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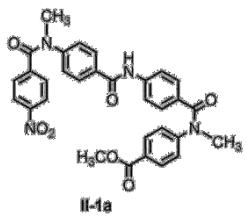
第 7 章　補遺

7. 1. 結晶データ

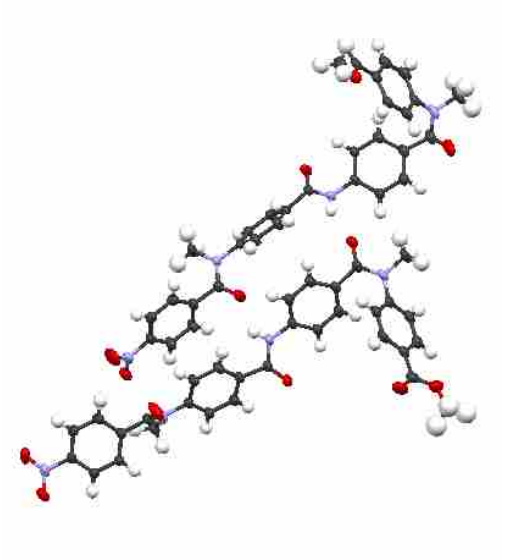
7. 1. 1. Crystal data and structure refinement for compound **II-1a** recrystallized from DMSO-d_6

Identification code	131129mis1	
Recryst. solvent	DMSO-d_6	
Empirical formula	$C_{31}H_{26}N_4O_7$	
Formula weight	566.56	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 39.018(6) Å	α = 90°
	b = 5.6456(9) Å	β = 91.196(3)°
	c = 23.038(4) Å	γ = 90°
Volume	5074.7(14) Å^3	
Z	8	
Density	1.483 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
Crystal size	0.20 × 0.05 × 0.02 mm^3	
Theta range for data collection	1.044 to 28.333°	
Reflections collected	4798	
Independent reflections	5082 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.1393　wR_2 = 0.3187	
R indices (all data)	R_1 = 0.1617　wR_2 = 0.3292	
CCDC number	1848115	

7. 1. 2. Crystal data and structure refinement for compound **II-1a** recrystallized from CH_2Cl_2/*n*-hexane

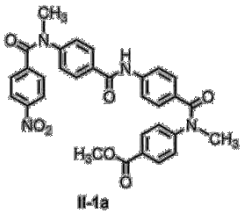


II-1a

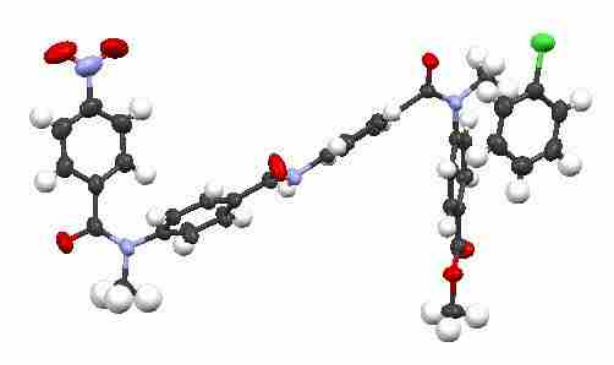


Identification code	u140410uru1	
Recryst. solvent	CH_2Cl_2/*n*-hexane	
Empirical formula	$C_{31}H_{26}N_4O_7$	
Formula weight	566.56	
Temperature	173 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	*P-1*	
Unit cell dimensions	a = 9.4411(5) Å	α = 95.928(3)°
	b = 13.9132(7) Å	β = 97.099(3)°
	c = 20.7293(10) Å	γ = 93.724(3)°
Volume	2679.2(2) Å^3	
Z	4	
Density	1.405 Mg/m^3	
Absorption coefficient	0.840 mm^{-1}	
Crystal size	0.20 x 0.30 x 0.03 mm^3	
Theta range for data collection	4.326 to 68.458°	
Reflections collected	7411	
Independent reflections	9426 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.0533 wR_2 = 0.1491	
R indices (all data)	R_1 = 0.0684 wR_2 = 0.1608	
CCDC number	1848128	

7. 1. 3. Crystal data and structure refinement for compound **II-1a** recrystallized from C_6H_5Cl/*n*-hexane

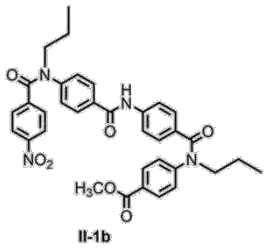


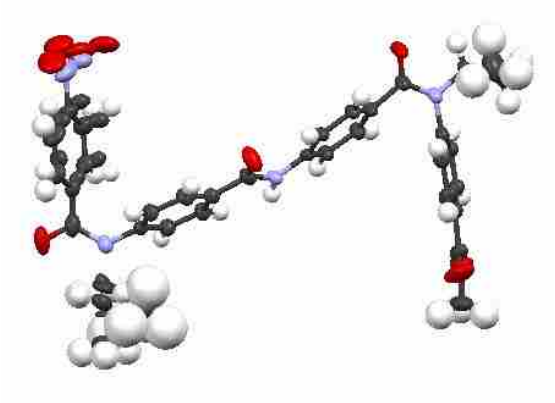
II-1a



Identification code	u140501uru2	
Recryst. solvent	C_6H_5Cl/*n*-hexane	
Empirical formula	$C_{31}H_{26}N_4O_7 \cdot C_6H_5Cl$	
Formula weight	679.11	
Temperature	223 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a =19.2513(8) Å	α = 90°
	b = 11.5028(5) Å	β = 106.146(3)°
	c = 15.5440(7) Å	γ=90°
Volume	3306.4(3) Å^3	
Z	4	
Density	1.364 Mg/m^3	
Absorption coefficient	1.501 mm^{-1}	
Crystal size	0.40 x 0.10 x 0.02 mm^3	
Theta range for data collection		
Reflections collected	4145	
Independent reflections	5999 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.0478 wR_2 = 0.1210	
R indices (all data)	R_1 = 0.0755 wR_2 = 0.1352	
CCDC number	1583148	

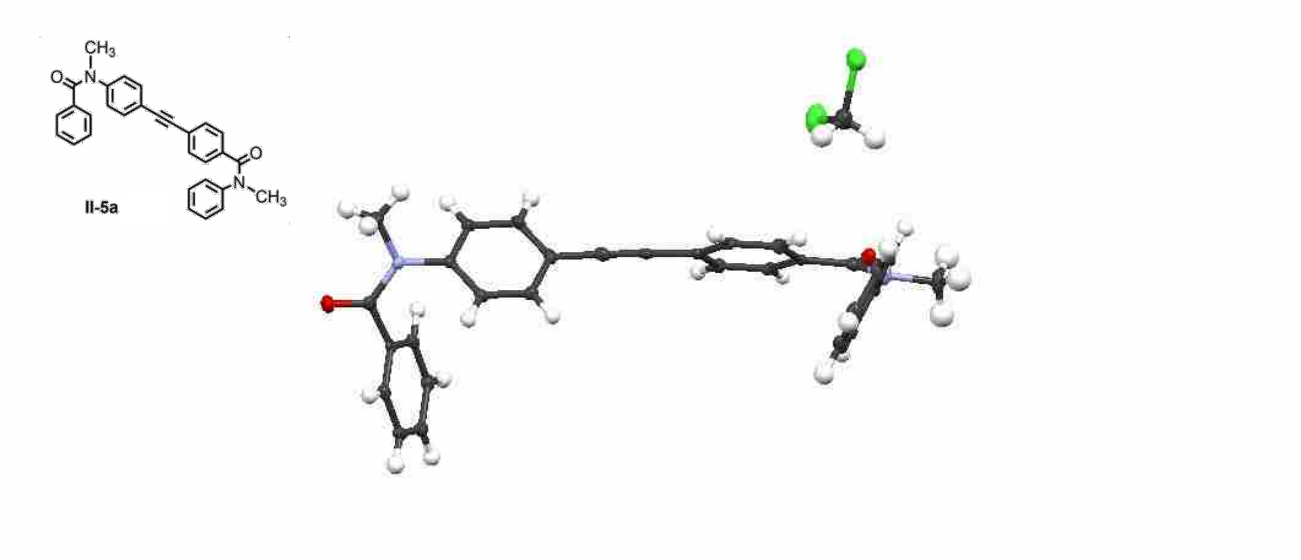
7. 1. 4. Crystal data and structure refinement for compound **II-1b** recrystallized from $CHCl_3$/*n*-hexane





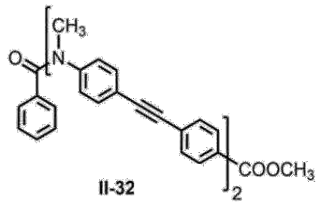
Identification code	u140501uru1	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{35}\ H_{34}\ N_4\ O_7$	
Formula weight	622.66	
Temperature	173 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.0264(6) Å	α = 90°
	b = 10.9646(4) Å	β = 101.399(2)°
	c = 15.9060(4) Å	γ = 90°
Volume	3252.81(18) $Å^3$	
Z	4	
Density	1.271 Mg/m^3	
Absorption coefficient	0.736 mm^{-1}	
Crystal size	0.20 x 0.20 x 0.02 mm^3	
Theta range for data collection	4.68 to 68.21°	
Reflections collected	5708	
Independent reflections	3876 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0486 wR_2 = 0.1243	
R indices (all data)	R_1 = 0.0759 wR_2 = 0.1414	
CCDC number	1583151	

