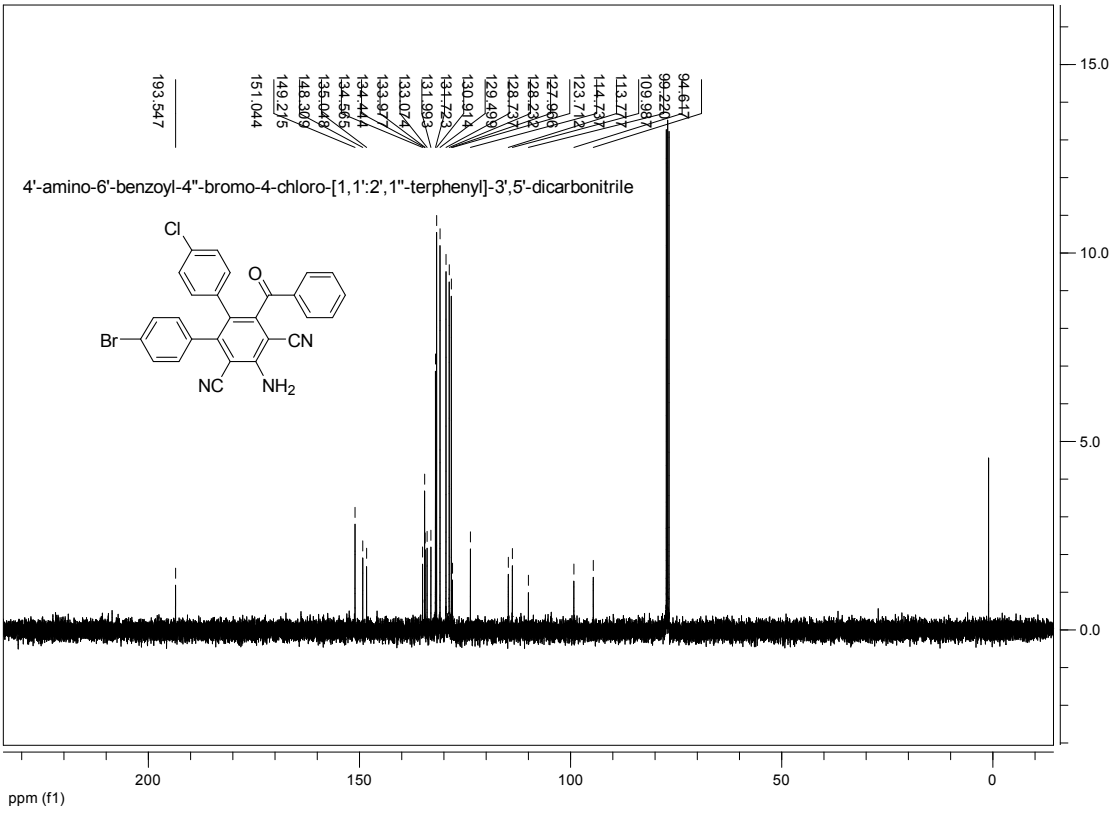
4'-amino-6'-benzoyl-4-chloro-3"-methyl-[1,1':2',1"-terphenyl]-3',5'-dicarbonitrile(**3g**)





4'-amino-6'-benzoyl-4''-bromo-4-chloro-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile(**3h**)





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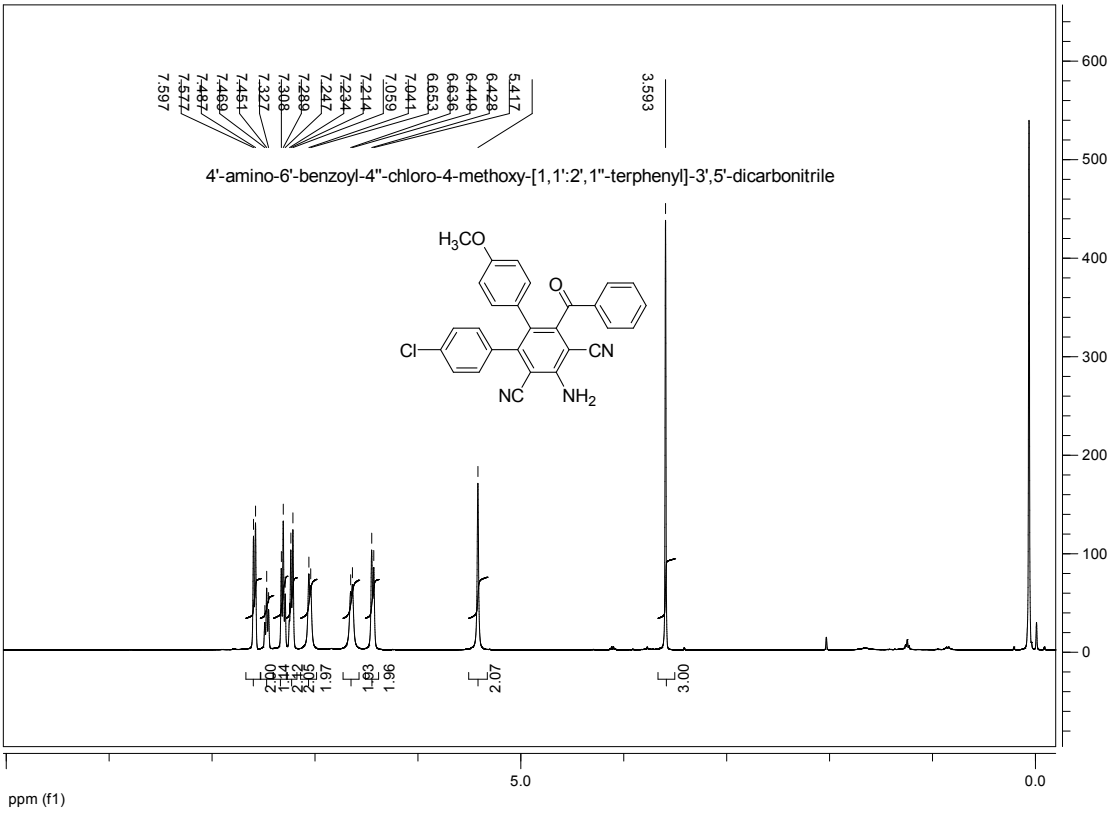

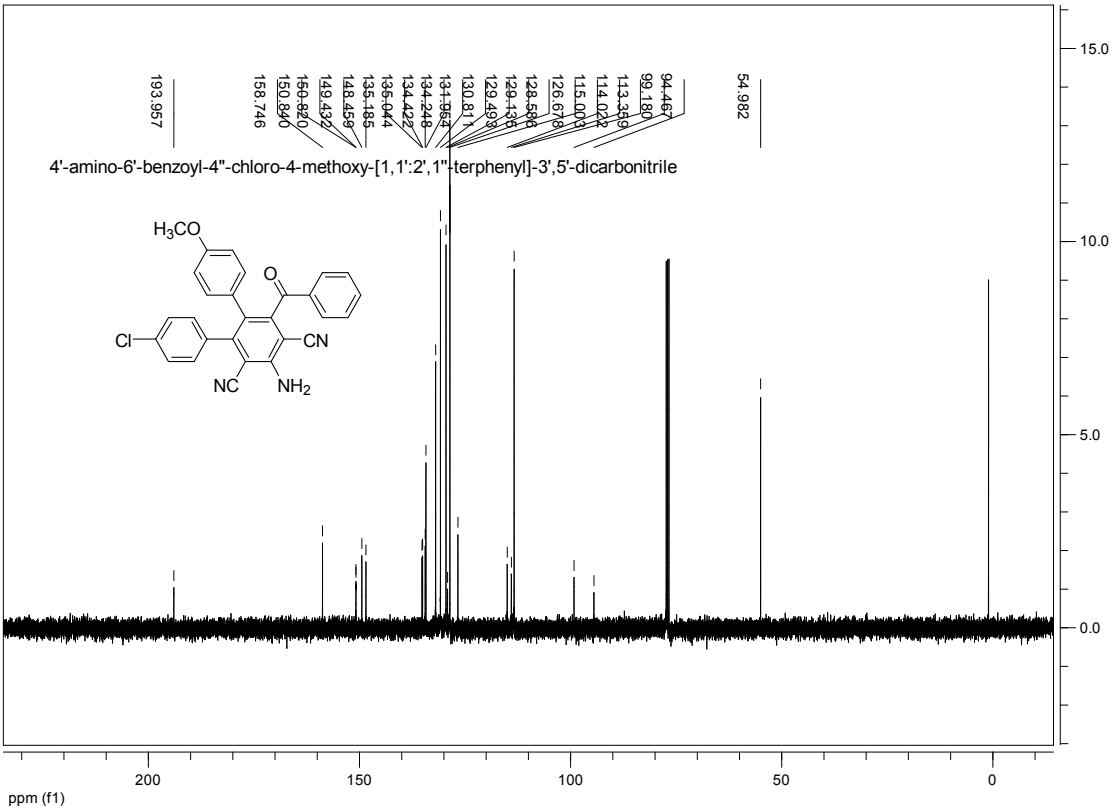

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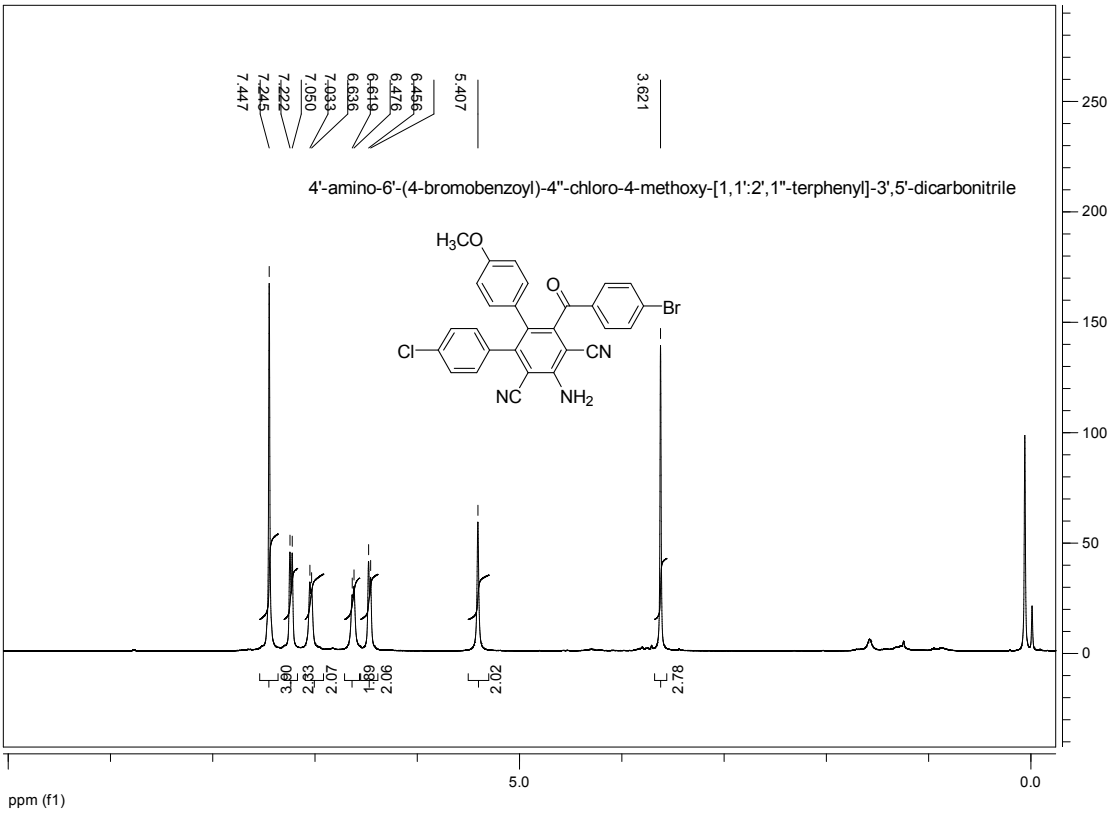
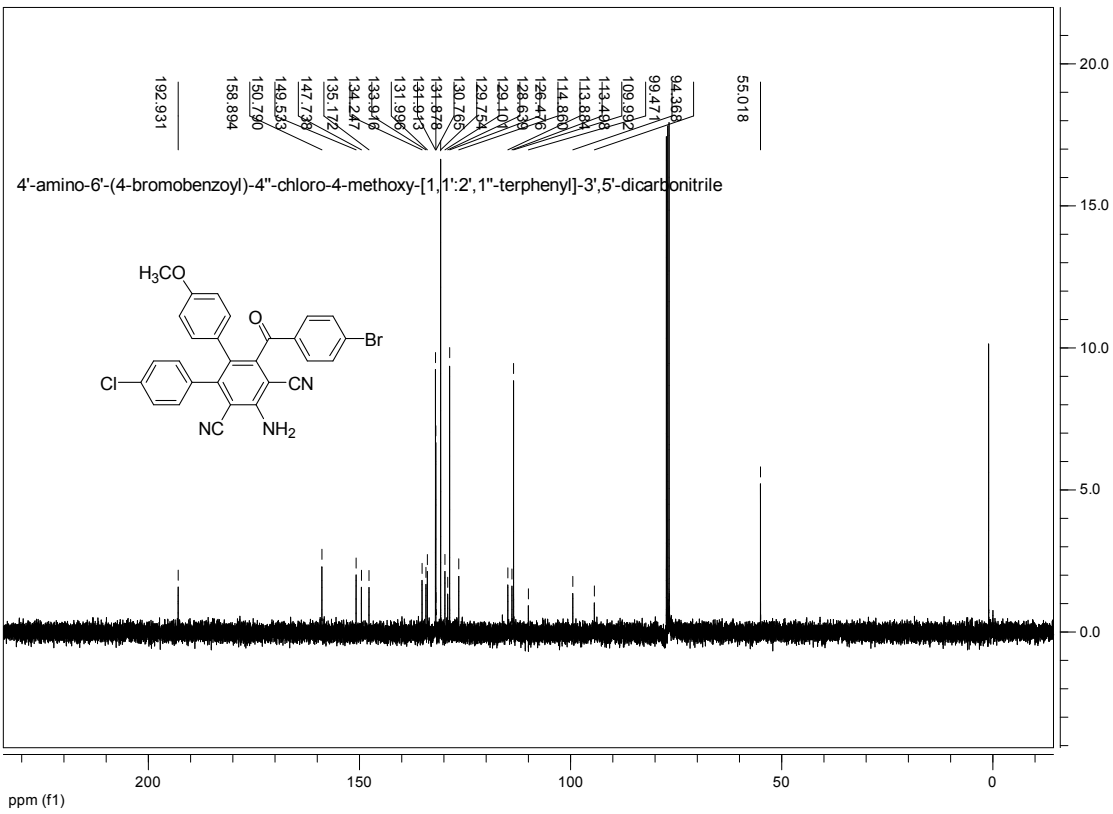
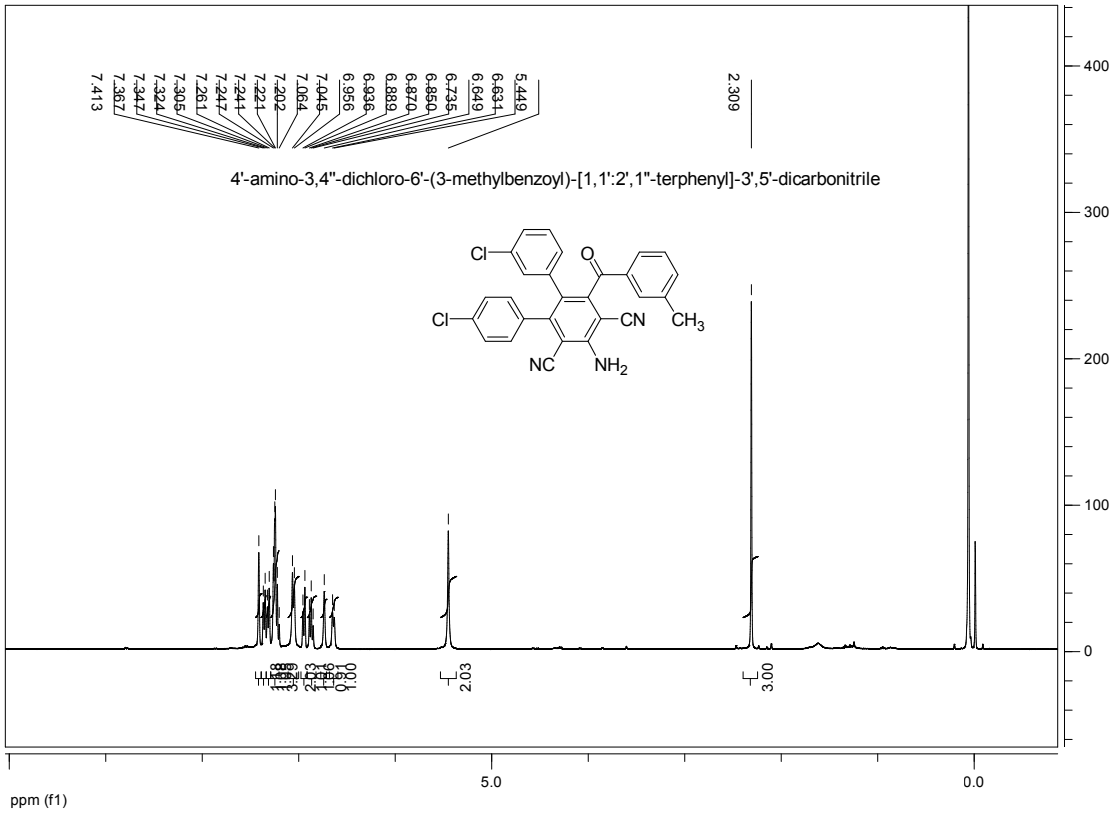
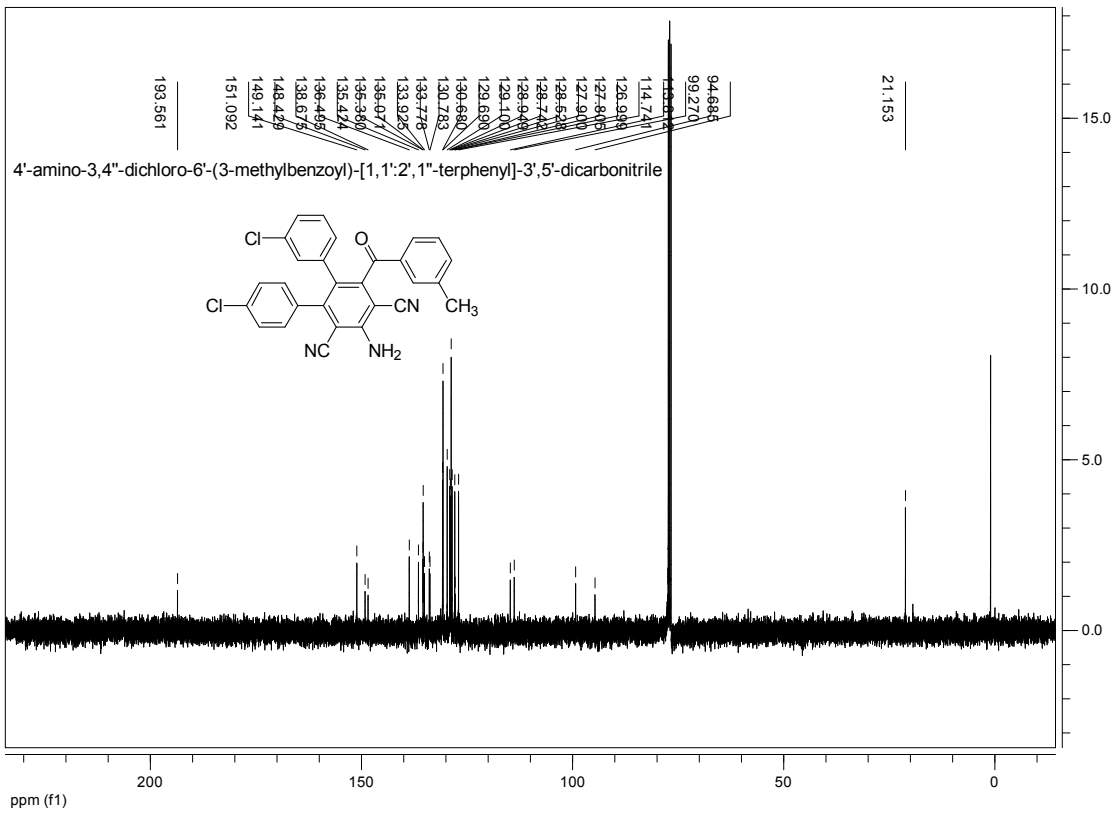


