Discovery of highly active imidotitanium ethylene polymerisation catalysts and their evaluation using high throughput catalyst screening

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Supporting information: selected characterising data

Characterising data for [Ti(N^{t}Bu)(Me$_3$[9]aneN$_3$)Me$_2$] (2a)

Anal. found (calcd. for $C_{15}H_{36}N_4Ti$): C, 52.4 (56.2); H, 11.0 (11.3); N, 17.1 (17.5) %. The low %C is attributed to carbide formation. ^{1}H NMR (C_6D_6, 300.1 MHz, 298 K): 2.65 (s, 6 H, NMe cis), 2.52 (m, 2 H, CH_2 ring), 2.43 (s, 3 H, NMe trans), 2.35 (m, 2 H, CH_2 ring), 2.19 (m, 2 H, CH_2 ring), 1.69 (m, 2 H, CH_2 ring), 1.66 (m, 2 H, CH_2 ring), 1.65 (s, 9 H, $NCMe_3$), 1.61 (m, 2 H, CH_2 ring), 0.36 (s, 6 H, TiMe. ^{13}C-{^{1}H} NMR (C_6D_6, 75.5 MHz, 298 K): 64.7 (N<u>C</u>Me$_3$), 55.5 (CH_2 ring), 55.1 (CH_2 ring), 54.8 (CH_2 ring), 51.8 (NMe cis), 48.5 (NMe trans), 33.5 (NC<u>Me</u>$_3$), 26.4 (TiMe). This compound has been crystallographically characterised.

Characterising data for [Ti(N^{t}Bu)(Me$_3$[9]aneN$_3$)(CH$_2$SiMe$_3$)$_2$] (2b)

Anal. found (calcd. for $C_{21}H_{52}N_4Si_2Ti$): C, 52.6 (54.3); H 11.4 (11.3); N 11.8 (12.1) %. The low %C is attributed to carbide formation. ^{1}H NMR (C_6D_6, 300.1 MHz, 298 K): 2.65 (s, 6 H, NMe cis), 2.51 (m, 2 H, CH_2 ring), 2.28 (s, 3 H, NMe trans), 2.27 (m, 2 H,CH_2 ring), 2.24 (m, 2 H,CH_2 ring), 1.65 (m, 2 H,CH_2 ring), 1.62 (m, 2 H,CH_2 ring), 1.58 (m, 2 H, CH_2 ring), 1.51 (s, 9 H, ^{t}Bu), 0.49 (s, 18 H, CH_2SiMe_3), 0.42 (d, ^2J = 10.4 Hz, 2 H, C<u>H$_a$</u>H$_b$SiMe$_3$), -0.19 (d, ^2J = 10.4 Hz, 2 H, CH$_a$<u>H$_b$</u>SiMe$_3$). ^{13}C-{^{1}H} NMR (C_6D_6, 75.5 MHz, 298 K): 66.1 (N<u>C</u>Me$_3$), 56.0 (CH_2 ring), 55.3 (CH_2 ring), 55.1 (CH_2 ring), 52.6 (NMe cis), 49.4 (NMe trans), 41.6 (<u>C</u>H$_2$SiMe$_3$), 33.8 (NC<u>Me</u>$_3$), 4.7 (CH$_2$Si<u>Me</u>$_3$). ^{29}Si NMR (HMQC ^{1}H-observed, C_6D_5Br, 299.9 MHz, 293 K): -1.76 (CH$_2$<u>Si</u>Me$_3$).

Characterising data for [Ti(N^{t}Bu)(Me$_3$[9]aneN$_3$)Me][B(Ar^F)$_4$] (3, NMR only)

^{1}H NMR (C_6D_5Br, 299.9 MHz, 293 K): 2.34 (br. m, 6 H, CH_2 ring), 2.20 (s, 9 H, NMe), 2.15 (br. m, 6 H, CH_2 ring), 0.93 (s, 9 H, ^{t}Bu), 0.69 (s, 3 H, TiMe). ^{13}C-{^{1}H} NMR (C_6D_5Br, 75.4 MHz, 293 K): 148.8 (br. d, $^1J_{C\text{-}F}$ = 239 Hz, *o*-C_6F_5), 138.6 (br. d, $^1J_{C\text{-}F}$ = 251 Hz, *p*-C_6F_5), 136.7 (br. d, $^1J_{C\text{-}F}$ = 246 Hz, *m*-C_6F_5), 69.9 (N<u>C</u>Me$_3$), 55.0 (CH_2 ring), 50.5 (NMe), 40.3 (TiMe), 31.4 (NC<u>Me</u>$_3$). ^{19}F NMR (C_6D_5Br, 282.1 MHz, 293

K): -131.82 (d, ^3J = 10.6 Hz, *o*-C_6F_5), -161.85 (t, ^3J = 21.2 Hz, *p*-C_6F_5), -165.79 (app.t, app. ^3J = 18.1 Hz, *m*-C_6F_5).