7. 1. 5. Crystal data and structure refinement for compound **II-5a**

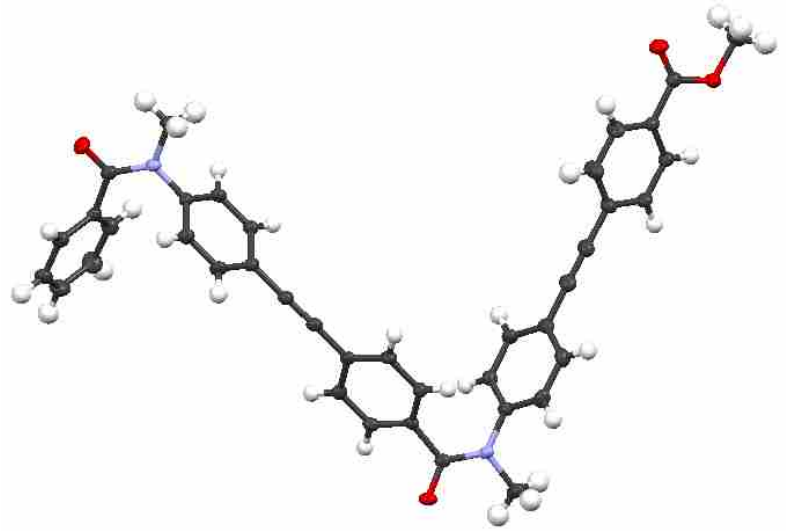


Identification code	150129uru1	
Recryst. solvent	CH_2Cl_2/*n*-hexane	
Empirical formula	$C_{30}H_{24}N_2O_2 \cdot CH_2Cl_2$	
Formula weight	529.46	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.6568(17) Å	α = 90°
	b = 15.768(3) Å	β = 96.890(4)°
	c = 22.082(5) Å	γ = 90°
Volume	2646.8(10) $Å^3$	
Z	4	
Density	1.329 Mg/m^3	
Absorption coefficient	0.277 mm^{-1}	
Crystal size	0.10 x 0.05 x 0.03 mm^3	
Theta range for data collection	1.59 to 27.48°	
Reflections collected	6041	
Independent reflections	2978 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0775 wR_2 = 0.1851	
R indices (all data)	R_1 = 0.1725 wR_2 = 0.2316	

7. 1. 6. Crystal data and structure refinement for compound **II-32**

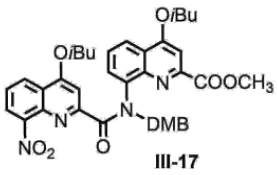


II-32

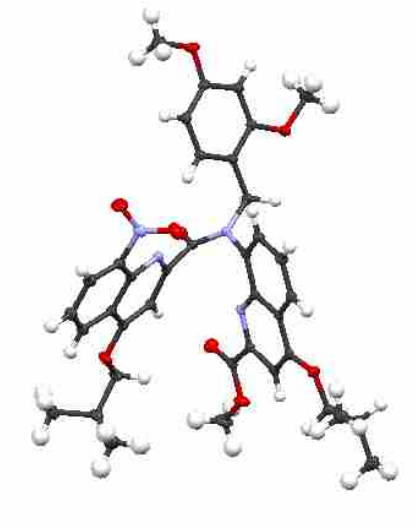


Identification code	170207uru1	
Recryst. solvent	THF/*n*-hexane	
Empirical formula	$C_{40}H_{30}N_2O_4$	
Formula weight	602.66	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 7.7894(13) Å	α = 88.829(3)°
	b = 9.2514(15) Å	β = 79.555(3)°
	c = 23.546(4) Å	γ = 69.208(2)°
Volume	1558.2(4) Å^3	
Z	2	
Density	1.284 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
Crystal size	0.10 x 0.05 x 0.10 mm^3	
Theta range for data collection	2.6418 to 27.4652°	
Reflections collected	7021	
Independent reflections	4476 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.0504	wR_2 = 0.1153
R indices (all data)	R_1 = 0.0931	wR_2 = 0.1317

7. 1. 7. Crystal data and structure refinement for compound **III-17**

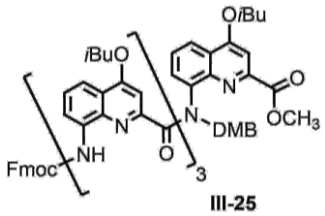


III-17

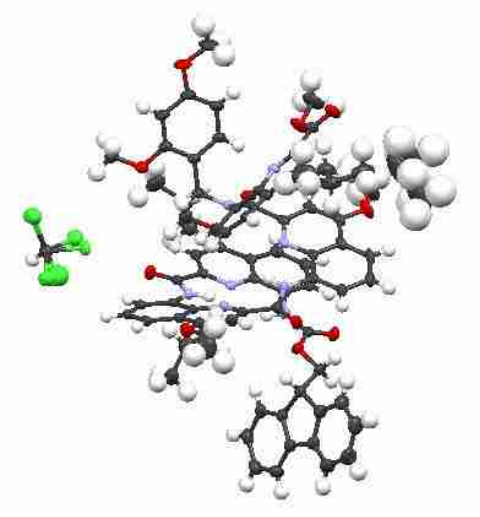


Identification code	KU-20	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{38}H_{40}N_4O_9$	
Formula weight	696.74	
Temperature	293 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.4000(12) Å	α = 90°
	b = 21.935(2) Å	β = 91.177(4)°
	c = 12.9987(18) Å	γ = 90°
Volume	3507.9(7) $Å^3$	
Z	4	
Density	1.319 Mg/m^3	
Absorption coefficient	0.783 mm^{-1}	
Crystal size		
Theta range for data collection	3.976 to 72.970°	
Reflections collected	6899	
Independent reflections	6593 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0329 wR_2 = 0.0844	
R indices (all data)	R_1 = 0.0329 wR_2 = 0.0853	

7. 1. 8. Crystal data and structure refinement for compound **III-25**

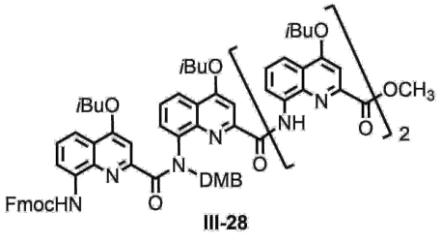


III-25

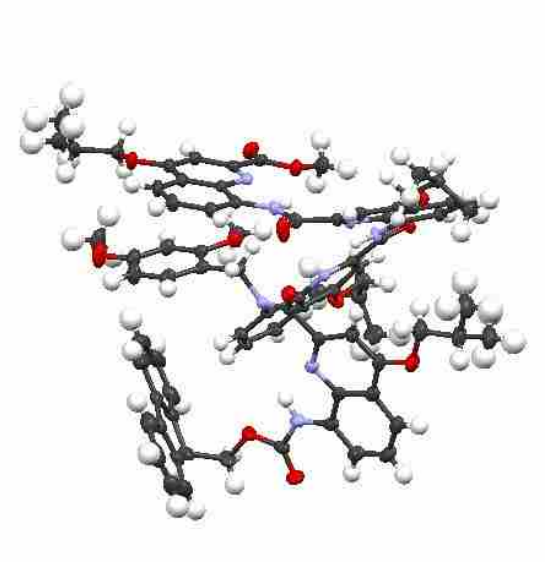


Identification code	KU-40	
Recryst. solvent	$CHCl_3/CH_3OH$	
Empirical formula	$C_{81}H_{80}N_8O_{13}$ · $CHCl_3$	
Formula weight	1492.89	
Temperature	173 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	*P-1*	
Unit cell dimensions	a = 14.027(6) Å	α = 102.307(7)°
	b = 17.201(7) Å	β = 102.373(10)°
	c = 18.706(7) Å	γ = 107.917(10)°
Volume	4001(3) $Å^3$	
Z	2	
Density	1.239 Mg/m^3	
Absorption coefficient	1.574 mm^{-1}	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.830 to 68.244°	
Reflections collected	14491	
Independent reflections	13225 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0497 wR_2 = 0.1350	
R indices (all data)	R_1 = 0.0527 wR_2 = 0.1374	

7. 1. 9. Crystal data and structure refinement for compound **III-28**

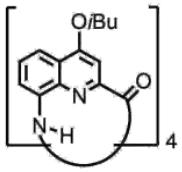


III-28

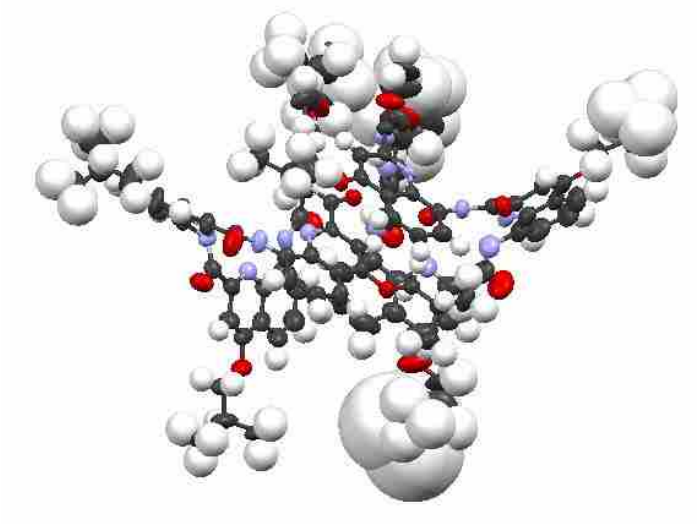


Identification code	KU-70	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{81}H_{80}N_8O_{13}$	
Formula weight	1373.53	
Temperature	173 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 13.6177(15) Å	α = 90°
	b = 18.7279(18) Å	β = 90°
	c = 27.868(3) Å	γ = 90°
Volume	7106.6(12) Å^3	
Z	4	
Density	1.284 Mg/m^3	
Absorption coefficient	0.713 mm^{-1}	
Crystal size		
Theta range for data collection	2.843 to 73.001°	
Reflections collected	12885	
Independent reflections	11880 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.0335 wR_2 = 0.0870	
R indices (all data)	R_1 = 0.0379 wR_2 = 0.0909	