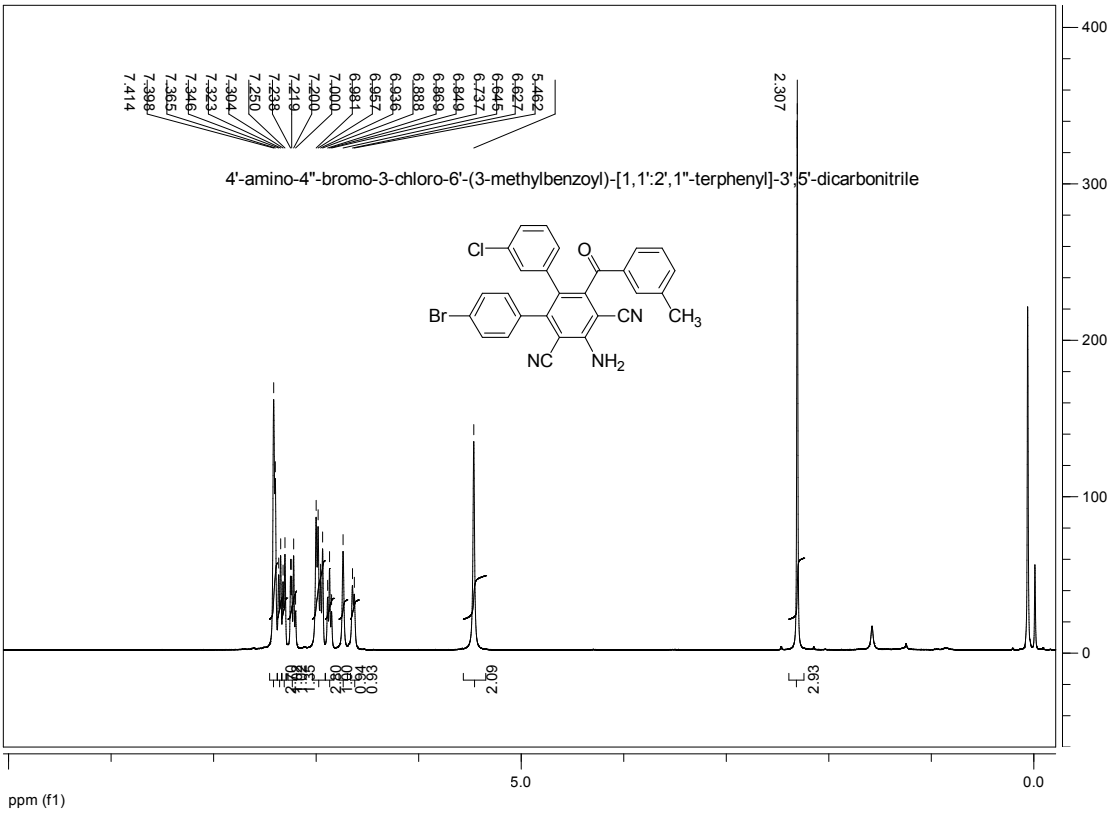


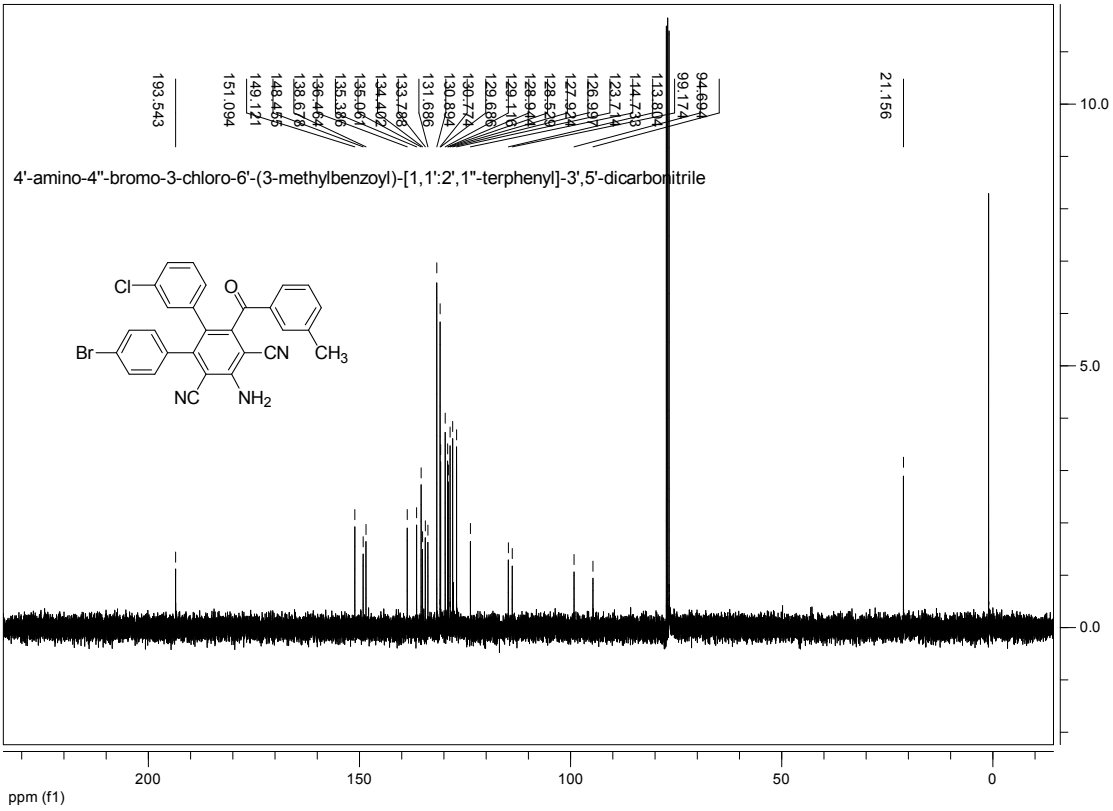
4'-amino-3,4''-dichloro-6'-(3-methylbenzoyl)-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3k**)



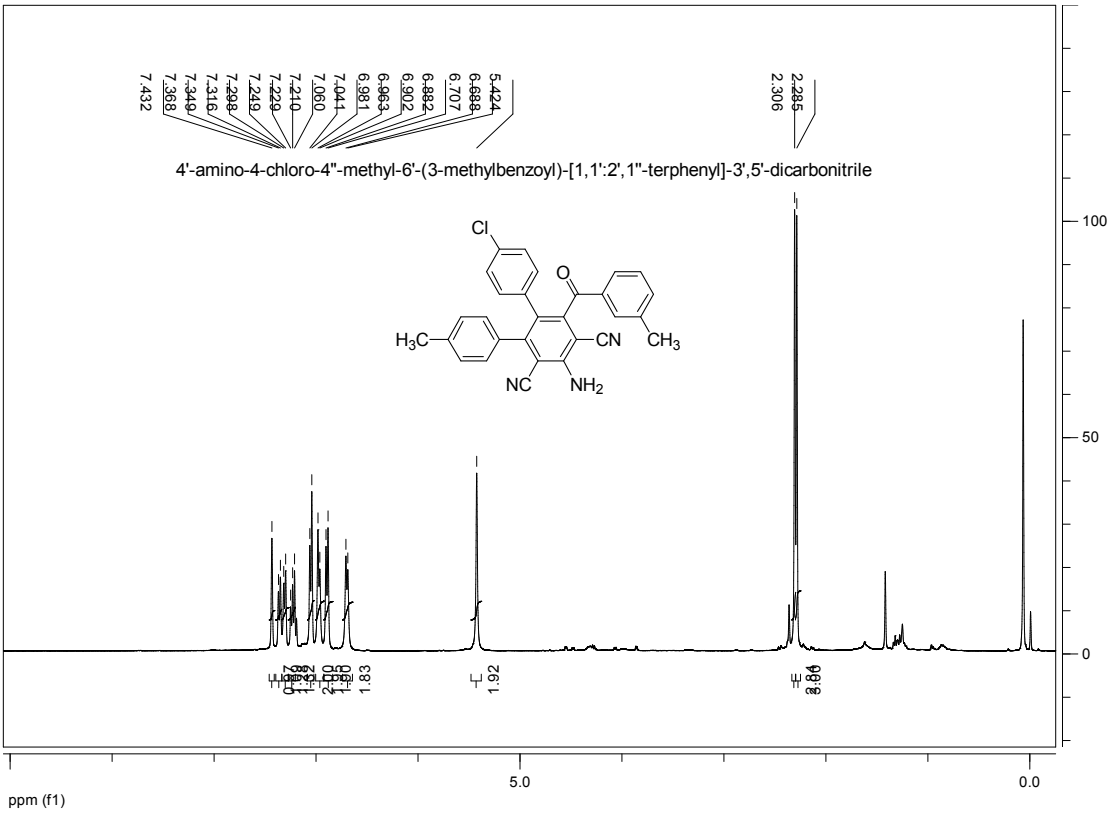


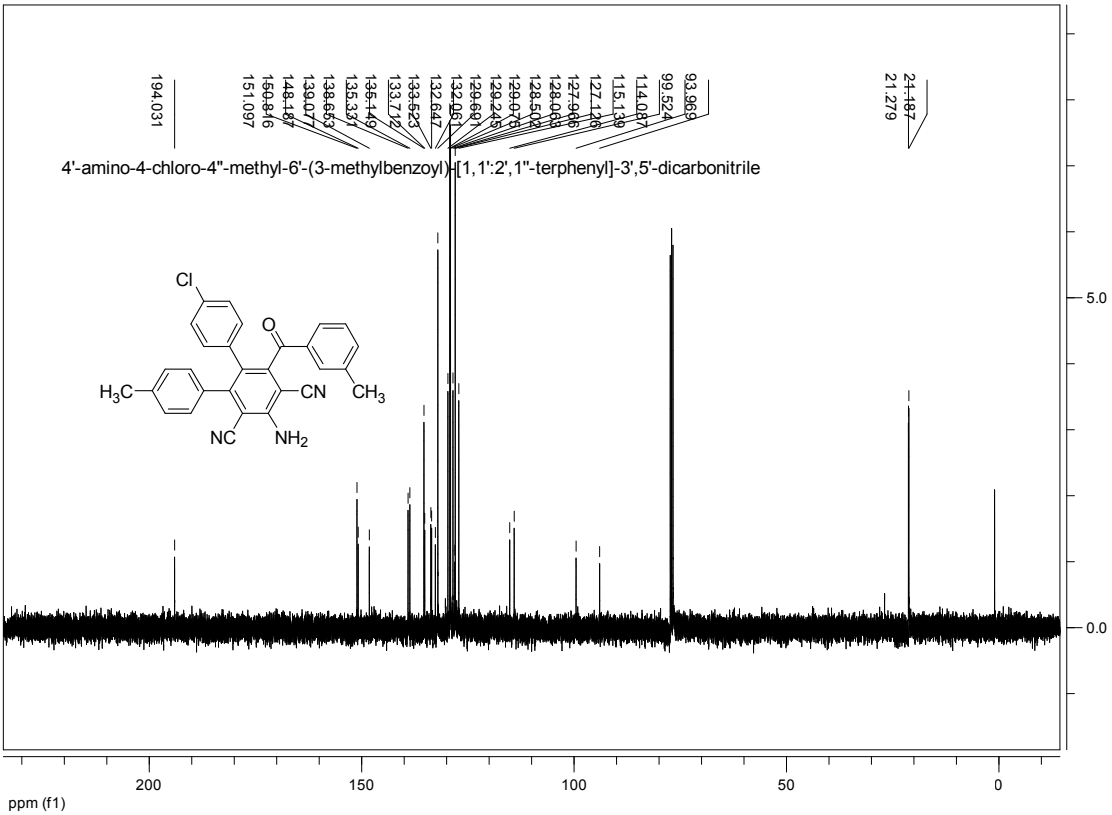
4'-amino-4''-bromo-3-chloro-6'-(3-methylbenzoyl)-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3l**)