7. 1. 10. Crystal data and structure refinement for compound **C4**

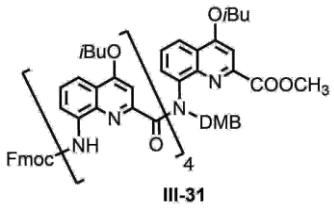


C4

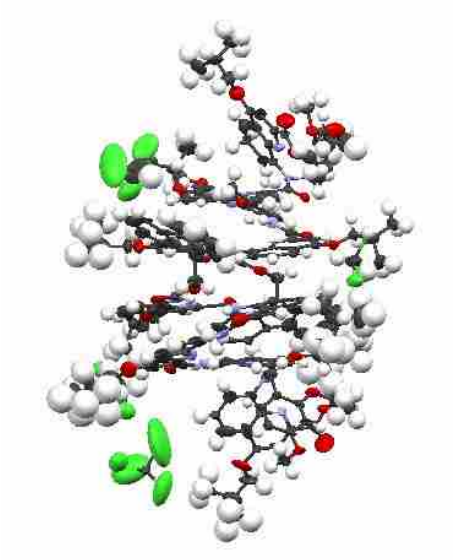


Identification code	KU-75	
Recryst. solvent	$CHCl_3/CH_3OH$	
Empirical formula	$C_{56}H_{56}N_8O_8$	
Formula weight	989.34	
Temperature	173 K	
Wavelength	1.54178 Å	
Crystal system	Trigonal	
Space group	*R*-3	
Unit cell dimensions	a = 33.092(6) Å	α = 120°
	b = 33.092(6) Å	β = 96.69(3)°
	c = 56.566(13) Å	γ = 120°
Volume	53645(22) $Å^3$	
Z	18	
Density	1.286 Mg/m^3	
Absorption coefficient	0.975 mm^{-1}	
Crystal size	0.20 x 0.20 x 0.02 mm^3	
Theta range for data collection	2.195 to 50.434°	
Reflections collected	12235	
Independent reflections	7938 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.2068 wR_2 = 0.5072	
R indices (all data)	R_1 = 0.2481 wR_2 = 0.5264	

7. 1. 11. Crystal data and structure refinement for compound **III-31**

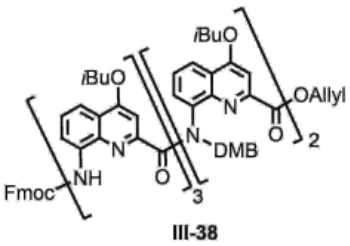


III-31

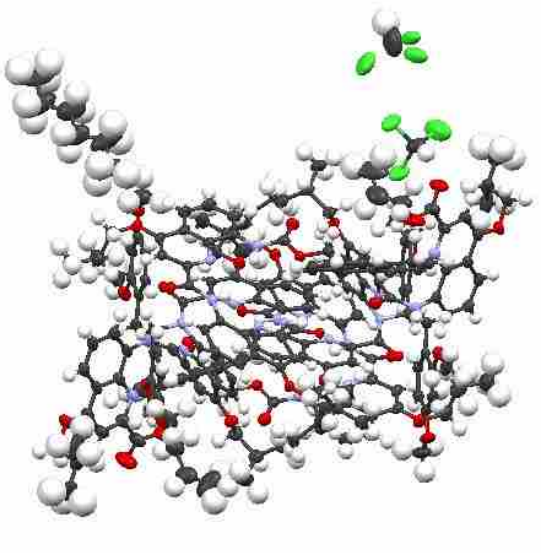


Identification code	170125uru1	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{95}H_{94}N_{10}O_{15}$ · $2CHCl_3$	
Formula weight	1828.50	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 22.472(9) Å	α = 90°
	b = 29.768(13) Å	β = 101.434(5)°
	c = 27.526(12) Å	γ = 90°
Volume	18048(13) $Å^3$	
Z	8	
Density	1.346 Mg/m^3	
Absorption coefficient	0.262 mm^{-1}	
Crystal size	0.20 x 0.05 x 0.01 mm^3	
Theta range for data collection	1.07 to 21.14°	
Reflections collected	19647	
Independent reflections	9761 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.1512 wR_2 = 0.3540	
R indices (all data)	R_1 = 0.2493 wR_2 = 0.4173	

7. 1. 12. Crystal data and structure refinement for compound **III-38**

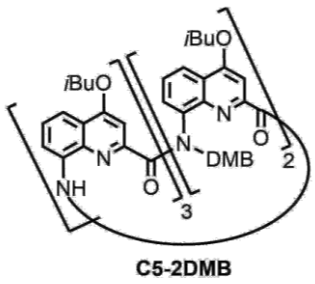


III-38

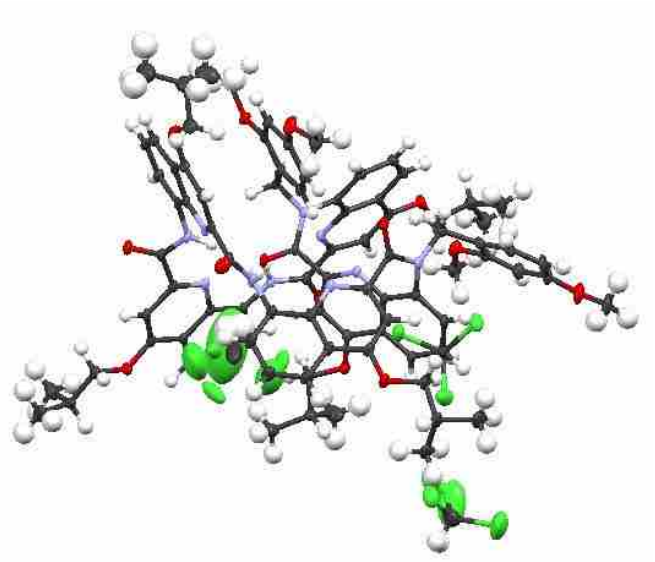


Identification code	170731uru1	
Recryst. solvent	$CHCl_3$/ CH_3OH	
Empirical formula	$2(C_{106}H_{106}N_{10}O_{17}) \cdot CHCl_3 \cdot 0.5(C_6H_{14})$	
Formula weight	3746.46	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 21.753(4) Å	α = 90°
	b = 29.135(6) Å	β = 105.30(3)°
	c = 33.043(7) Å	γ = 90°
Volume	20200.(8) $Å^3$	
Z	4	
Density	1.232 Mg/m^3	
Absorption coefficient	0.122 mm^{-1}	
Crystal size	0.10 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.398 to 25.350	
Reflections collected	36969	
Independent reflections	22845 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0844 wR_2 = 0.2478	
R indices (all data)	R_1 = 0.1332 wR_2 = 0.2857	
CCDC number	1824124	

7. 1. 13. Crystal data and structure refinement for compound **C5-2DMB**

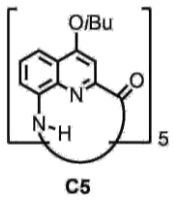


C5-2DMB

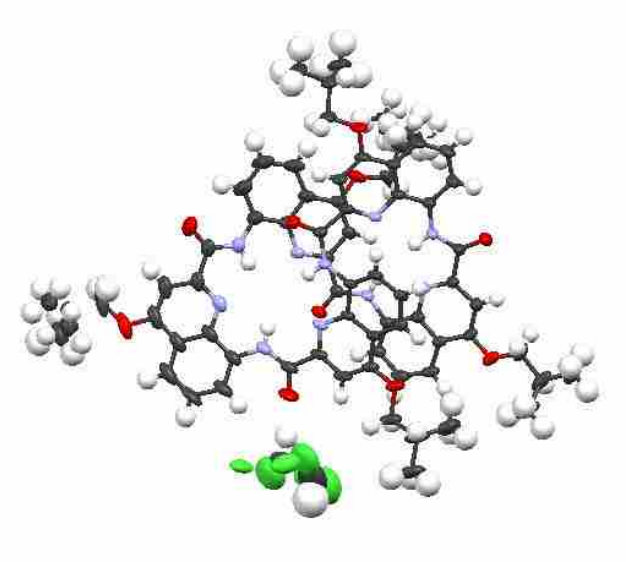


Identification code	170527uru1	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{88}H_{30}N_{10}O_{14}$ · $3CHCl_3$	
Formula weight	1869.80	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 13.2665(15) Å	α = 67.8772(18)°
	b = 19.254(2) Å	β = 86.1256(18)°
	c = 20.173(2) Å	γ = 70.748(2)°
Volume	4497.1(9) $Å^3$	
Z	2	
Density	1.381 Mg/m^3	
Absorption coefficient	0.349 mm^{-1}	
Crystal size	0.15 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.3193 to 27.2964°	
Reflections collected	20783	
Independent reflections	13142 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0735 wR_2 = 0.1766	
R indices (all data)	R_1 = 0.1230 wR_2 = 0.1996	
CCDC number	1585727	

7. 1. 14. Crystal data and structure refinement for compound **C5**

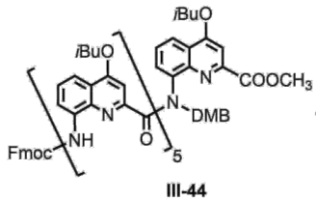


C5

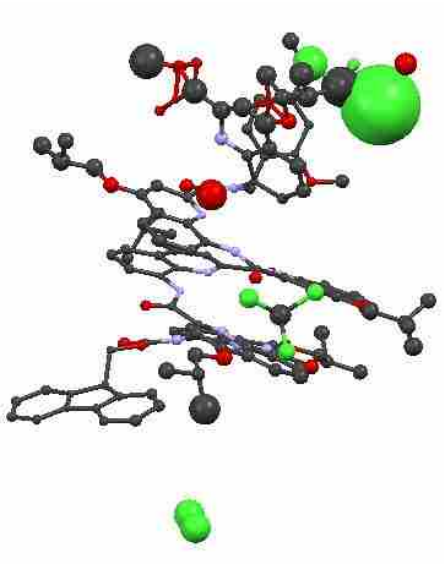


Identification code	170622uru1	
Recryst. solvent	$CHCl_3$/ CH_3OH	
Empirical formula	$C_{70}H_{70}N_{10}O_{10}$ · 0.5($CHCl_3$)	
Formula weight	1271.04	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.5024(8) Å	α = 90°
	b = 52.491(3) Å	β = 102.2195(12)°
	c = 8.9069(5) Å	γ = 90°
Volume	6626.7(6) $Å^3$	
Z	4	
Density	1.274 Mg/m^3	
Absorption coefficient	0.144 mm^{-1}	
Crystal size	0.15 x 0.01 x 0.01 mm^3	
Theta range for data collection	2.7223 to 26.2971°	
Reflections collected	15297	
Independent reflections	7985 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.0717 wR_2 = 0.1743	
R indices (all data)	R_1 = 0.1531 wR_2 = 0.2111	
CCDC number	1585728	

7. 1. 15. Crystal data and structure refinement for compound **III-44**

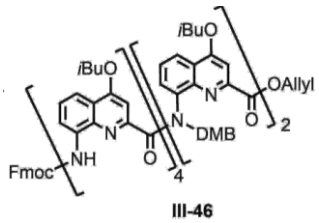


III-44

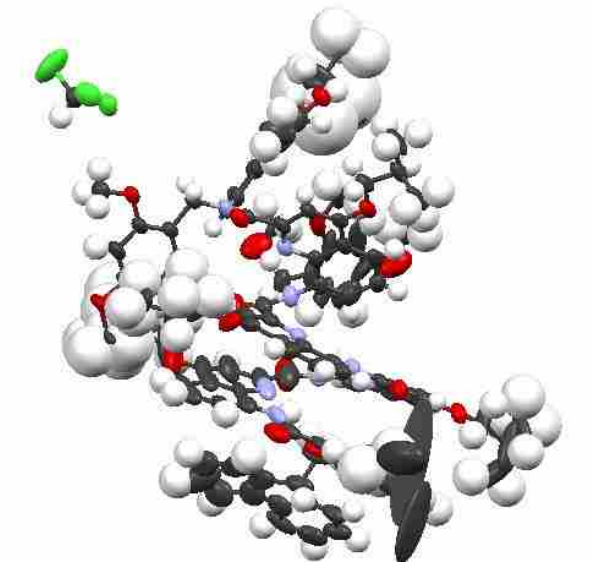


Identification code	170529uru2	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{109}H_{108}ClN_{12}O_{17}$	
Formula weight	1893.52	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 14.934(9) Å	α = 73.068(8)°
	b = 16.394(10) Å	β = 80.235(9)°
	c = 26.486(16) Å	γ = 66.046(8)°
Volume	5660(6) $Å^3$	
Z	2	
Density	1.111 Mg/m^3	
Absorption coefficient	0.098 mm^{-1}	
Crystal size	0.10 x 0.10 x 0.05 mm^3	
Theta range for data collection		
Reflections collected	25116	
Independent reflections	12990 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.2650 wR_2 = 0.5272	
R indices (all data)	R_1 = 0.3453 wR_2 = 0.5460	

7. 1. 16. Crystal data and structure refinement for compound **III-46**

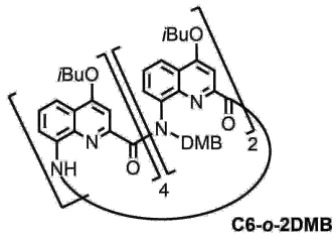


III-46

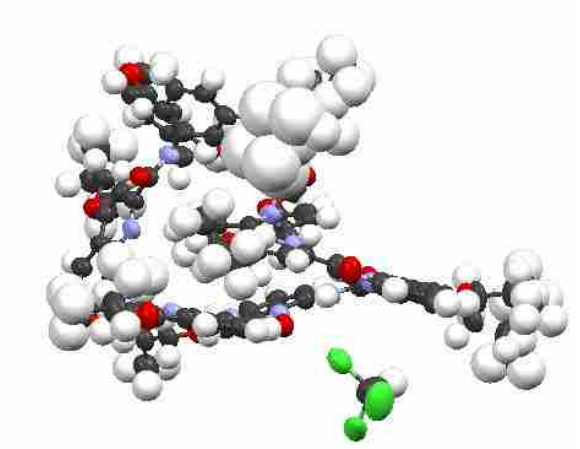


Identification code	170912uru2	
Recryst. solvent	$CHCl_3$/*n*-hexane	
Empirical formula	$C_{120}H_{120}N_{12}O_{19}$ · $CHCl_3$	
Formula weight	2153.64	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 17.4294(14) Å	α = 111.6320(10)°
	b = 18.2425(14) Å	β = 90.1380(10)°
	c = 20.1864(16) Å	γ = 105.4890(10)°
Volume	5713.1(8) $Å^3$	
Z	2	
Density	1.252 Mg/m^3	
Absorption coefficient	0.152 mm^{-1}	
Crystal size	0.10 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.476 to 25.927°	
Reflections collected	22106	
Independent reflections	12543 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.1713 wR_2 = 0.4680	
R indices (all data)	R_1 = 0.2306 wR_2 = 0.5132	

7. 1. 17. Crystal data and structure refinement for compound **C6-*o*-2DMB**

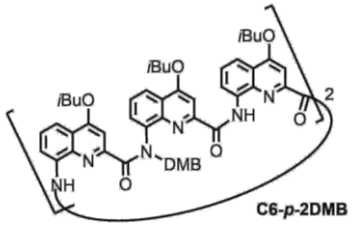


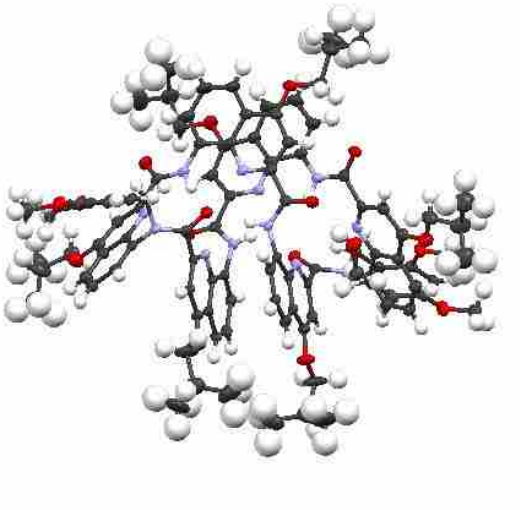
C6-*o*-2DMB



Identification code	17B03urs02	
Recryst. solvent	$CHCl_3$/ CH_3OH	
Empirical formula	$C_{102}H_{104}N_{12}O_{16}$ · 0.41($CHCl_3$)	
Formula weight	1803.00	
Temperature	100 K	
Wavelength	0.850 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.678(4) Å	α = 90°
	b = 14.216(3) Å	β = 96.69(3)°
	c = 37.768(8) Å	γ = 90°
Volume	9427(3) $Å^3$	
Z	4	
Density	1.270 Mg/m^3	
Absorption coefficient	0.185 mm^{-1}	
Crystal size	0.10 x 0.04 x 0.01 mm^3	
Theta range for data collection	1.298 to 31.735°	
Reflections collected	11618	
Independent reflections	5004 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.1144 wR_2 = 0.2901	
R indices (all data)	R_1 = 0.2282 wR_2 = 0.3594	

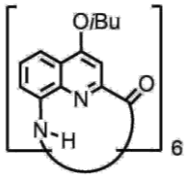
7. 1. 18. Crystal data and structure refinement for compound **C6-*p*-2DMB**

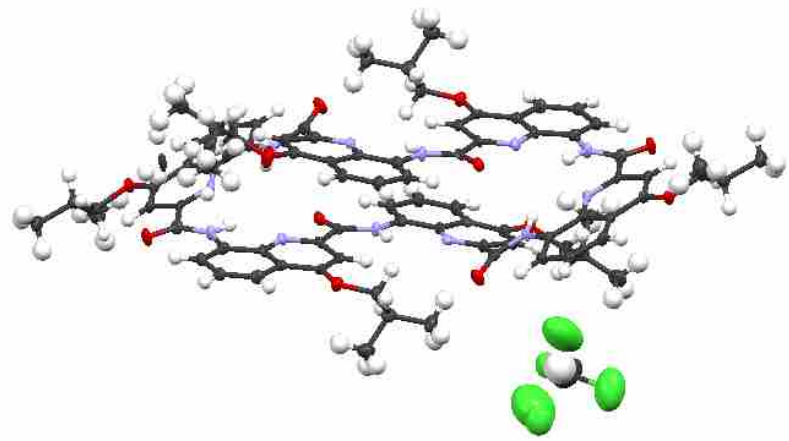




Identification code	171111uru1	
Recryst. solvent	$CHCl_3$/ CH_3OH	
Empirical formula	$C_{102}H_{104}N_{12}O_{16}$ · CH_3OH	
Formula weight	1790.04	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 32.719(6) Å	α = 90°
	b = 17.980(4) Å	β = 101.043(3)°
	c = 16.476(3) Å	γ = 90°
Volume	9513.(3) $Å^3$	
Z	4	
Density	1.250 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
Crystal size	0.20 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.27 to 23.40°	
Reflections collected	6908	
Independent reflections	4633 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0717 wR_2 = 0.1945	
R indices (all data)	R_1 = 0.1103 wR_2 = 0.2192	

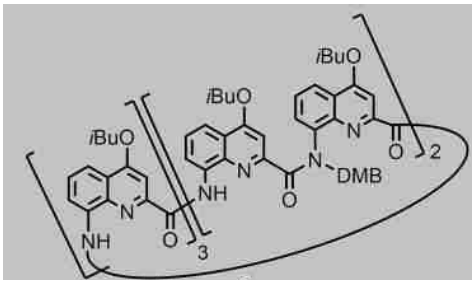
7. 1. 19. Crystal data and structure refinement for compound **C6**



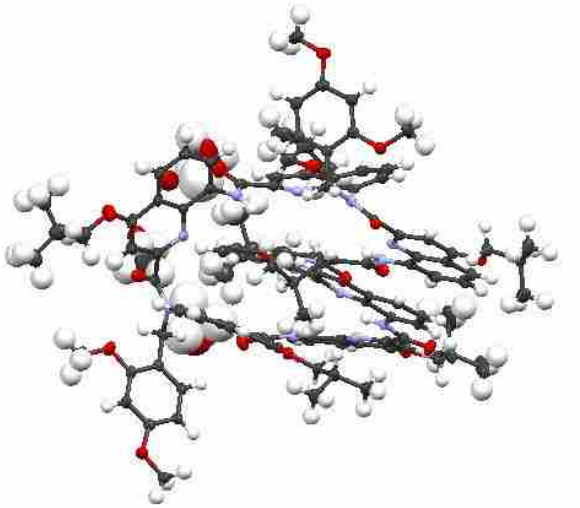


Identification code	171106uru3	
Recryst. solvent	$CHCl_3$/ CH_3OH	
Empirical formula	$C_{84}H_{84}N_{12}O_{12}$ · $CHCl_3$	
Formula weight	1572.99	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 8.602(4) Å	α = 93.218(8)°
	b = 12.502(6) Å	β = 91.180(7)°
	c = 18.968(9) Å	γ = 103.516(9)°
Volume	1979.0(16) $Å^3$	
Z	1	
Density	1.320 Mg/m^3	
Absorption coefficient	0.186 mm^{-1}	
Crystal size	0.10 x 0.01 x 0.01 mm^3	
Theta range for data collection	1.08 to 24.76°	
Reflections collected	6716	
Independent reflections	3172 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.1133 wR_2 = 0.3010	
R indices (all data)	R_1 = 0.2202 wR_2 = 0.3682	