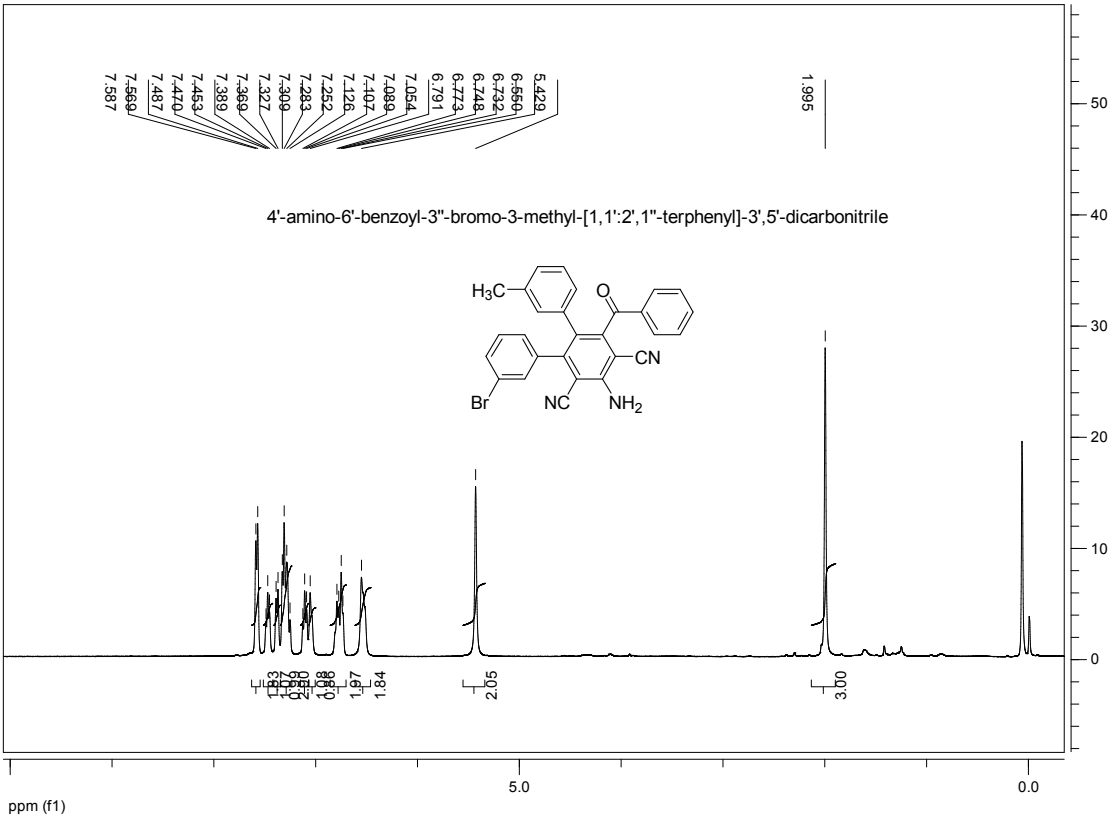


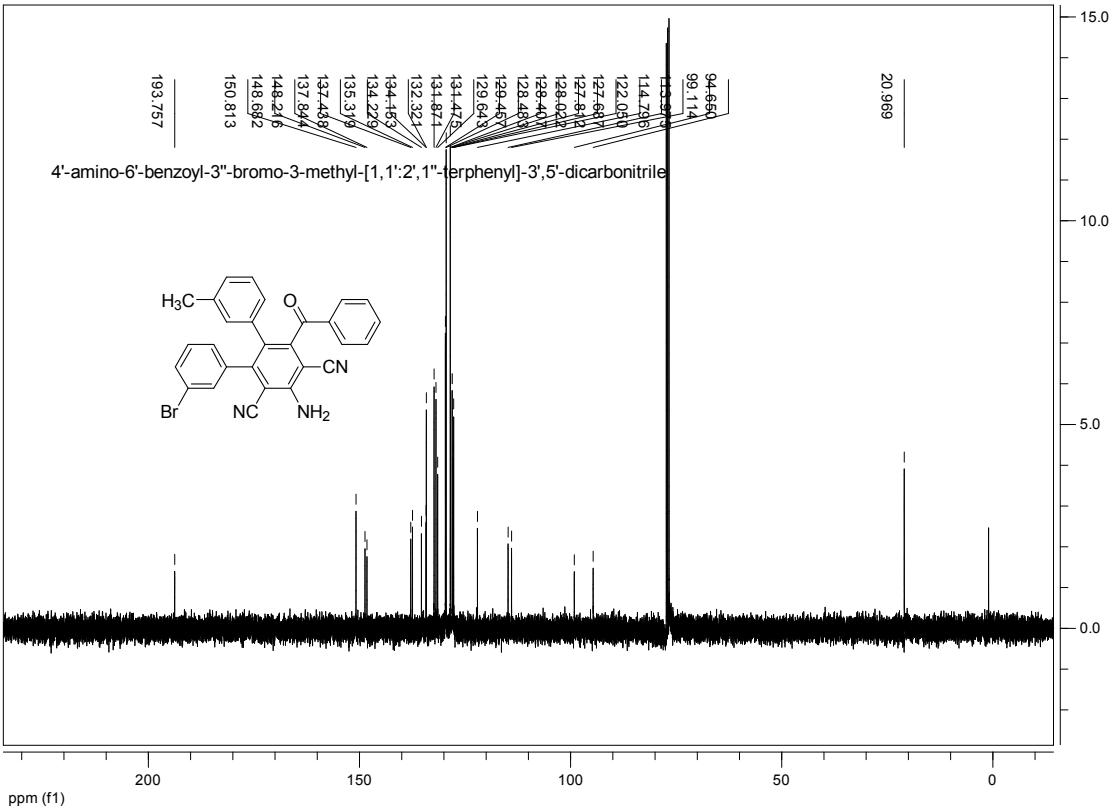
4'-amino-4-chloro-4''-methyl-6'-(3-methylbenzoyl)-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3m**)



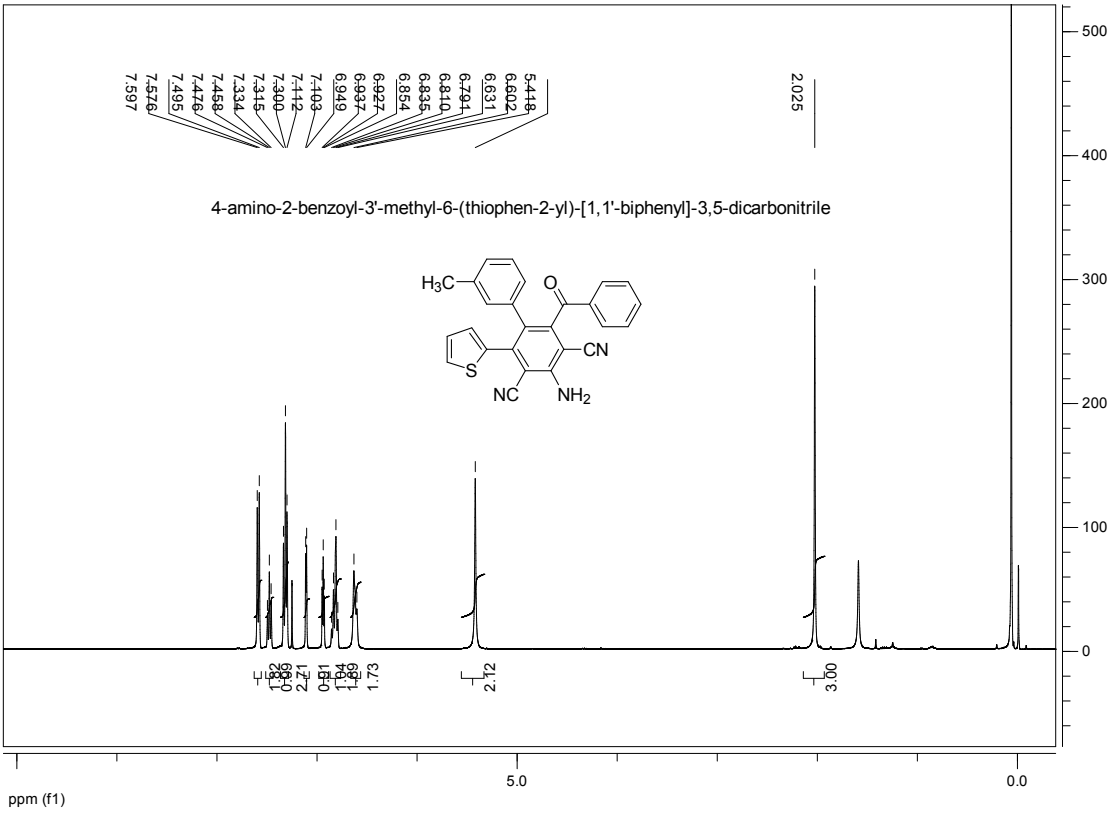


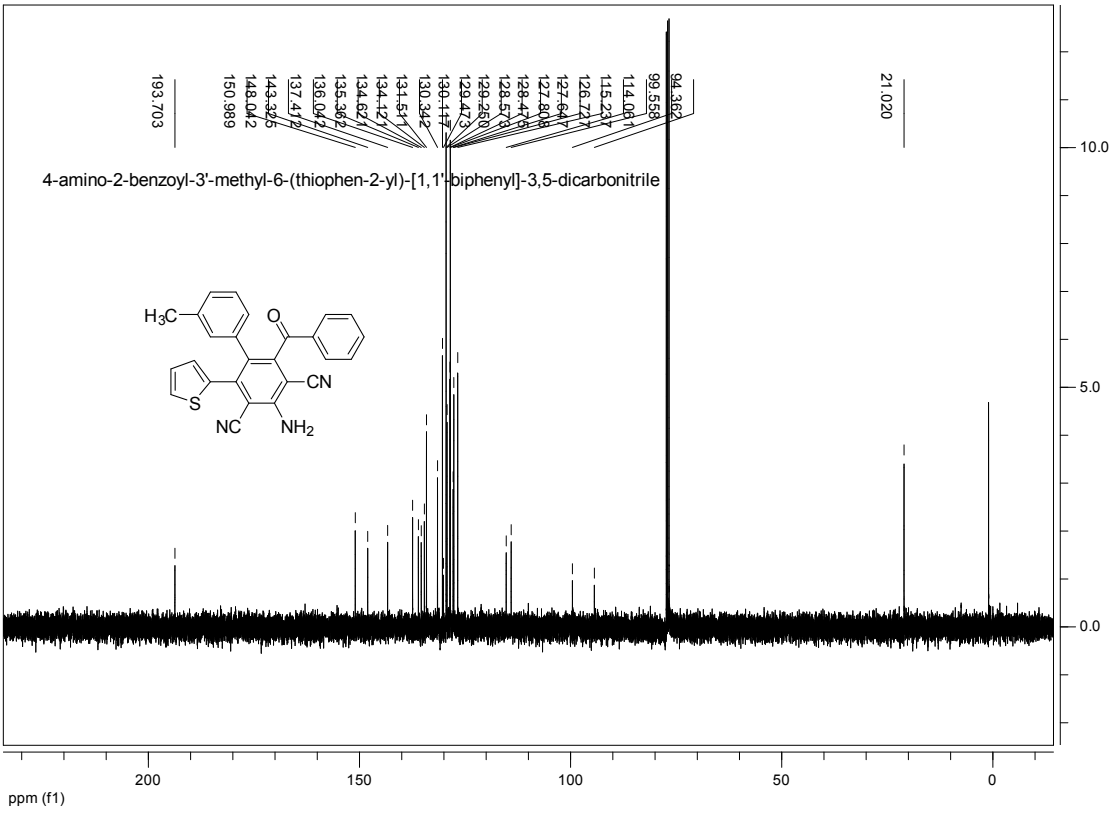
4'-amino-6'-benzoyl-3''-bromo-3-methyl-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3n**)