7. 1. 20. Crystal data and structure refinement for compound **C7-2DMB**

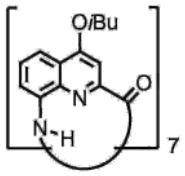


C7-2DMB

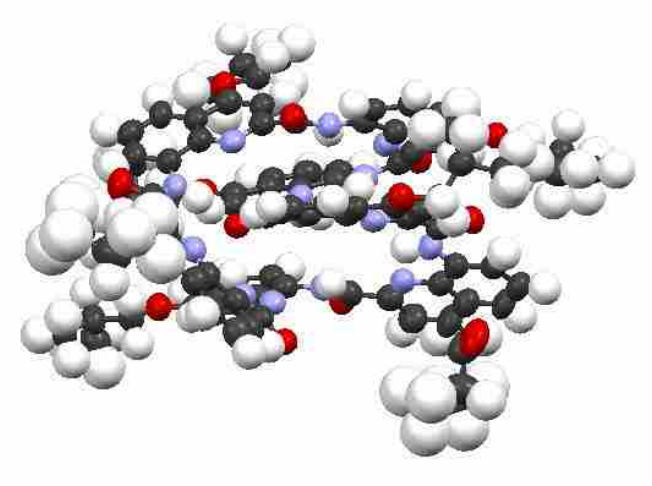


Identification code	180704uru1	
Recryst. solvent	$CHCl_3$/ CH_3CN / CH_3OH	
Empirical formula	$C_{116}H_{118}N_{14}O_{18}$ · $3CH_3OH$ · $(H_2)O$	
Formula weight	2108.36	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.1053(11) Å	α = 90°
	b = 21.5495(14) Å	β = 98.8050(10)°
	c = 28.1674(18) Å	γ = 90°
Volume	10860.3(12) $Å^3$	
Z	4	
Density	1.289 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
Crystal size	0.20 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.20 to 30.76°	
Reflections collected	32309	
Independent reflections	19498 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0939	wR_2 = 0.2338
R indices (all data)	R_1 = 0.1524	wR_2 = 0.2705

7. 1. 21. Crystal data and structure refinement for compound **C7** recrystallized from $CHCl_3/CH_3OH$

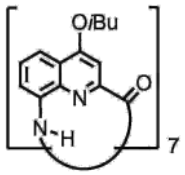


C7

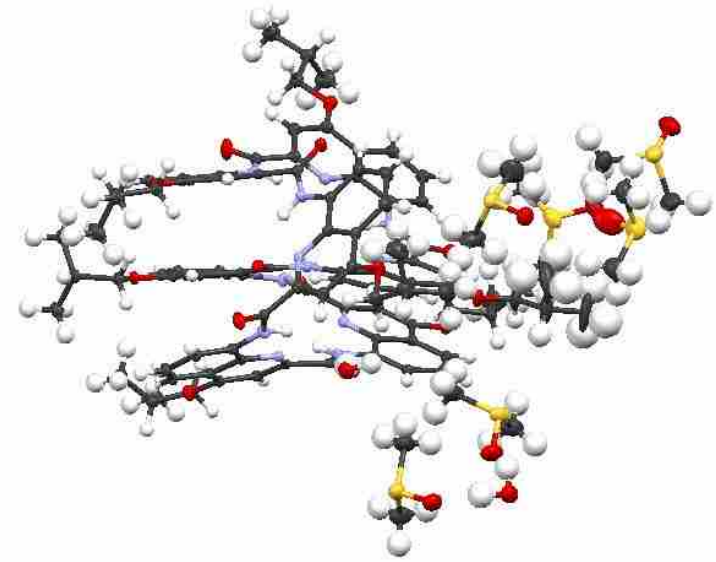


Identification code	17B03urs01	
Recryst. solvent	$CHCl_3$/ CH_3OH	
Empirical formula	$C_{98}H_{98}N_{14}O_{14}$	
Formula weight	1695.90	
Temperature	100 K	
Wavelength	0.850 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 19.856(4) Å	α = 90°
	b = 18.444(4) Å	β = 96.39(3)°
	c = 24.271(5) Å	γ = 90°
Volume	8833(3) $Å^3$	
Z	4	
Density	1.275 Mg/m^3	
Absorption coefficient	0.130 mm^{-1}	
Crystal size	0.10 x 0.04 x 0.03 mm^3	
Theta range for data collection	1.662 to 31.759°	
Reflections collected	12425	
Independent reflections	5454 [R_{int} = 0.0224]	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.1313 wR_2 = 0.3666	
R indices (all data)	R_1 = 0.2314 wR_2 = 0.4383	

7. 1. 22. Crystal data and structure refinement for compound **C7** recrystallized from DMSO-d_6



C7



Identification code	180516uru1	
Recryst. solvent	DMSO-d_6	
Empirical formula	$C_{98}H_{98}N_{14}O_{14}$ · $6(C_2H_6SO)$ · $2(H_2O)$	
Formula weight	2200.70	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 21.3798(14) Å	α = 90°
	b = 17.9932(12) Å	β = 96.6490(10)°
	c = 29.2144(19) Å	γ = 90°
Volume	11162.9(13) Å^3	
Z	4	
Density	1.309 Mg/m^3	
Absorption coefficient	0.198 mm^{-1}	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.2103 to 30.1355°	
Reflections collected	32660	
Independent reflections	22416 [R_{int} = 0.0224]	
Final R indices [I>2σ(I)]	R_1 = 0.0742 wR_2 = 0.1980	
R indices (all data)	R_1 = 0.1086 wR_2 = 0.2156	

7. 2. NMR データ

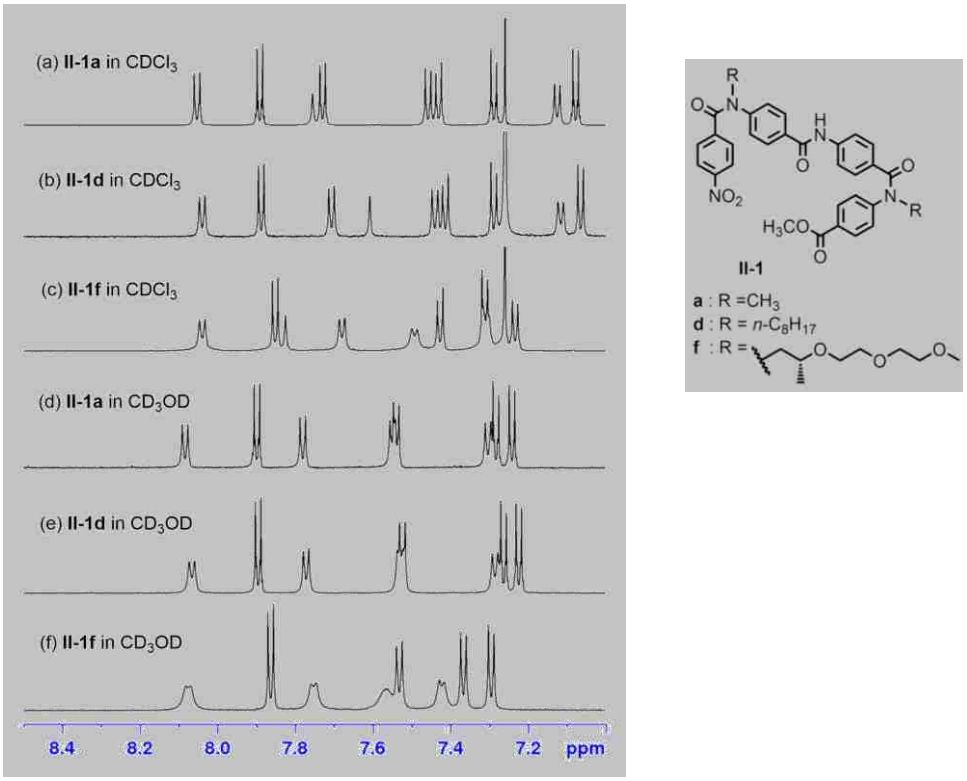


Figure S-1. Aromatic regions of 600 MHz ^{1}H NMR spectra of (a) **II-1a**, (b) **II-1d**, (c) **II-1f** in $CDCl_3$ and (d) **II-1a**, (e) **II-1d**, (f) **II-1f** in CD_3OD at 293 K.