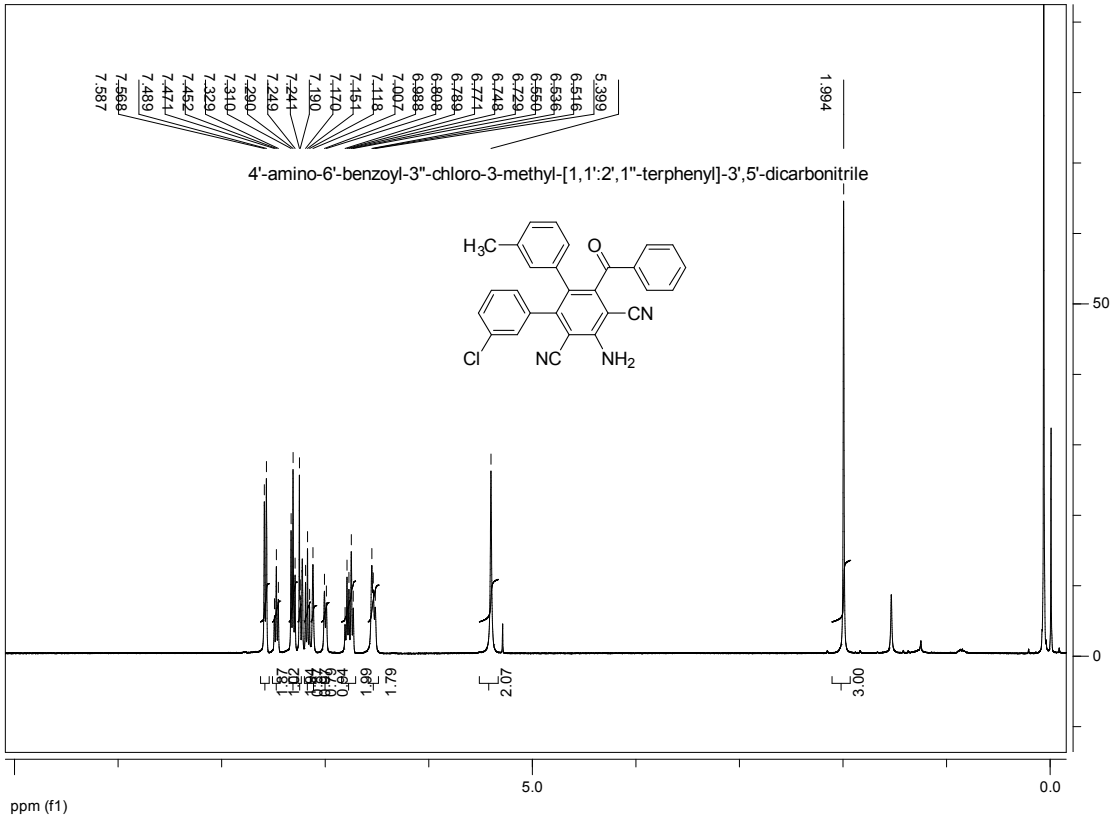


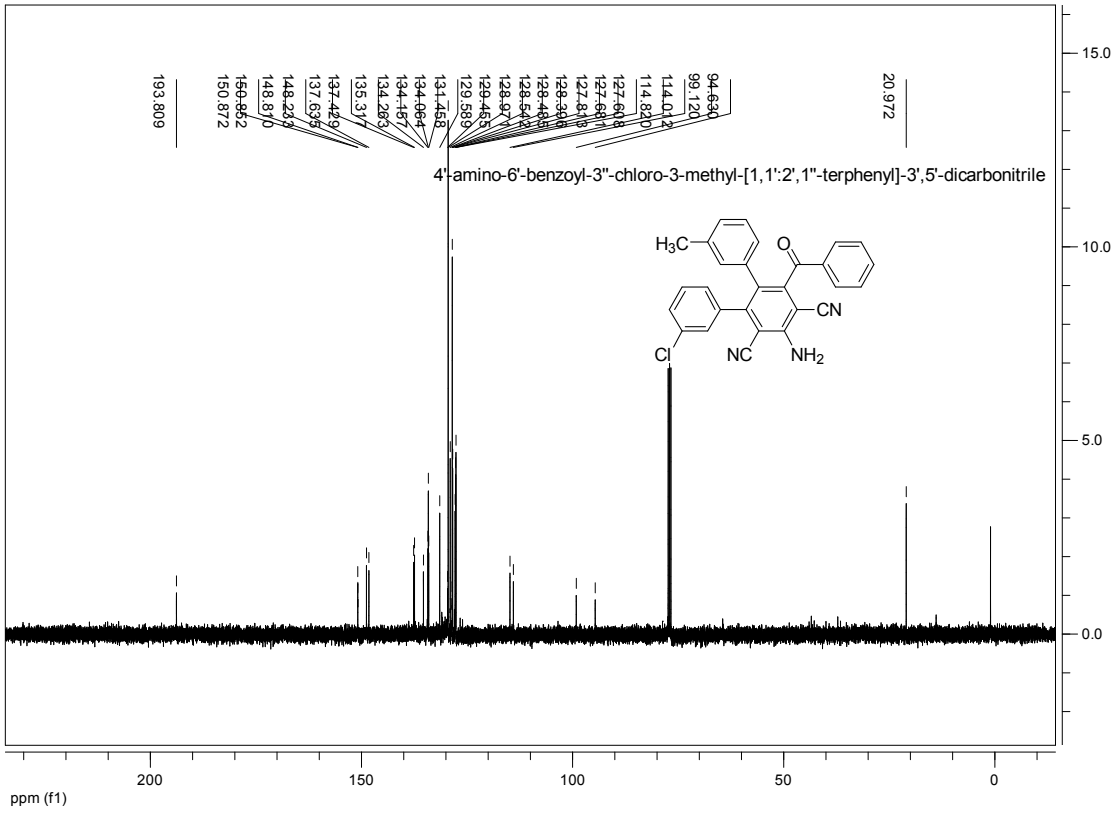
4-amino-2-benzoyl-3'-methyl-6-(thiophen-2-yl)-[1,1'-biphenyl]-3,5-dicarbonitrile(**3o**)



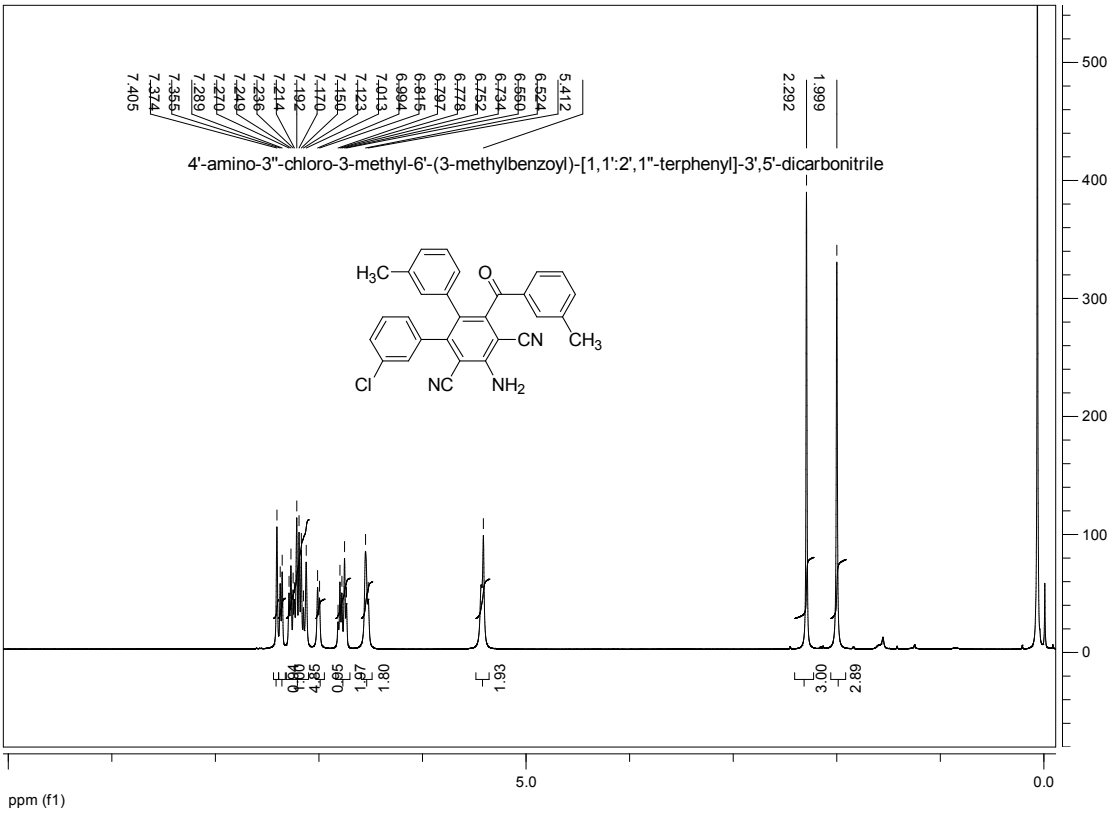


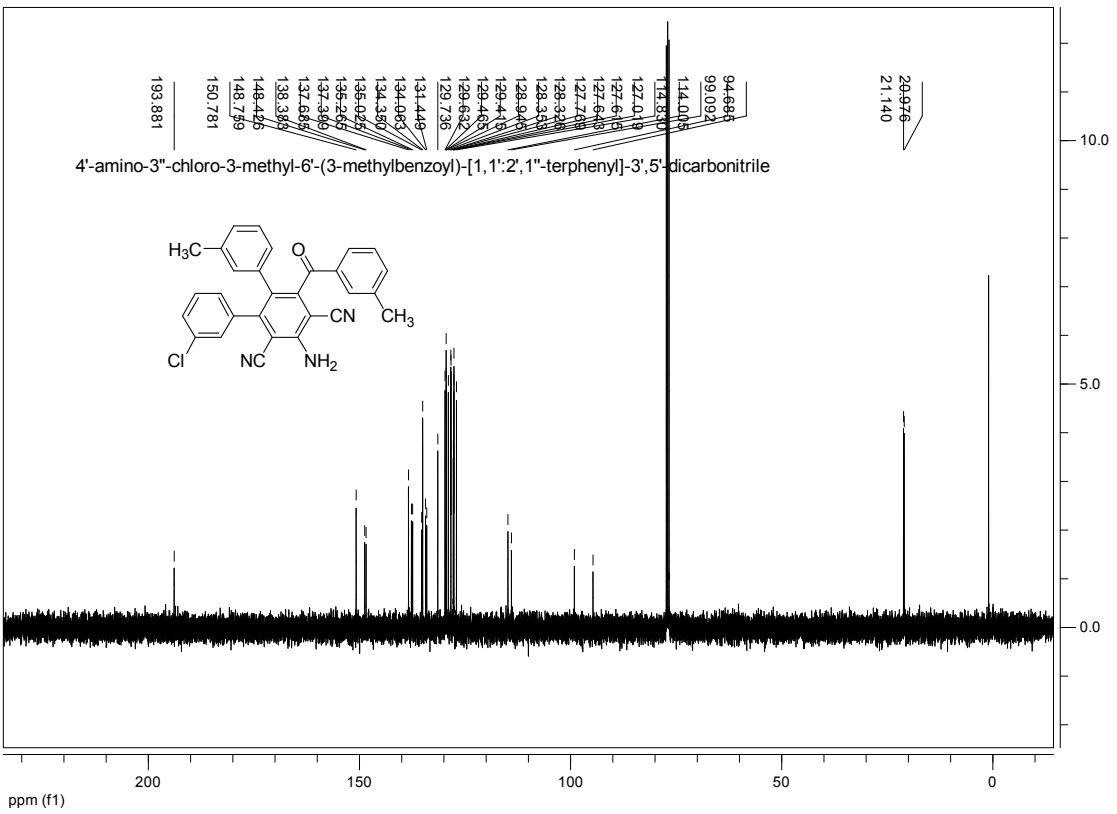
4'-amino-6'-benzoyl-3''-chloro-3-methyl-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile(**3p**)



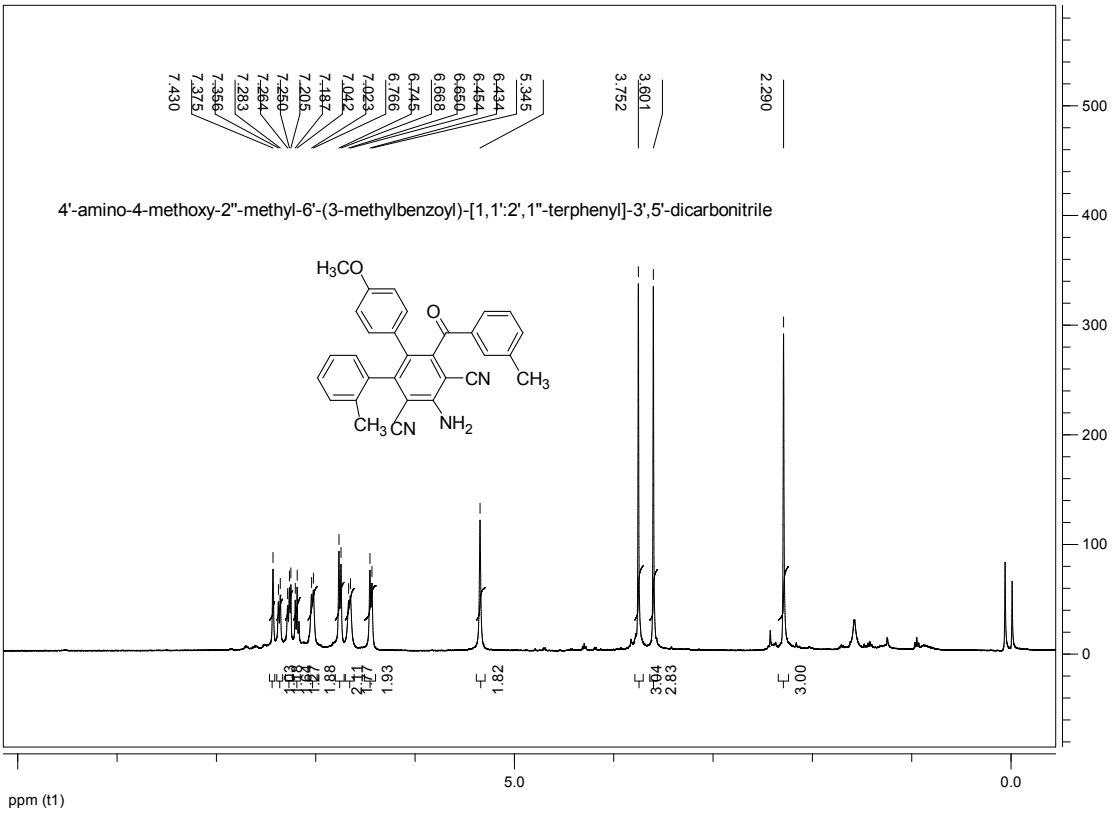


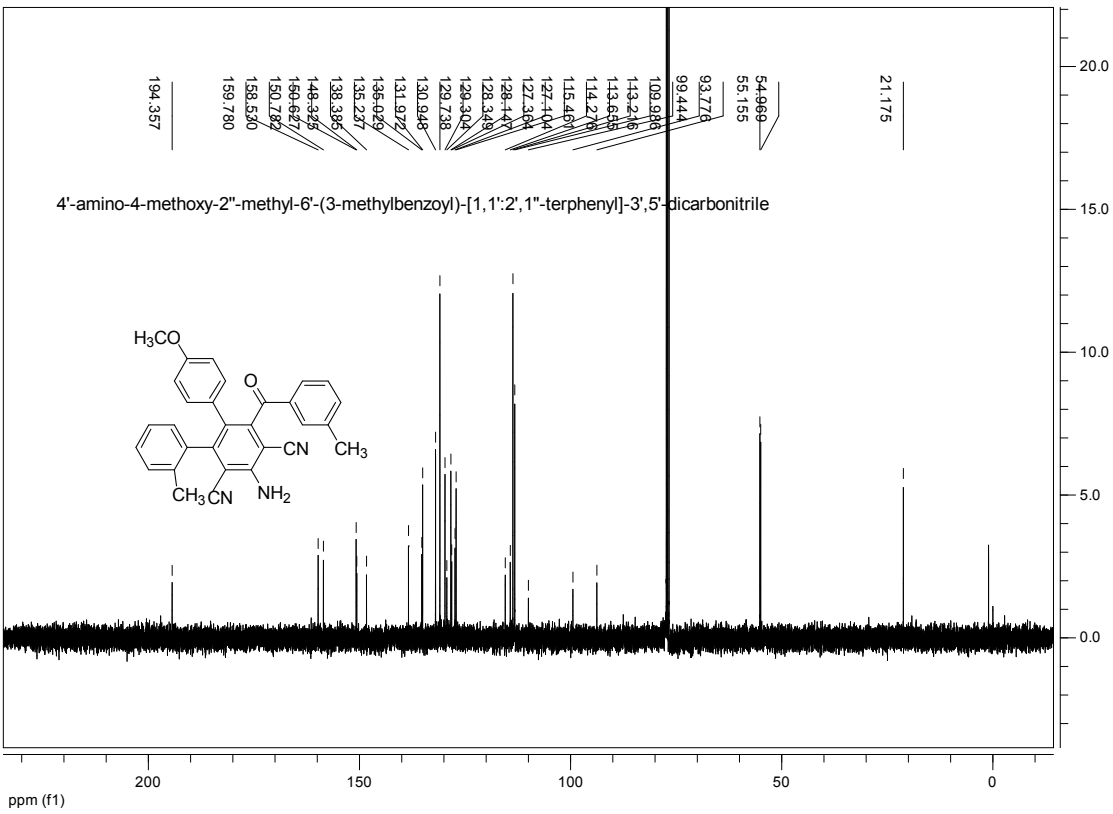
4'-amino-3"-chloro-3-methyl-6'-(3-methylbenzoyl)-[1,1':2',1"-terphenyl]-3',5'-dicarbonitrile(**3q**)