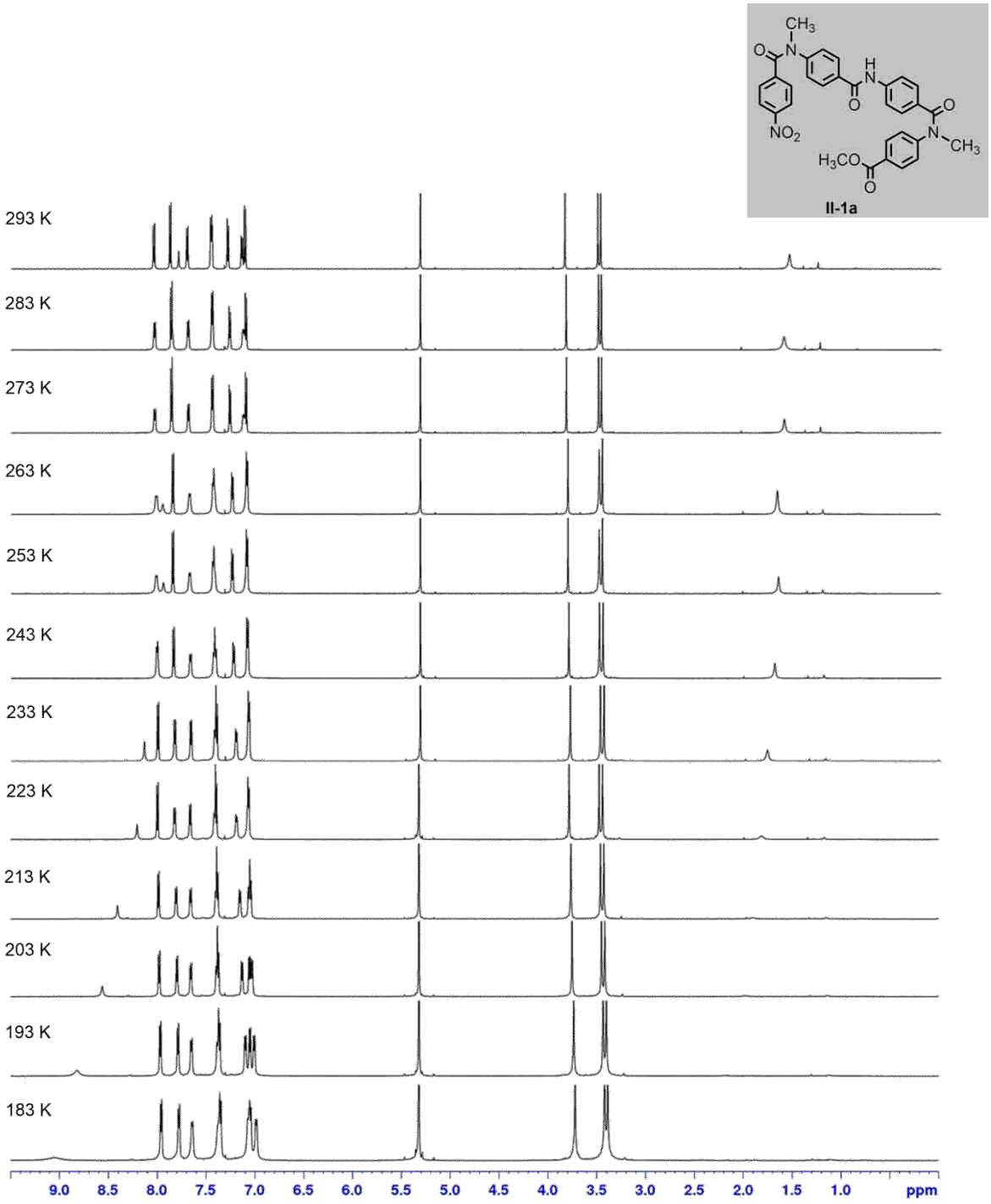
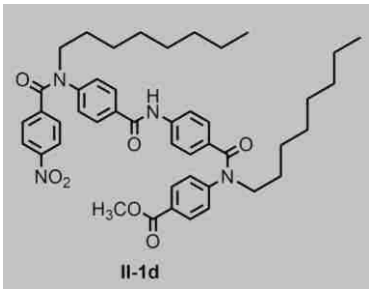


Figure S-2. VT ^{1}H NMR spectra of monomer **II-1a** at 183 - 293 K in CD_2Cl_2.



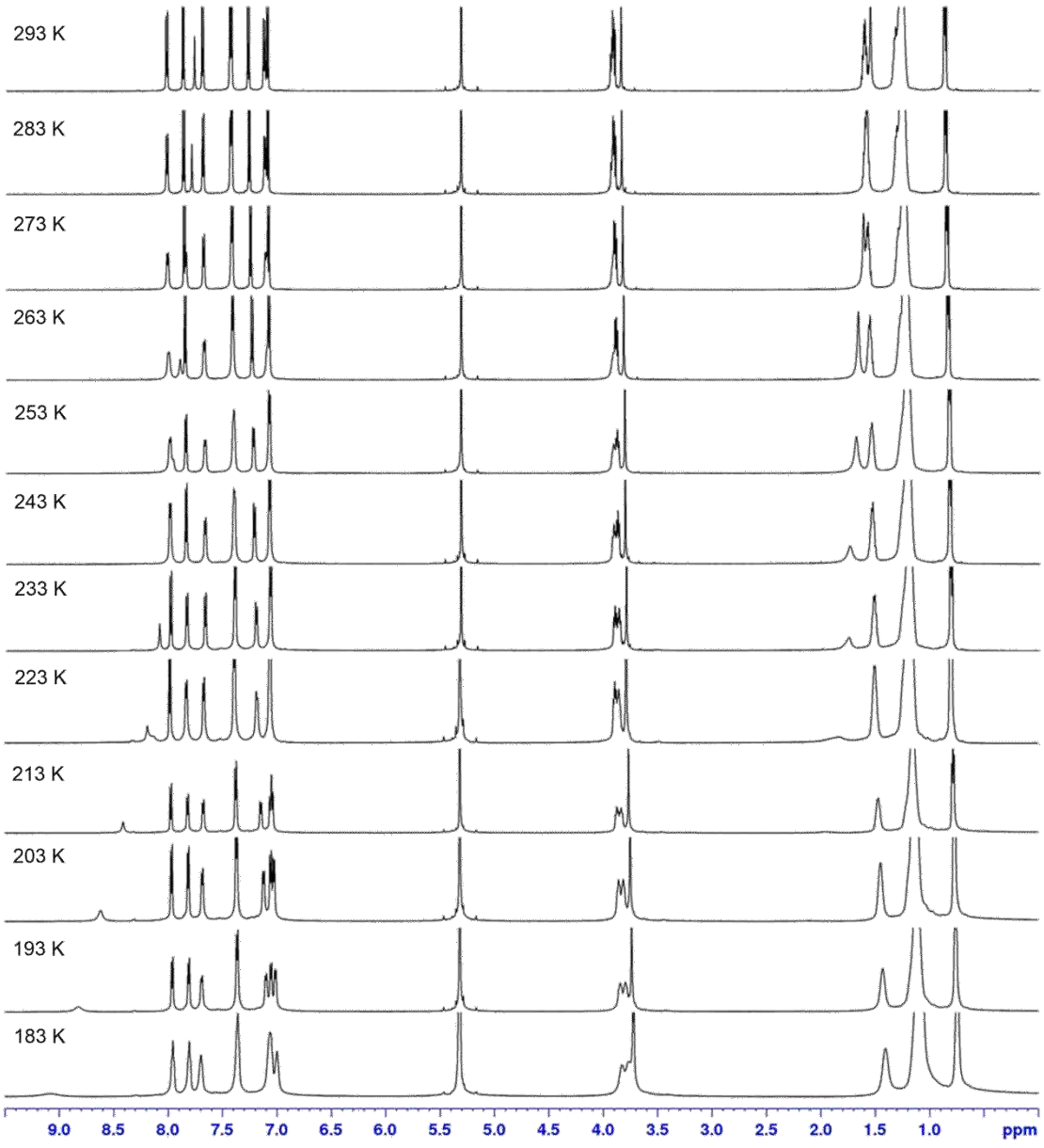
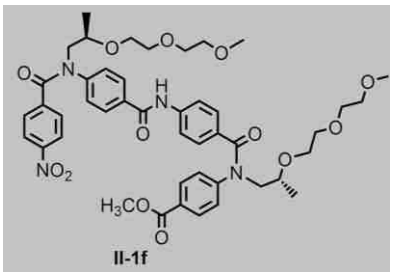


Figure S-3. VT ^{1}H NMR spectra of monomer **II-1d** at 183 - 293 K in CD_2Cl_2.