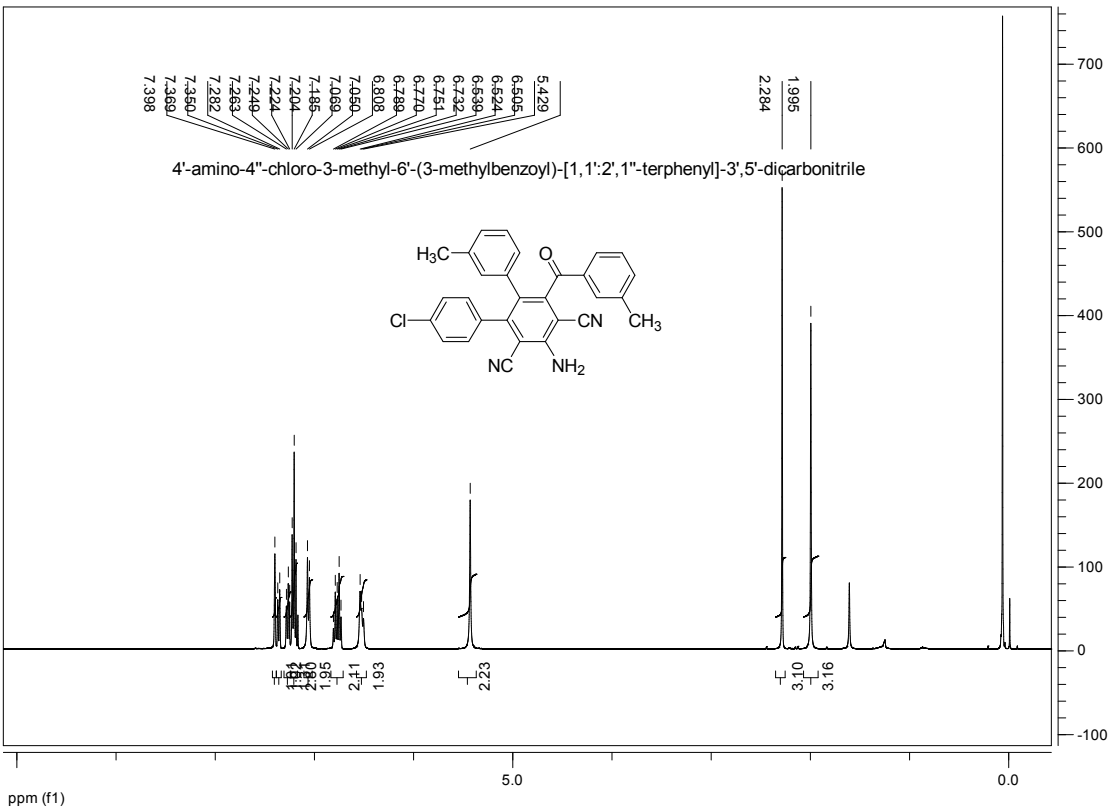


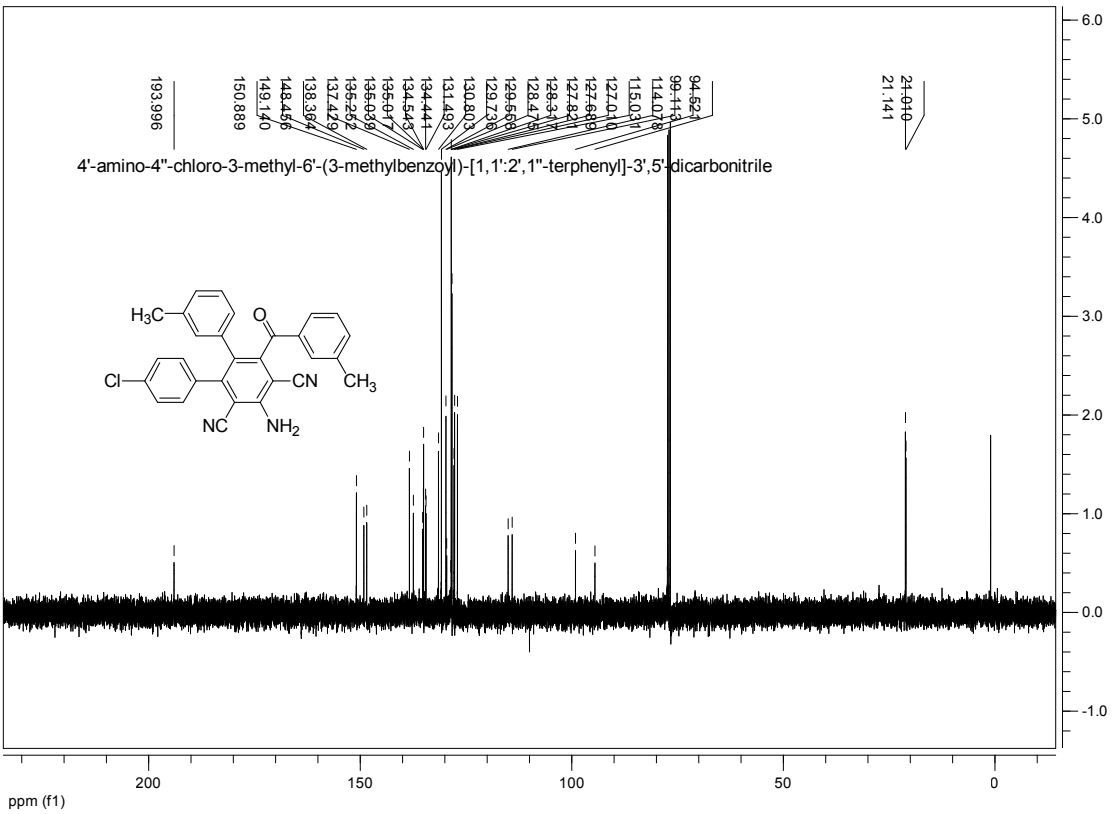
4'-amino-4-methoxy-2''-methyl-6'-(3-methylbenzoyl)-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3r**)



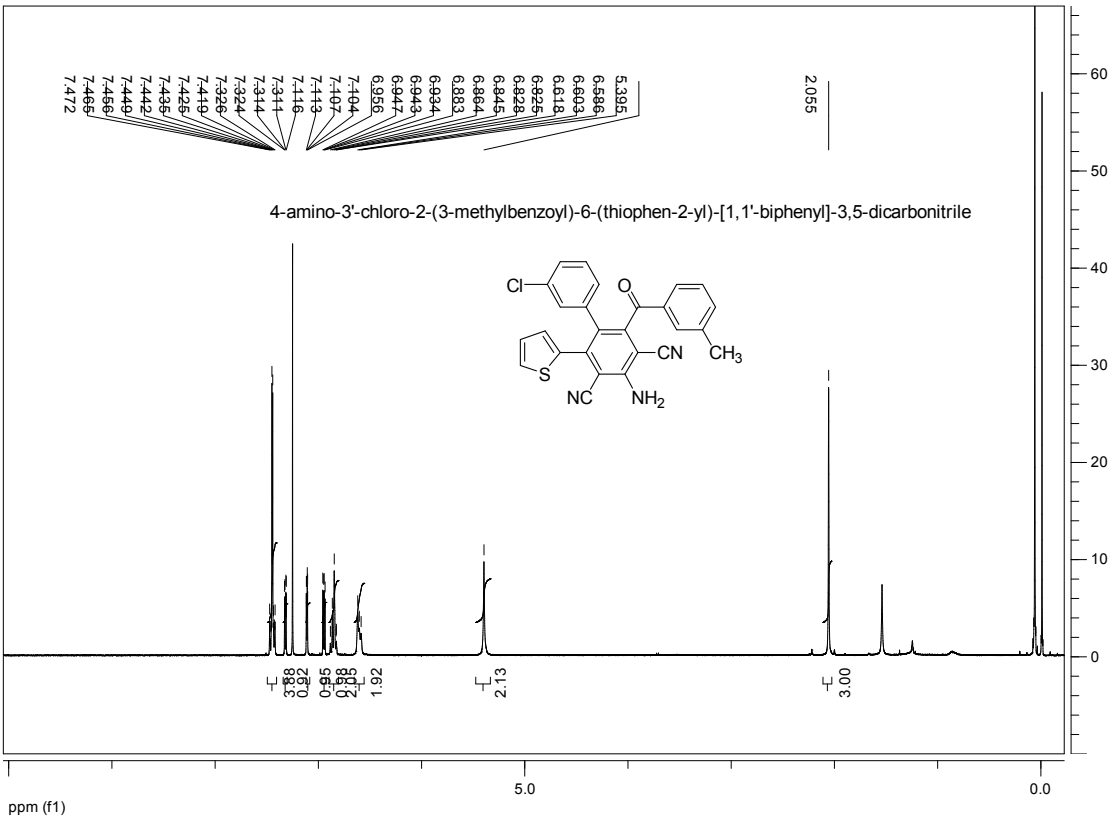


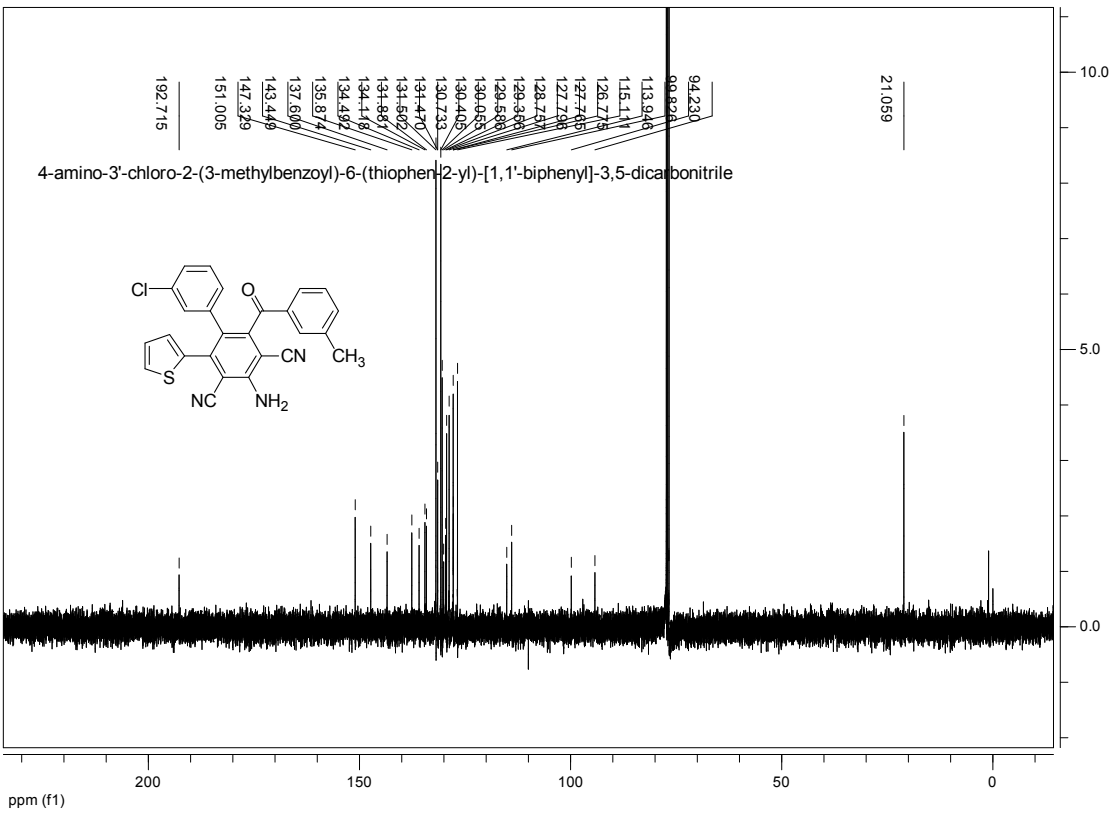
4'-amino-4''-chloro-3-methyl-6'-(3-methylbenzoyl)-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3s**)