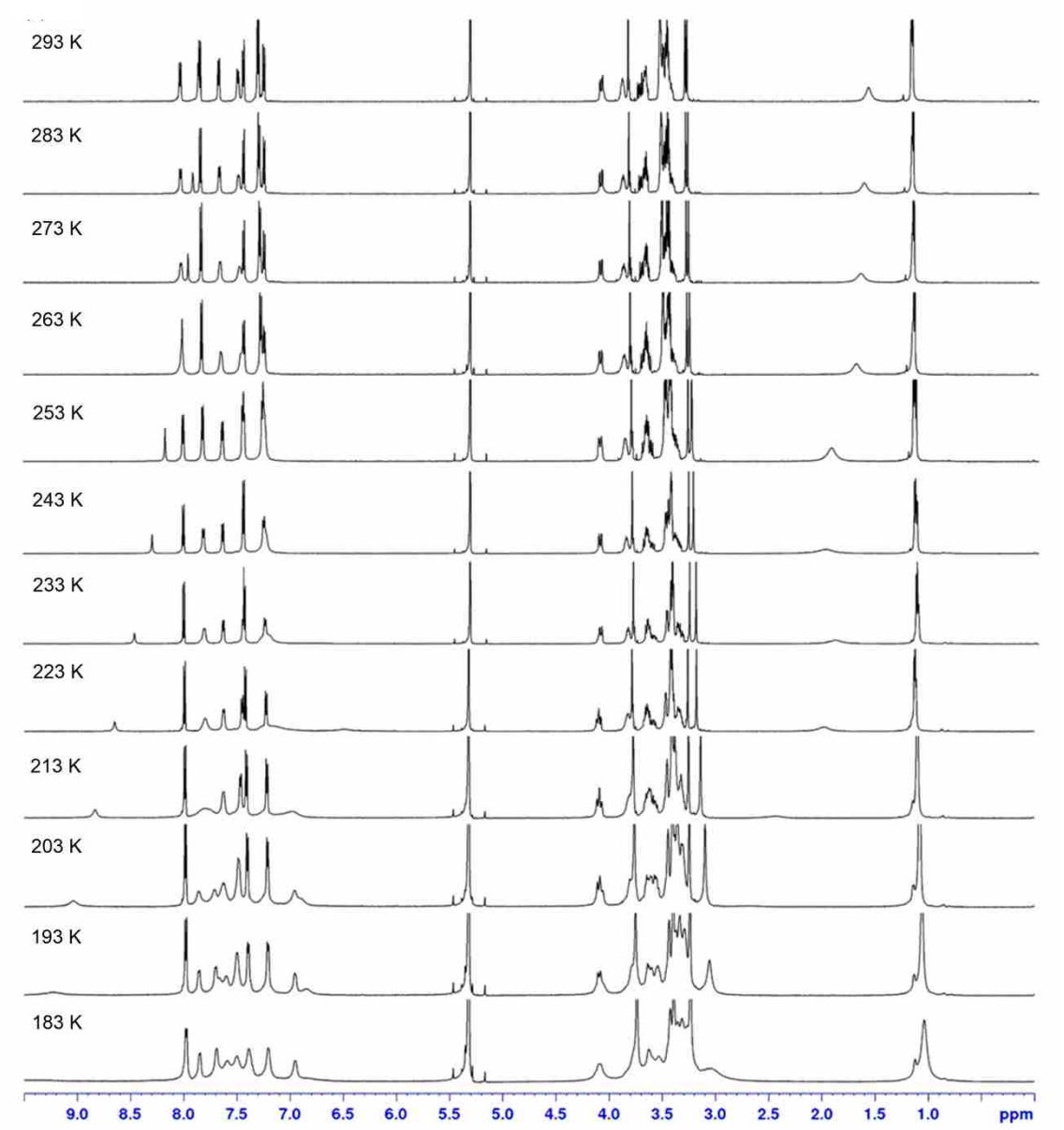


Figure S-4. VT ^{1}H NMR spectra of monomer **II-1f** at 183 - 293 K in CD_2Cl_2.

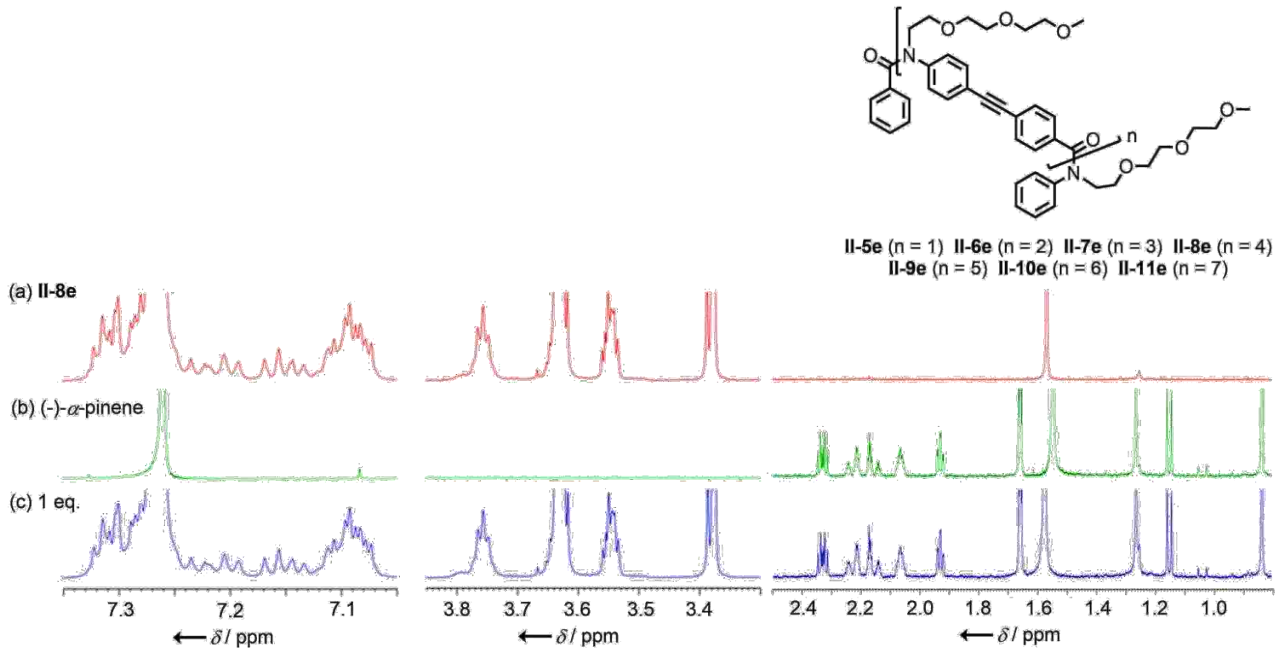


Figure S-5. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-8e** (1 mM), (b) (-)-α-pinene (1 mM), (c) **II-8e** with 1 eq. of pinene at 25^{o}C.

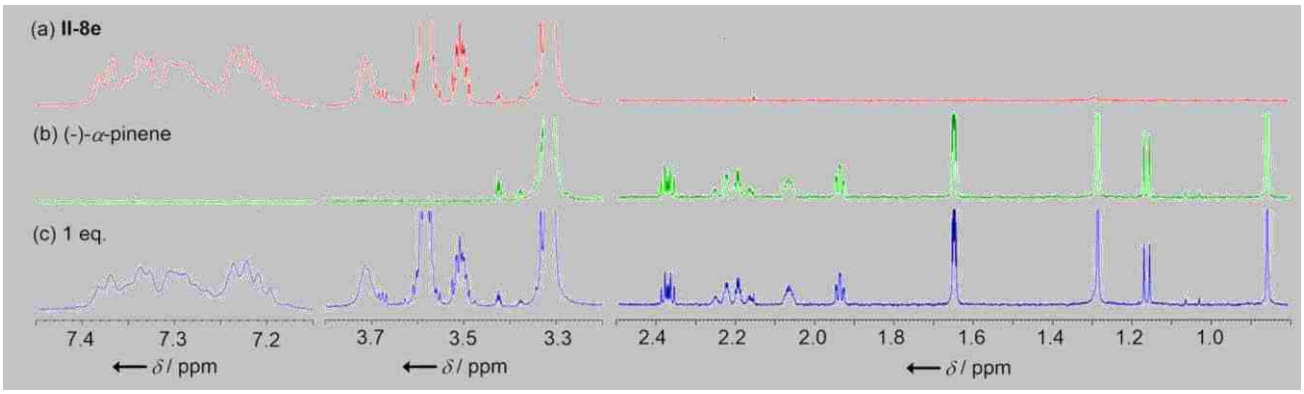


Figure S-6. ^{1}H NMR spectra (600 MHz, CD_3OD) spectra of (a) **II-8e** (1 mM), (b) (-)-α-pinene (1 mM), (c) **II-8e** with 1 eq. of pinene at 25^{o}C.

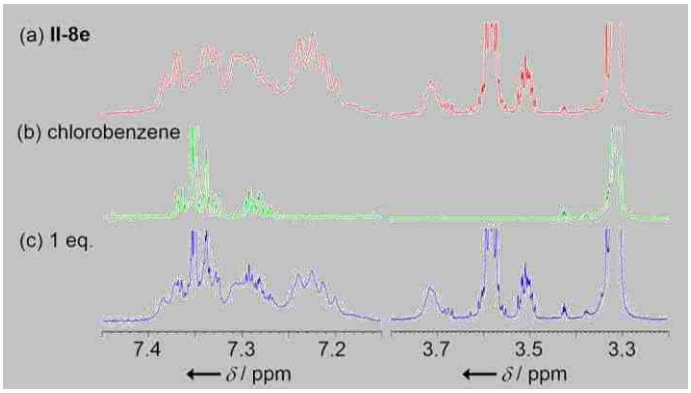


Figure S-7. ^{1}H NMR spectra (600 MHz, CD_3OD) spectra of (a) **II-8e** (1 mM), (b) chlorobenzene (1 mM), (c) **II-8e** with 1 eq. of chlorobenzene at 25^{o}C.

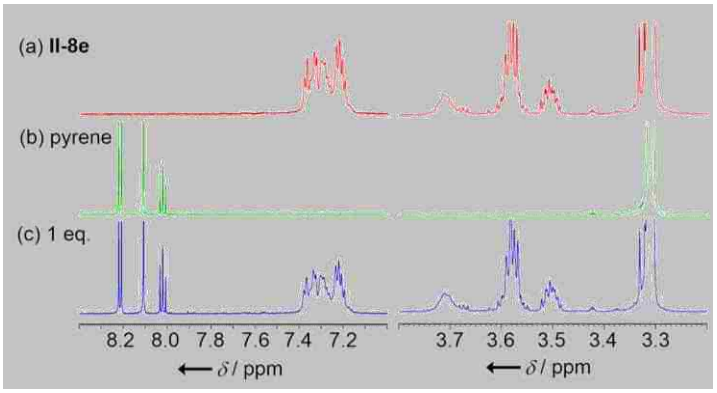


Figure S-8. ^{1}H NMR spectra (600 MHz, CD_3OD) spectra of (a) **II-8e** (1 mM), (b) pyrene (1 mM), (c) **II-8e** with 1 eq. of pyrene at 25^{o}C.

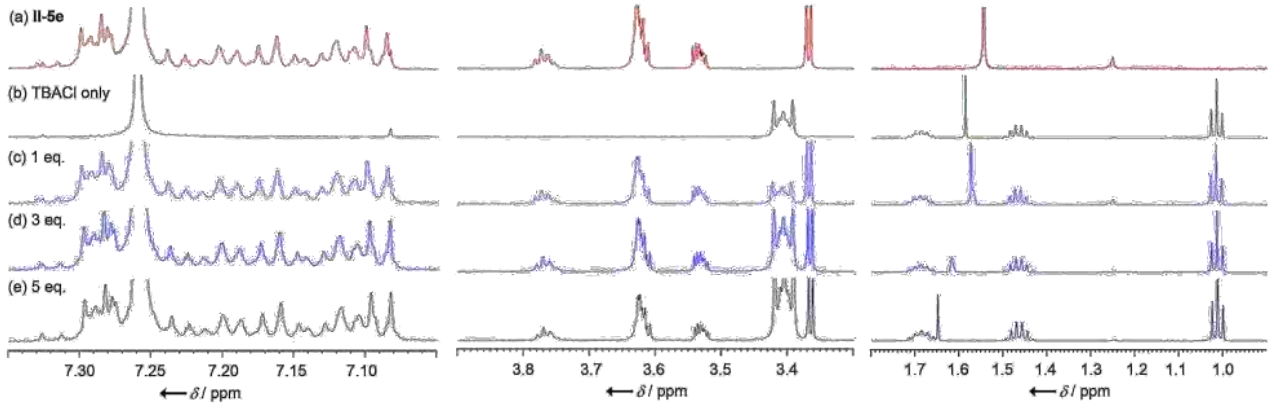


Figure S-9. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-5e** (1 mM), (b) TBACl (1 mM), (c) **II-5e** with 1 eq., (d) 3 eq. and (e) 5 eq. of TBACl at 25^{o}C.