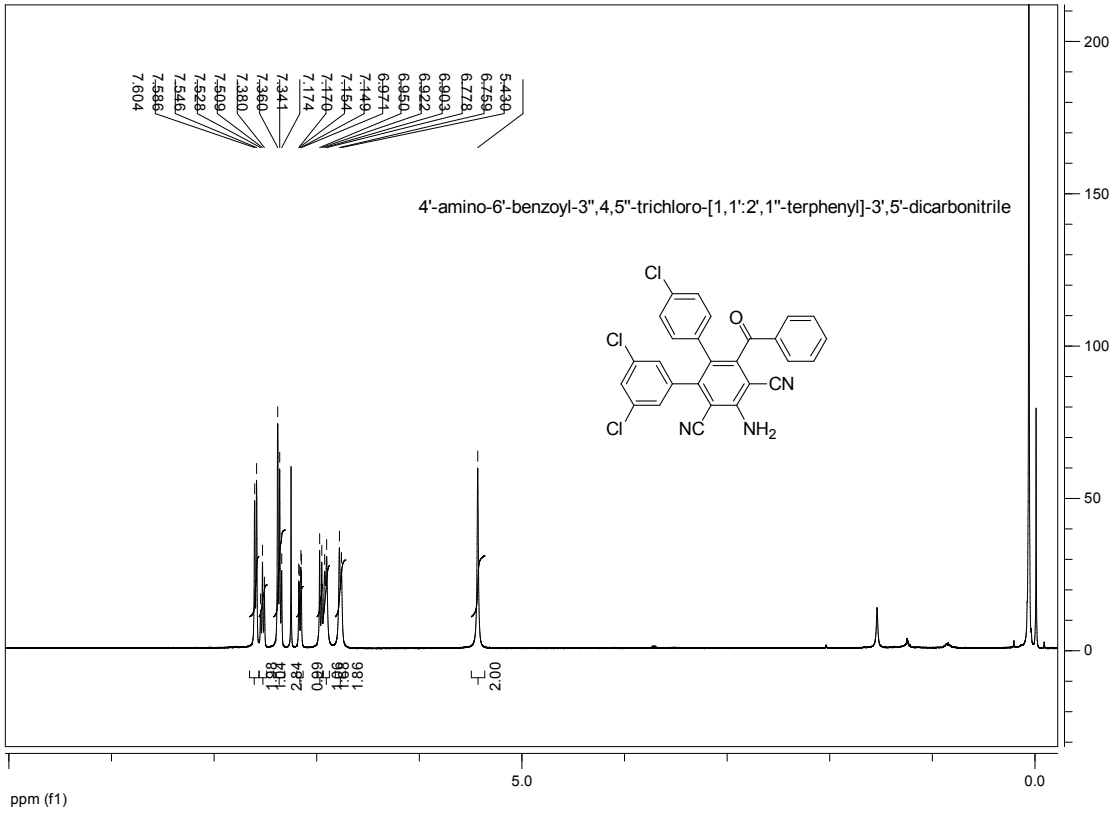


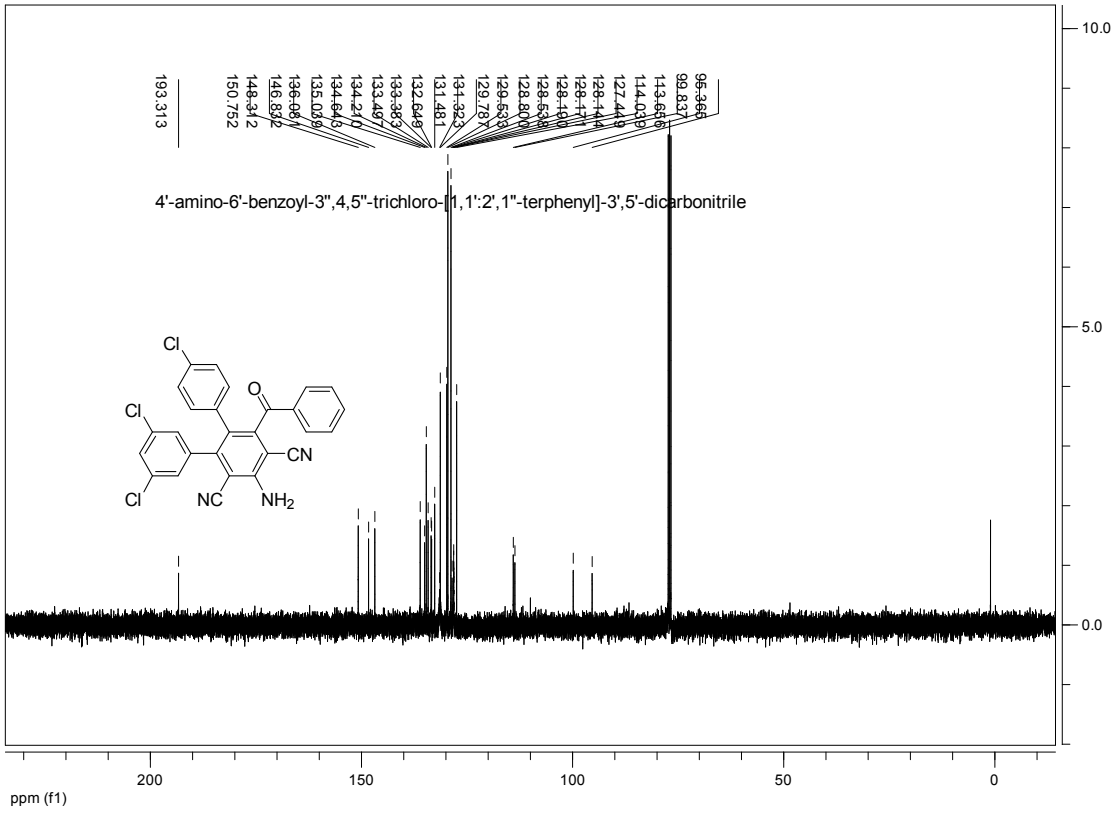
4-amino-3'-chloro-2-(3-methylbenzoyl)-6-(thiophen-2-yl)-[1,1'-biphenyl]-3,5-dicarbonitrile (**3t**)



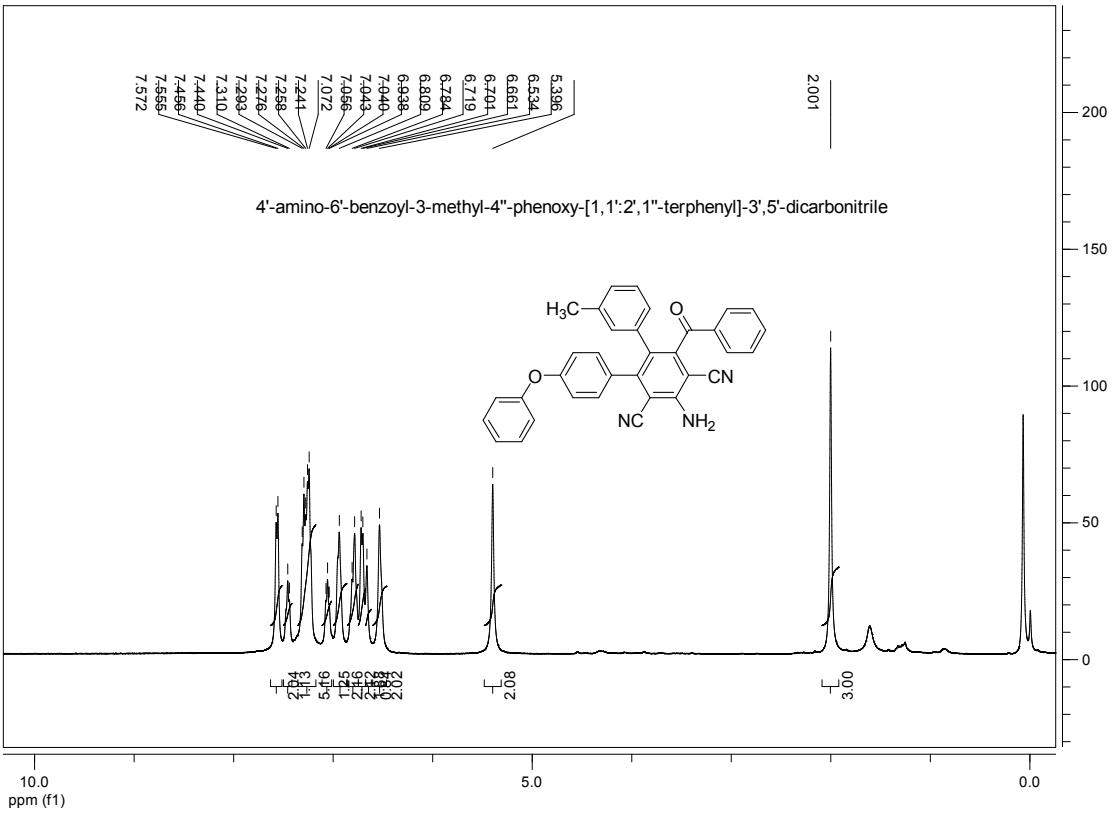


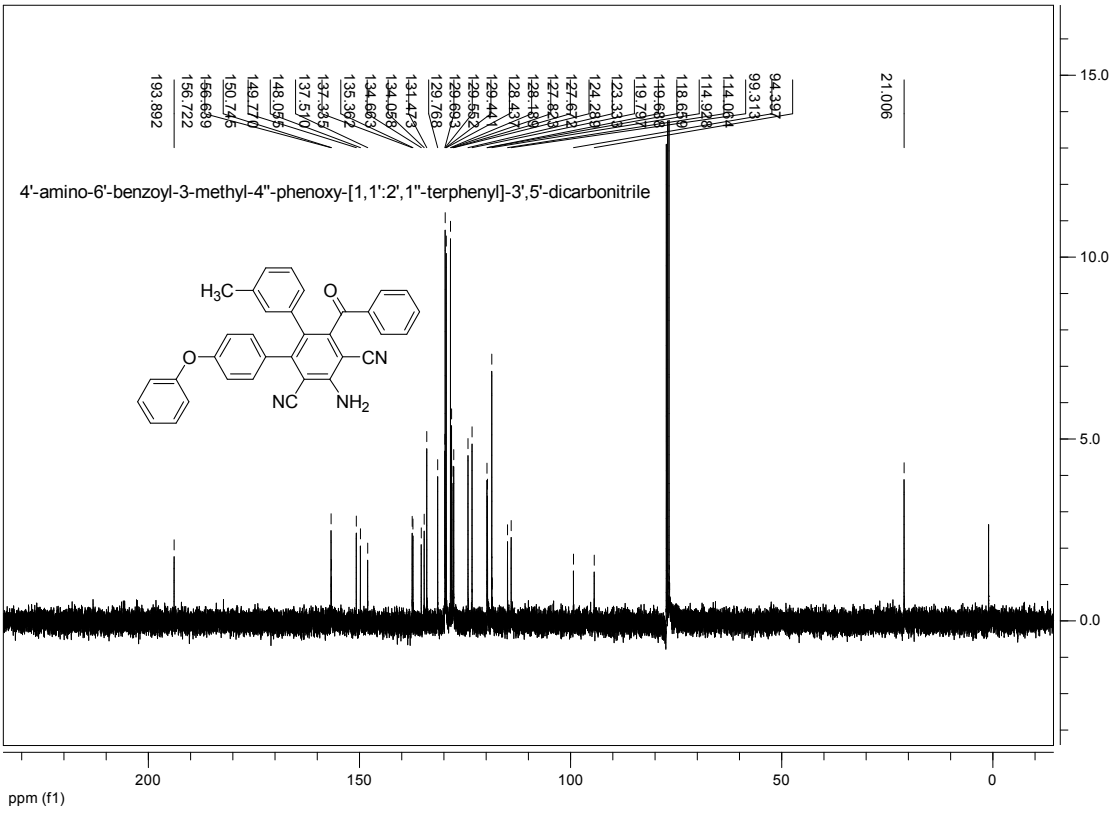
4'-amino-6'-benzoyl-3",4,5"-trichloro-[1,1':2',1"-terphenyl]-3',5'-dicarbonitrile (**3u**)



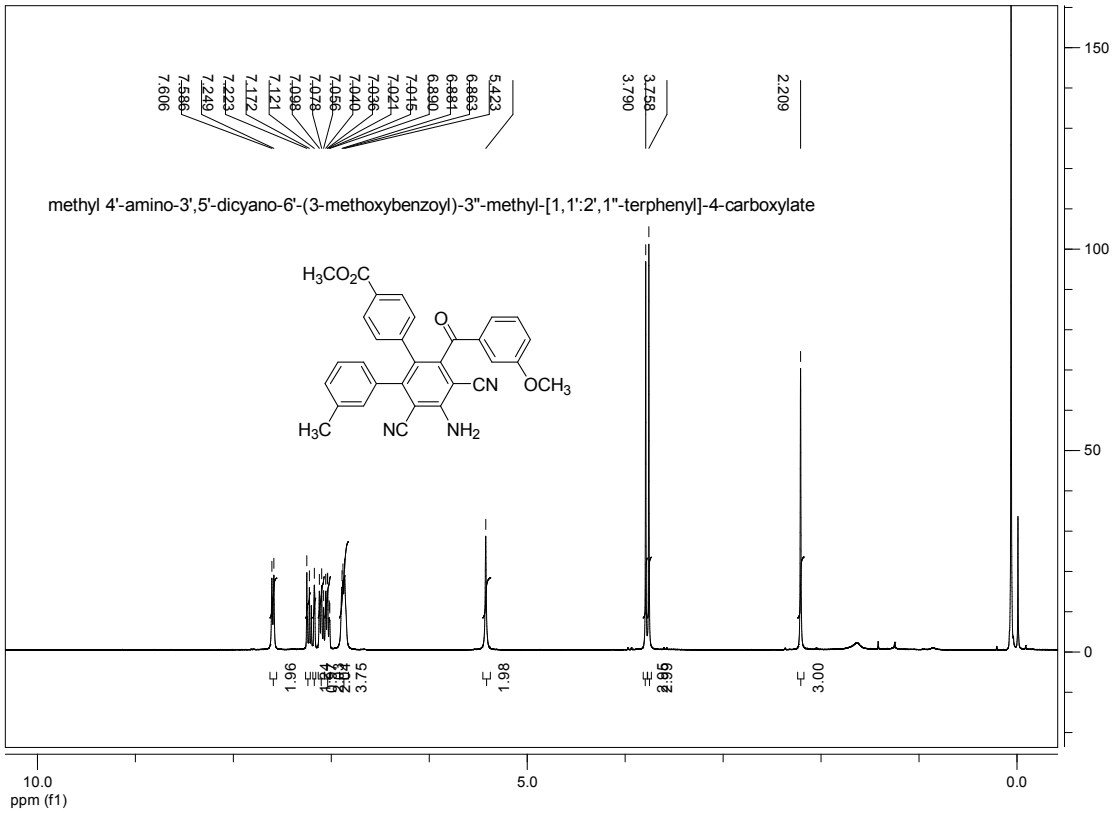


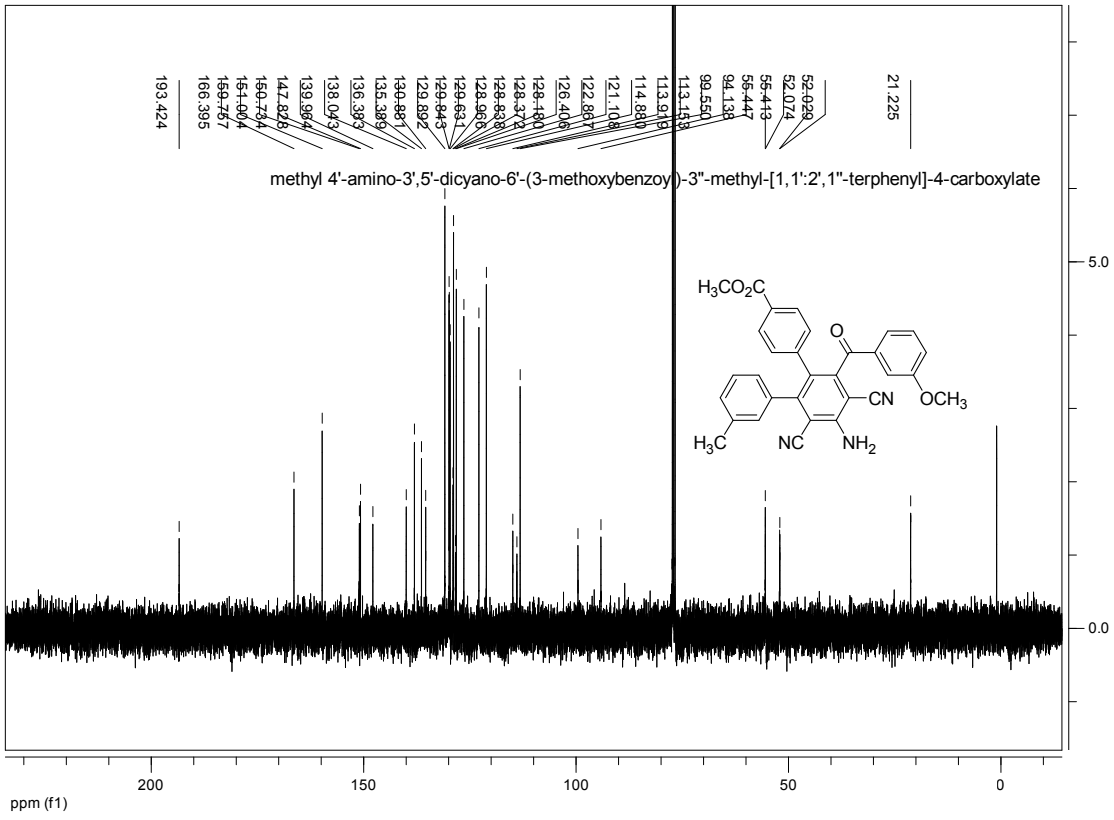
4'-amino-6'-benzoyl-3-methyl-4''-phenoxy-[1,1':2',1''-terphenyl]-3',5'-dicarbonitrile (**3v**)





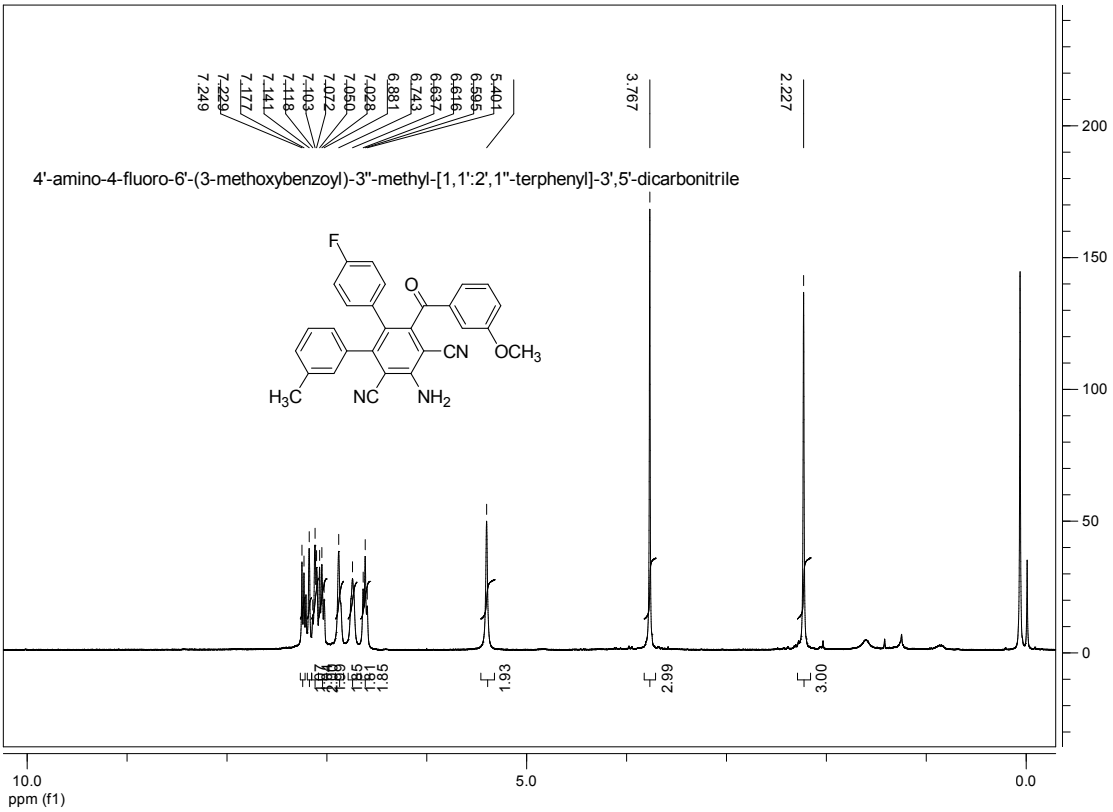
methyl 4'-amino-3',5'-dicyano-6'-(3-methoxybenzoyl)-3"-methyl-[1,1':2',1"-terphenyl]-4-carboxylate (**3w**)

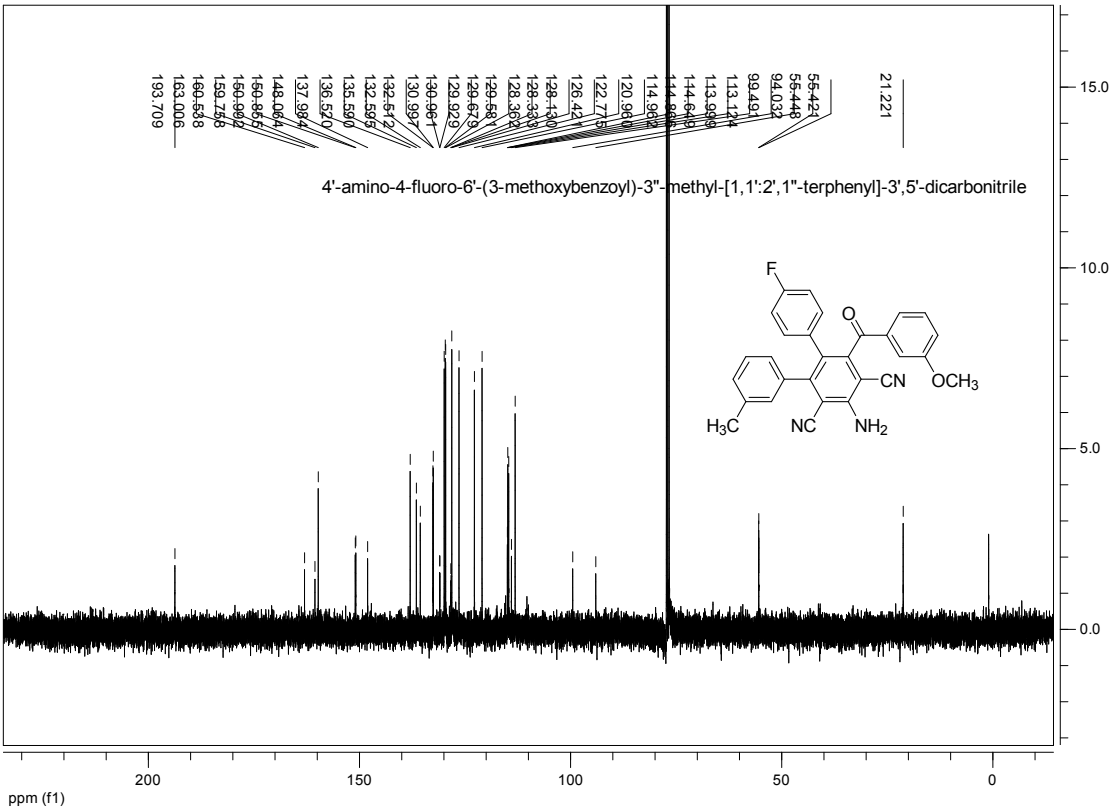




4'-amino-4-fluoro-6'-(3-methoxybenzoyl)-3"-methyl-[1,1':2',1"-terphenyl]-3',5'-

dicarbonitrile (**3x**)





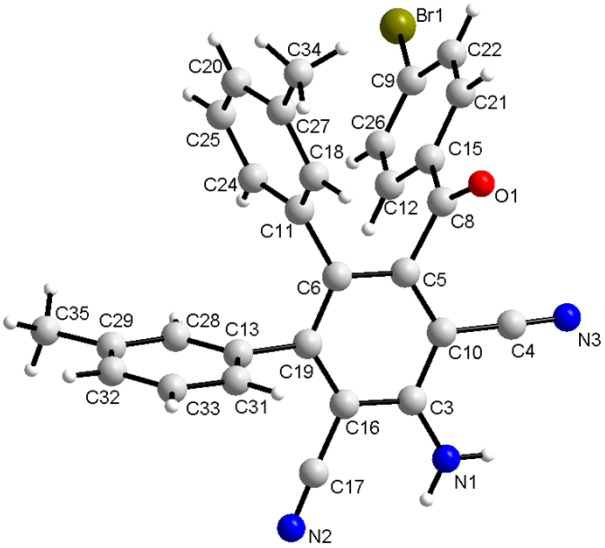


Table S1. Crystal data and structure refinement for **3b**.

Identification code	**3b**
Empirical formula	$C_{29}H_{20}BrN_3O$
Formula weight	506.38
Temperature	296 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.6727(5) A alpha = 90 deg. b = 21.9456(14) A beta = 94.984(2) deg. c = 12.5567(7) A gamma = 90 deg.
Volume	2380.9(2) A^3
Z, Calculated density	4, 1.413 Mg/m^3
Absorption coefficient	1.754 mm^-1
F(000)	1032
Crystal size	0.35 x 0.33 x 0.3 mm

Theta range for data collection	1.87 to 25.00 deg.
Limiting indices	-10<=h<=10, -26<=k<=21, -14<=l<=14
Reflections collected / unique	20655 / 4198 [R(int) = 0.0391]
Completeness to theta = 25.00	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4185 / 0 / 309
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1431
R indices (all data)	R1 = 0.0838, wR2 = 0.1590
Largest diff. peak and hole	1.135 and -0.490 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	900(1)	2688(1)	-2569(1)	76(1)
O(1)	5726(4)	4431(2)	793(2)	66(1)
C(3)	6099(5)	3137(2)	3528(3)	49(1)
C(4)	7097(5)	3157(2)	1756(3)	49(1)
C(5)	4871(4)	3780(2)	2109(3)	43(1)
C(6)	3764(4)	3997(2)	2764(3)	47(1)
N(1)	7164(5)	2717(2)	3878(3)	69(1)
C(8)	4882(5)	4013(2)	973(3)	47(1)
C(9)	2135(5)	3098(2)	-1472(3)	54(1)
C(10)	6003(4)	3364(2)	2474(3)	44(1)
C(11)	2540(5)	4426(2)	2308(3)	53(1)
C(12)	3052(6)	3183(2)	352(3)	61(1)
C(13)	2861(6)	4059(2)	4624(4)	59(1)
N(3)	7960(5)	3000(2)	1176(3)	63(1)
C(15)	3895(4)	3701(2)	130(3)	43(1)
C(16)	5030(5)	3389(2)	4204(3)	51(1)
C(17)	5151(6)	3205(2)	5309(4)	60(1)
C(18)	2855(5)	5034(2)	2198(3)	59(1)
C(19)	3888(5)	3806(2)	3836(3)	50(1)
C(20)	315(6)	5185(3)	1340(4)	71(1)
C(21)	3825(5)	3908(2)	-916(3)	57(1)
C(22)	2955(5)	3605(2)	-1714(3)	62(1)
N(2)	5282(6)	3058(2)	6181(3)	80(1)
C(24)	1092(5)	4207(2)	1923(4)	64(1)
C(25)	-19(6)	4589(3)	1446(4)	76(2)
C(26)	2164(6)	2884(2)	-453(4)	67(1)
C(27)	1708(7)	5431(2)	1699(4)	68(1)
C(28)	1323(6)	3891(2)	4601(4)	71(1)
C(29)	392(6)	4146(3)	5359(5)	82(2)
C(31)	3445(7)	4467(2)	5384(4)	76(2)
C(32)	1010(10)	4564(3)	6079(5)	96(2)

C(33)	2509(9)	4727(3)	6114(5)	94(2)
C(34)	2070(8)	6087(3)	1559(6)	100(2)
C(35)	-1197(8)	3975(4)	5372(6)	126(3)

Table S3. Bond lengths [A] and angles [deg] for **3b**.

Br(1)-C(9)	1.896(4)
O(1)-C(8)	1.206(5)
C(3)-N(1)	1.351(5)
C(3)-C(10)	1.410(5)
C(3)-C(16)	1.422(6)
C(4)-N(3)	1.141(5)
C(4)-C(10)	1.438(6)
C(5)-C(10)	1.389(5)
C(5)-C(6)	1.400(5)
C(5)-C(8)	1.517(5)
C(6)-C(19)	1.406(6)
C(6)-C(11)	1.497(6)
C(8)-C(15)	1.471(6)
C(9)-C(26)	1.362(6)
C(9)-C(22)	1.369(6)
C(11)-C(18)	1.371(6)
C(11)-C(24)	1.392(6)
C(12)-C(26)	1.382(6)
C(12)-C(15)	1.392(6)
C(13)-C(31)	1.373(7)
C(13)-C(28)	1.382(7)
C(13)-C(19)	1.495(6)
C(15)-C(21)	1.386(5)
C(16)-C(19)	1.397(6)
C(16)-C(17)	1.440(6)
C(17)-N(2)	1.137(6)
C(18)-C(27)	1.427(7)
C(20)-C(25)	1.348(8)
C(20)-C(27)	1.365(8)
C(21)-C(22)	1.373(6)
C(24)-C(25)	1.375(7)
C(27)-C(34)	1.486(7)
C(28)-C(29)	1.416(7)
C(29)-C(32)	1.364(9)
C(29)-C(35)	1.430(8)
C(31)-C(33)	1.398(7)
C(32)-C(33)	1.346(9)
N(1)-C(3)-C(10)	122.0(4)

N(1)-C(3)-C(16)	122.2(4)
C(10)-C(3)-C(16)	115.8(4)
N(3)-C(4)-C(10)	178.9(5)
C(10)-C(5)-C(6)	122.0(3)
C(10)-C(5)-C(8)	118.0(3)
C(6)-C(5)-C(8)	119.9(3)
C(5)-C(6)-C(19)	117.5(4)
C(5)-C(6)-C(11)	119.3(3)
C(19)-C(6)-C(11)	123.2(3)
O(1)-C(8)-C(15)	122.9(4)
O(1)-C(8)-C(5)	119.1(4)
C(15)-C(8)-C(5)	117.9(4)
C(26)-C(9)-C(22)	121.4(4)
C(26)-C(9)-Br(1)	118.8(4)
C(22)-C(9)-Br(1)	119.7(3)
C(5)-C(10)-C(3)	121.6(3)
C(5)-C(10)-C(4)	119.2(3)
C(3)-C(10)-C(4)	119.2(4)
C(18)-C(11)-C(24)	118.9(4)
C(18)-C(11)-C(6)	120.7(4)
C(24)-C(11)-C(6)	120.2(4)
C(26)-C(12)-C(15)	120.7(4)
C(31)-C(13)-C(28)	119.1(4)
C(31)-C(13)-C(19)	119.8(5)
C(28)-C(13)-C(19)	121.1(5)
C(21)-C(15)-C(12)	118.4(4)
C(21)-C(15)-C(8)	120.3(4)
C(12)-C(15)-C(8)	121.3(4)
C(19)-C(16)-C(3)	122.5(4)
C(19)-C(16)-C(17)	119.5(4)
C(3)-C(16)-C(17)	118.0(4)
N(2)-C(17)-C(16)	178.4(5)
C(11)-C(18)-C(27)	120.1(5)
C(16)-C(19)-C(6)	120.3(4)
C(16)-C(19)-C(13)	118.1(4)
C(6)-C(19)-C(13)	121.5(4)
C(25)-C(20)-C(27)	122.9(5)
C(22)-C(21)-C(15)	120.6(4)
C(9)-C(22)-C(21)	119.7(4)
C(25)-C(24)-C(11)	121.1(5)
C(20)-C(25)-C(24)	119.1(5)
C(9)-C(26)-C(12)	119.1(4)
C(20)-C(27)-C(18)	117.8(5)
C(20)-C(27)-C(34)	122.4(5)