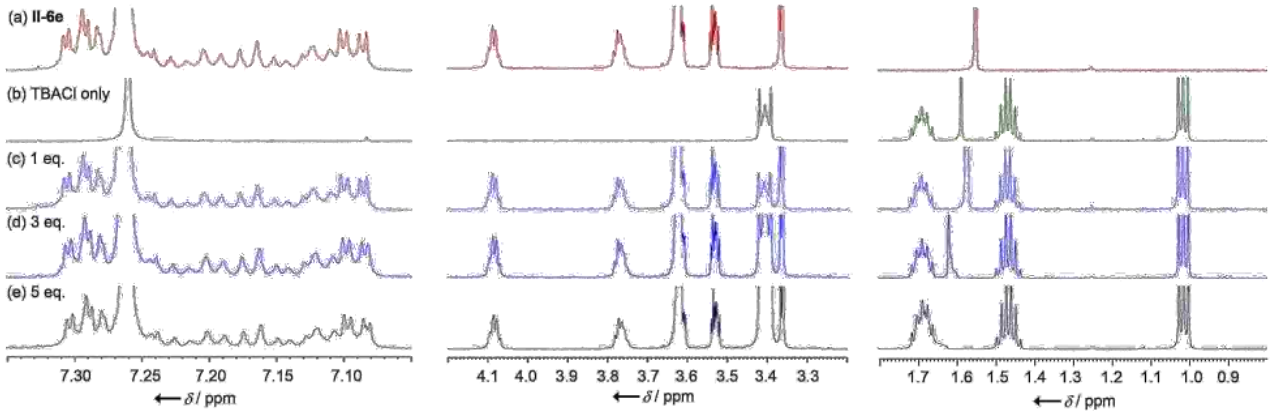


Figure S-10. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-6e** (1 mM), (b) TBACl (1 mM), (c) **II-6e** with 1 eq., (d) 3 eq. and (e) 5 eq. of TBACl at 25^{o}C.

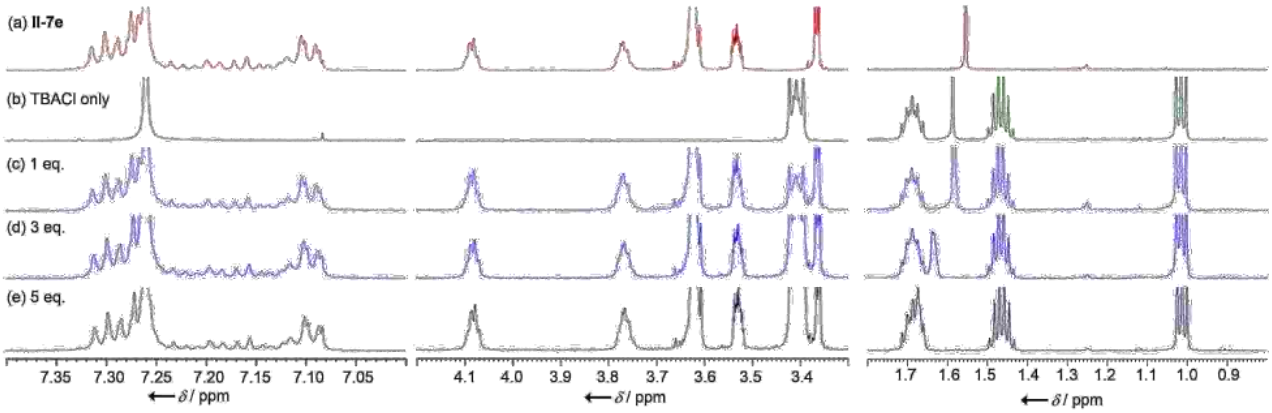


Figure S-11. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-7e** (1 mM), (b) TBACl (1 mM), (c) **II-7e** with 1 eq., (d) 3 eq. and (e) 5 eq. of TBACl at 25^{o}C.

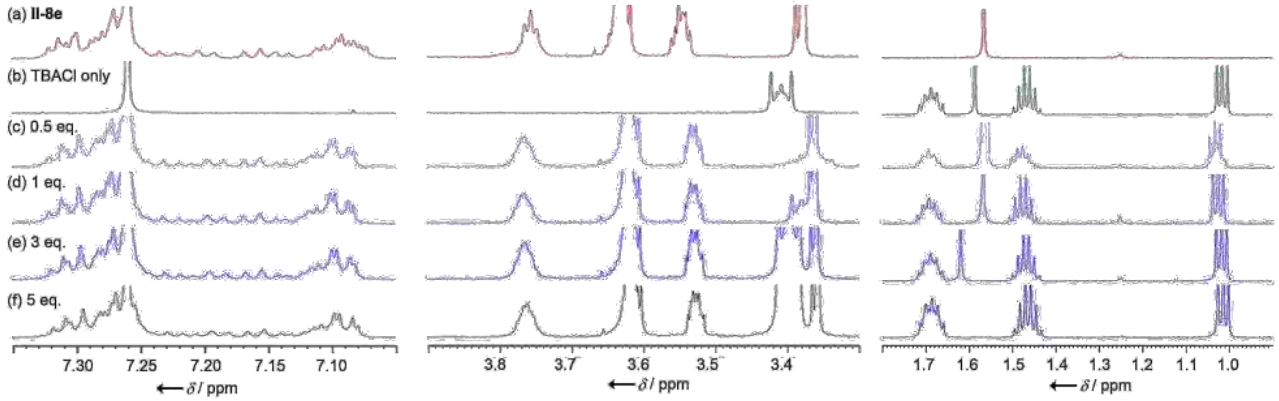


Figure S-12. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-8e** (1 mM), (b) TBACl (1 mM), (c) **II-8e** with 0.5 eq., (d) 1 eq., (e) 3 eq. and (f) 5 eq. of TBACl at 25^{o}C.

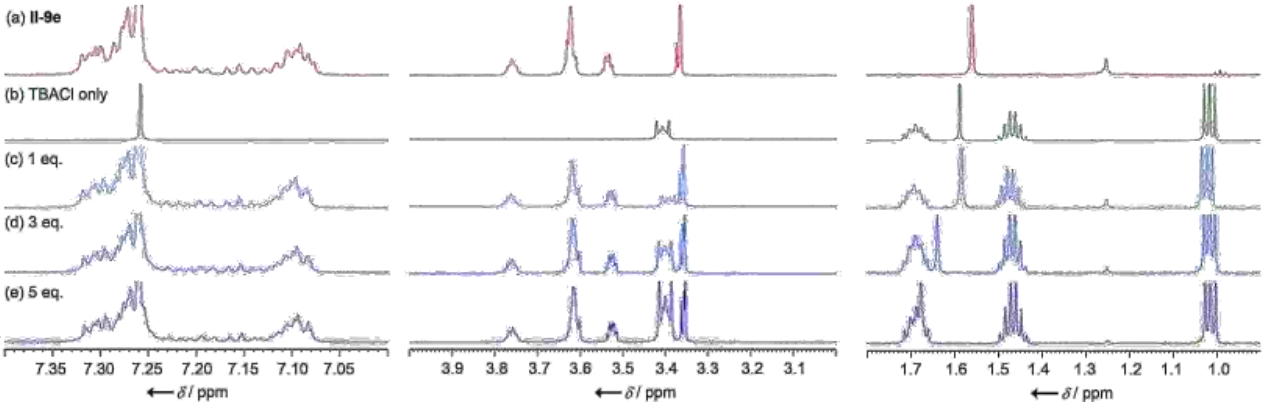


Figure S-13. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-9e** (1 mM), (b) TBACl (1 mM), (c) **II-9e** with 1 eq., (d) 3 eq. and (e) 5 eq. of TBACl at 25^{o}C.

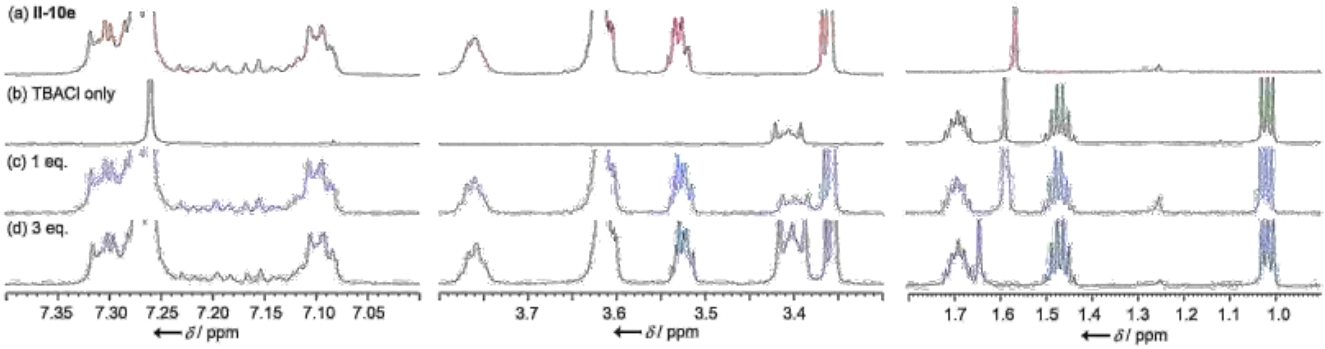


Figure S-14. ^{1}H NMR spectra (600 MHz, $CDCl_3$) spectra of (a) **II-10e** (1 mM), (b) TBACl (1 mM), (c) **II-10e** with 1 eq. and (d) 3 eq. of TBACl at 25^{o}C.

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