C(18)-C(27)-C(34)	119.8(5)
C(13)-C(28)-C(29)	119.1(6)
C(32)-C(29)-C(28)	119.9(6)
C(32)-C(29)-C(35)	119.5(6)
C(28)-C(29)-C(35)	120.6(7)
C(13)-C(31)-C(33)	121.4(6)
C(33)-C(32)-C(29)	121.5(6)
C(32)-C(33)-C(31)	119.0(7)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **3b**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	82(1)	85(1)	61(1)	-20(1)	-5(1)	2(1)
O(1)	77(2)	64(2)	58(2)	12(2)	5(2)	-17(2)
C(3)	56(3)	45(2)	45(2)	1(2)	4(2)	4(2)
C(4)	53(3)	47(2)	45(2)	4(2)	0(2)	3(2)
C(5)	50(2)	42(2)	38(2)	0(2)	7(2)	-1(2)
C(6)	48(2)	48(2)	45(2)	6(2)	10(2)	7(2)
N(1)	86(3)	70(3)	51(2)	13(2)	12(2)	35(2)
C(8)	49(2)	44(2)	48(2)	5(2)	11(2)	6(2)
C(9)	57(3)	60(3)	44(2)	-5(2)	5(2)	6(2)
C(10)	49(2)	44(2)	39(2)	-1(2)	9(2)	1(2)
C(11)	64(3)	55(3)	42(2)	5(2)	18(2)	13(2)
C(12)	84(3)	60(3)	41(2)	7(2)	8(2)	-13(2)
C(13)	74(3)	53(3)	53(3)	19(2)	25(2)	18(2)
N(3)	65(2)	72(3)	55(2)	-1(2)	16(2)	16(2)
C(15)	45(2)	44(2)	43(2)	3(2)	11(2)	7(2)
C(16)	63(3)	50(2)	39(2)	7(2)	10(2)	5(2)
C(17)	76(3)	56(3)	49(3)	8(2)	16(2)	17(2)
C(18)	64(3)	61(3)	53(3)	5(2)	17(2)	12(2)
C(19)	57(3)	47(2)	46(2)	3(2)	14(2)	8(2)
C(20)	67(3)	99(4)	49(3)	5(3)	12(2)	29(3)
C(21)	60(3)	60(3)	50(3)	14(2)	10(2)	0(2)
C(22)	70(3)	78(3)	38(2)	11(2)	2(2)	3(3)
N(2)	110(4)	81(3)	50(3)	15(2)	19(2)	28(3)
C(24)	61(3)	77(3)	55(3)	5(2)	7(2)	14(3)
C(25)	71(3)	101(5)	55(3)	-4(3)	2(2)	11(3)
C(26)	85(4)	60(3)	57(3)	0(2)	9(2)	-19(3)
C(27)	94(4)	57(3)	58(3)	14(2)	34(3)	20(3)
C(28)	78(3)	78(3)	58(3)	21(3)	19(3)	24(3)
C(29)	65(3)	105(5)	81(4)	46(4)	39(3)	37(3)
C(31)	114(4)	55(3)	63(3)	5(2)	40(3)	7(3)

C(32)	149(7)	83(4)	62(4)	8(3)	45(4)	47(4)
C(33)	139(6)	72(4)	78(4)	15(3)	52(4)	21(4)
C(34)	111(5)	70(4)	124(5)	12(4)	37(4)	21(3)
C(35)	105(5)	151(7)	124(6)	4(5)	20(5)	9(5)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3b**.

	x	y	z	U(eq)
H(1A)	7809	2580	3454	82
H(1B)	7196	2587	4525	82
H(12)	3087	3037	1049	74
H(18)	3819	5187	2448	70
H(20)	-439	5439	1007	85
H(21)	4372	4256	-1079	68
H(22)	2923	3743	-2416	75
H(24)	872	3794	1990	77
H(25)	-987	4438	1200	91
H(26)	1595	2541	-300	81
H(28)	905	3614	4095	85
H(31)	4486	4572	5413	91
H(32)	380	4740	6558	115
H(33)	2917	5008	6616	113
H(34A)	2634	6137	940	150
H(34B)	2685	6232	2180	150
H(34C)	1124	6315	1467	150
H(35A)	-1265	3599	5757	189
H(35B)	-1646	3922	4652	189
H(35C)	-1746	4288	5716	189

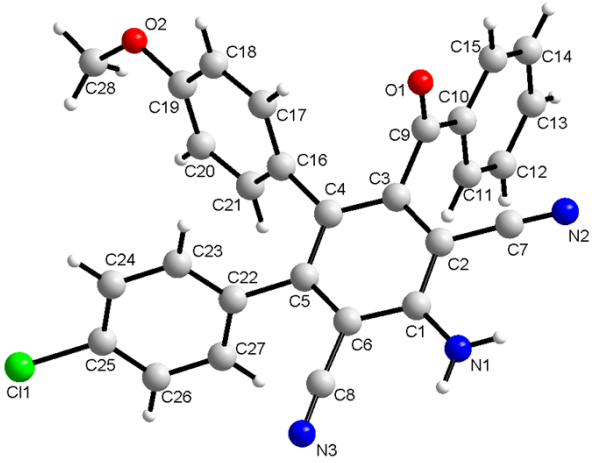


Table S6. Crystal data and structure refinement for **3i**.

Identification code	**3i**
Empirical formula	$C_{28}H_{18}ClN_3O_2$
Formula weight	463.90
Temperature	296 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.579(3) A alpha = 90 deg. b = 12.312(3) A beta = 107.948(10) deg. c = 17.454(4) A gamma = 90 deg.
Volume	2367.0(11) A^3
Z, Calculated density	4, 1.302 Mg/m^3
Absorption coefficient	0.192 mm^-1
F(000)	960
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	2.06 to 27.45 deg.

Limiting indices	-12<=h<=15, -12<=k<=15, -18<=l<=22
Reflections collected / unique	11690 / 5391 [R(int) = 0.0319]
Completeness to theta = 27.45	97.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5233 / 0 / 308
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1166
R indices (all data)	R1 = 0.0785, wR2 = 0.1299
Largest diff. peak and hole	0.226 and -0.353 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3i**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	4410(1)	11169(1)	1104(1)	95(1)
C(3)	9038(1)	6153(1)	3039(1)	33(1)
C(22)	7229(2)	8751(1)	2449(1)	34(1)
C(4)	8195(1)	6894(1)	2572(1)	33(1)
C(16)	7382(2)	6629(1)	1744(1)	35(1)
C(10)	8544(1)	4102(1)	2892(1)	35(1)
N(1)	10501(2)	7713(1)	4890(1)	60(1)
C(2)	9787(2)	6417(1)	3812(1)	37(1)
O(1)	9941(1)	4954(1)	2344(1)	61(1)
C(5)	8133(1)	7924(1)	2901(1)	33(1)
C(9)	9216(2)	5044(1)	2716(1)	37(1)
C(11)	7711(2)	4218(1)	3315(1)	42(1)
O(2)	5183(2)	6215(1)	-629(1)	74(1)
C(27)	6336(2)	9110(1)	2770(1)	42(1)
C(14)	8169(2)	2182(2)	2806(1)	60(1)
C(6)	8911(2)	8194(1)	3668(1)	35(1)
N(3)	8922(2)	10125(1)	4235(1)	58(1)
C(21)	6126(2)	6666(1)	1565(1)	40(1)
C(1)	9754(2)	7449(1)	4149(1)	39(1)
C(23)	7252(2)	9153(2)	1712(1)	44(1)
C(8)	8899(2)	9279(1)	3969(1)	41(1)
C(25)	5508(2)	10240(2)	1629(1)	53(1)
N(2)	11334(2)	5040(2)	4669(1)	70(1)
C(26)	5473(2)	9855(2)	2356(1)	50(1)
C(7)	10644(2)	5639(2)	4281(1)	46(1)
C(20)	5355(2)	6529(2)	783(1)	47(1)
C(15)	8774(2)	3072(1)	2641(1)	49(1)
C(13)	7330(2)	2309(2)	3214(1)	58(1)
C(17)	7851(2)	6425(2)	1114(1)	51(1)
C(19)	5843(2)	6355(2)	167(1)	51(1)
C(12)	7098(2)	3314(2)	3470(1)	54(1)

C(24)	6391(2)	9902(2)	1297(1)	55(1)
C(18)	7091(2)	6294(2)	338(1)	62(1)
C(28)	3923(2)	6423(2)	-867(2)	88(1)

Table S8. Bond lengths [A] and angles [deg] for **3i**.

Cl(1)-C(25)	1.746(2)
C(3)-C(2)	1.400(2)
C(3)-C(4)	1.399(2)
C(3)-C(9)	1.515(2)
C(22)-C(23)	1.386(2)
C(22)-C(27)	1.391(2)
C(22)-C(5)	1.498(2)
C(4)-C(5)	1.404(2)
C(4)-C(16)	1.498(2)
C(16)-C(17)	1.390(2)
C(16)-C(21)	1.392(2)
C(10)-C(11)	1.390(2)
C(10)-C(15)	1.394(2)
C(10)-C(9)	1.481(2)
N(1)-C(1)	1.355(2)
C(2)-C(1)	1.406(2)
C(2)-C(7)	1.438(2)
O(1)-C(9)	1.215(2)
C(5)-C(6)	1.404(2)
C(11)-C(12)	1.391(3)
O(2)-C(19)	1.375(2)
O(2)-C(28)	1.413(3)
C(27)-C(26)	1.384(3)
C(14)-C(15)	1.378(3)
C(14)-C(13)	1.380(3)
C(6)-C(1)	1.412(2)
C(6)-C(8)	1.437(2)
N(3)-C(8)	1.137(2)
C(21)-C(20)	1.392(2)
C(23)-C(24)	1.387(3)
C(25)-C(26)	1.366(3)
C(25)-C(24)	1.386(3)
N(2)-C(7)	1.144(2)
C(20)-C(19)	1.376(3)
C(13)-C(12)	1.370(3)
C(17)-C(18)	1.379(3)
C(19)-C(18)	1.384(3)
C(2)-C(3)-C(4)	121.61(14)

C(2)-C(3)-C(9)	116.92(14)
C(4)-C(3)-C(9)	121.42(14)
C(23)-C(22)-C(27)	119.29(16)
C(23)-C(22)-C(5)	121.45(15)
C(27)-C(22)-C(5)	119.25(15)
C(3)-C(4)-C(5)	117.75(14)
C(3)-C(4)-C(16)	122.54(14)
C(5)-C(4)-C(16)	119.71(14)
C(17)-C(16)-C(21)	117.69(16)
C(17)-C(16)-C(4)	121.34(15)
C(21)-C(16)-C(4)	120.76(15)
C(11)-C(10)-C(15)	119.44(17)
C(11)-C(10)-C(9)	121.68(15)
C(15)-C(10)-C(9)	118.87(16)
C(3)-C(2)-C(1)	121.63(15)
C(3)-C(2)-C(7)	120.51(15)
C(1)-C(2)-C(7)	117.84(15)
C(6)-C(5)-C(4)	120.35(15)
C(6)-C(5)-C(22)	118.69(14)
C(4)-C(5)-C(22)	120.95(14)
O(1)-C(9)-C(10)	122.25(15)
O(1)-C(9)-C(3)	118.50(15)
C(10)-C(9)-C(3)	119.20(14)
C(12)-C(11)-C(10)	120.00(17)
C(19)-O(2)-C(28)	118.45(19)
C(26)-C(27)-C(22)	120.47(17)
C(15)-C(14)-C(13)	120.14(18)
C(5)-C(6)-C(1)	122.42(14)
C(5)-C(6)-C(8)	119.56(15)
C(1)-C(6)-C(8)	117.96(15)
C(20)-C(21)-C(16)	121.69(16)
N(1)-C(1)-C(2)	121.60(16)
N(1)-C(1)-C(6)	122.20(15)
C(2)-C(1)-C(6)	116.20(15)
C(24)-C(23)-C(22)	120.35(18)
N(3)-C(8)-C(6)	177.34(19)
C(26)-C(25)-C(24)	121.37(18)
C(26)-C(25)-Cl(1)	119.38(17)
C(24)-C(25)-Cl(1)	119.25(17)
C(25)-C(26)-C(27)	119.44(18)
N(2)-C(7)-C(2)	178.2(2)
C(19)-C(20)-C(21)	119.43(18)
C(14)-C(15)-C(10)	119.92(19)
C(12)-C(13)-C(14)	120.69(19)

C(18)-C(17)-C(16)	120.76(18)
O(2)-C(19)-C(20)	125.08(19)
O(2)-C(19)-C(18)	115.36(18)
C(20)-C(19)-C(18)	119.55(17)
C(13)-C(12)-C(11)	119.8(2)
C(23)-C(24)-C(25)	119.09(19)
C(17)-C(18)-C(19)	120.84(18)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for **3i**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	64(1)	75(1)	136(1)	50(1)	15(1)	22(1)
C(3)	37(1)	29(1)	36(1)	-4(1)	14(1)	-3(1)
C(22)	39(1)	26(1)	35(1)	-4(1)	8(1)	-3(1)
C(4)	36(1)	30(1)	33(1)	-3(1)	12(1)	-4(1)
C(16)	41(1)	29(1)	34(1)	-5(1)	11(1)	-2(1)
C(10)	34(1)	30(1)	35(1)	-4(1)	3(1)	3(1)
N(1)	75(1)	41(1)	45(1)	-13(1)	-10(1)	10(1)
C(2)	41(1)	31(1)	36(1)	-3(1)	9(1)	1(1)
O(1)	72(1)	48(1)	82(1)	-12(1)	49(1)	-1(1)
C(5)	38(1)	29(1)	33(1)	0(1)	13(1)	-3(1)
C(9)	39(1)	34(1)	36(1)	-6(1)	10(1)	3(1)
C(11)	43(1)	34(1)	49(1)	-3(1)	12(1)	4(1)
O(2)	85(1)	80(1)	39(1)	-9(1)	-6(1)	-1(1)
C(27)	48(1)	37(1)	40(1)	-6(1)	12(1)	1(1)
C(14)	71(1)	28(1)	73(1)	-9(1)	12(1)	2(1)
C(6)	42(1)	28(1)	35(1)	-4(1)	11(1)	-3(1)
N(3)	74(1)	35(1)	51(1)	-10(1)	0(1)	2(1)
C(21)	45(1)	36(1)	40(1)	-5(1)	15(1)	-6(1)
C(1)	44(1)	35(1)	35(1)	-5(1)	8(1)	-3(1)
C(23)	46(1)	40(1)	47(1)	4(1)	15(1)	-3(1)
C(8)	48(1)	34(1)	37(1)	-3(1)	6(1)	-1(1)
C(25)	42(1)	35(1)	73(1)	8(1)	5(1)	-1(1)
N(2)	78(1)	70(1)	55(1)	1(1)	10(1)	31(1)
C(26)	44(1)	39(1)	64(1)	-6(1)	14(1)	3(1)
C(7)	52(1)	44(1)	39(1)	-7(1)	8(1)	7(1)
C(20)	42(1)	43(1)	49(1)	-5(1)	5(1)	-5(1)
C(15)	53(1)	36(1)	58(1)	-11(1)	16(1)	5(1)
C(13)	54(1)	38(1)	73(1)	6(1)	8(1)	-8(1)
C(17)	47(1)	65(1)	43(1)	-9(1)	16(1)	2(1)
C(19)	66(1)	45(1)	33(1)	-6(1)	2(1)	-3(1)

C(12)	47(1)	47(1)	68(1)	6(1)	19(1)	-2(1)
C(24)	58(1)	47(1)	54(1)	16(1)	10(1)	-5(1)
C(18)	66(1)	85(2)	37(1)	-13(1)	20(1)	3(1)
C(28)	81(2)	88(2)	64(2)	2(1)	-23(1)	-7(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3i**.

	x	y	z	U(eq)
H(1A)	11011	7243	5166	72
H(1B)	10464	8349	5084	72
H(11)	7563	4900	3494	51
H(27)	6317	8847	3265	50
H(14)	8326	1494	2641	71
H(21)	5792	6786	1979	47
H(23)	7848	8919	1494	53
H(26)	4875	10092	2571	59
H(20)	4518	6556	677	56
H(15)	9336	2986	2363	59
H(13)	6917	1705	3317	69
H(17)	8687	6376	1218	61
H(12)	6532	3391	3746	65
H(24)	6405	10173	803	66
H(18)	7421	6163	-77	74
H(28A)	3536	5914	-608	131
H(28B)	3592	6347	-1441	131
H(28C)	3783	7148	-714	131