Characterising data for [Ti(N^{t}Bu)(Me$_3$[9]aneN$_3$)Me][MeB(Ar^F)$_3$] (4, NMR only)

^{1}H NMR (C_6D_5Br, 299.9 MHz, 293 K): As above with additional peak at 1.03 (br. s, 3 H, BMe). ^{19}F NMR (C_6D_5Br, 282.5 MHz, 293 K): -132.18 (d, ^3J = 18.3 Hz, *o*-C_6F_5), -163.73 (t, ^3J = 16.0 Hz, *p*-C_6F_5), -166.43 (app. t, app. ^3J = 19.8 Hz, *m*-C_6F_5).

Characterising data for [Ti$_2$(N^{t}Bu)$_2$(Me$_3$[9]aneN$_3$)$_2$Me$_2$(μ-Me)][B(Ar^F)$_4$] (NMR only)

The cation is observed as a mixture of two diastereomers, hereafter referred to as diastereomer A and diastereomer B, in a 2.3:1 ratio.

Data for diastereomer A: ^{1}H NMR (CD_2Cl_2, 500.0 MHz, 233 K): 3.50-2.60 (series of mutually overlapping m, some corresponding to diastereomer B, CH_2 ring), 2.91 (s, 6 H, NMe cis), 2.88 (s, 6 H, NMe cis), 2.48 (s, 6 H, NMe trans), 1.12 (s, 18 H, ^{t}Bu), 0.26 (s, 3 H, TiMe bridging), -0.06 (s, 6 H, TiMe terminal). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 125.7 MHz, 233 K): 66.6 (N<u>C</u>Me$_3$), 56.7-54.8 (series of singlets overlapping with diastereomer B, CH_2 ring), 52.7 (NMe cis), 51.8 (NMe cis), 48.7 (NMe trans), 32.3 (NC<u>Me</u>$_3$), 29.8 (TiMe terminal), 24.2 (TiMe bridging).

Data for isomer B: ^{1}H NMR (CD_2Cl_2, 500.0 MHz, 233 K): 3.50-2.60 (series of mutually overlapping m, some corresponding to diastereomer A, CH_2 ring), 2.90 (s, 6 H, NMe cis), 2.84 (s, 6 H, NMe cis), 2.59 (s, 6 H, NMe trans), 1.10 (s, 18 H, ^{t}Bu), 0.30 (s, 3 H, TiMe bridging), 0.04 (s, 6 H, TiMe terminal). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 125.7 MHz, 233 K): 66.8 (N<u>C</u>Me$_3$), 56.7-54.8 (series of singlets overlapping with diastereomer A, CH_2 ring), 51.8 (NMe cis), 51.6 (NMe cis), 49.1 (NMe trans), 32.2 (NC<u>Me</u>$_3$), 30.0 (TiMe terminal), 22.8 (TiMe bridging).

Data for [B(Ar^F)$_4$]$^-$ anion: ^{13}C-{^{1}H} NMR (CD_2Cl_2, 500.0 MHz, 233 K): 147.6 (br. d, $^1J_{C\text{-}F}$ = 247 Hz, *o*-C_6F_5), 137.8 (br. d, $^1J_{C\text{-}F}$ = 225 Hz, *p*-C_6F_5), 135.9 (br. d, $^1J_{C\text{-}F}$ = 247 Hz, *m*-C_6F_5). ^{19}F NMR (CD_2Cl_2, 282.5 MHz, 293 K): -133.52 (d, ^3J = 12.2 Hz, *o*-C_6F_5), -164.06 (t, ^3J = 20.6 Hz, *p*-C_6F_5), -167.91 (app. t, app. ^3J = 16.8 Hz, *m*-C_6F_5).

Characterising data for [Ti(N^{t}Bu)(Me$_3$[9]aneN$_3$)(CH$_2$SiMe$_3$)][B(Ar^F)$_4$] (NMR only)

^{1}H NMR (CD_2Cl_2, 500.0 MHz, 213 K): 3.63 (m, 2 H, CH_2 ring), 3.06 (m, 2 H, CH_2 ring), 2.95 (s, 6 H, NMe cis), 2.90-2.50 (series of mutually overlapping m, 8 H, CH_2 ring), 2.40 (s, 3 H, NMe trans), 2.02 (s, 2 H, C<u>H$_2$</u>SiMe$_3$), 1.11 (s, 9 H, ^{t}Bu), 0.17 (s, 9 H, CH$_2$Si<u>Me</u>$_3$). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 125.7 MHz, 213 K): 147.6 (br. d, $^1J_{C\text{-}F}$ = 247 Hz, *o*-C_6F_5), 137.8 (br. d, $^1J_{C\text{-}F}$ = 225 Hz, *p*-C_6F_5), 135.9 (br. d, $^1J_{C\text{-}F}$ = 247 Hz, *m*-C_6F_5), 69.8 (N<u>C</u>Me$_3$), 55.9-54.9 (series of overlapping singlets, CH_2 ring and <u>C</u>H$_2$SiMe$_3$), 51.5 (NMe cis), 48.7 (NMe trans), 30.7 (NC<u>Me</u>$_3$), 1.3 (CH$_2$Si<u>Me</u>$_3$). ^{19}F NMR (CD_2Cl_2, 282.1 MHz, 293 K): -132.89 (d, ^3J

= 9.1 Hz, *o*-C_6F_5), -163.00 (t, ^3J = 19.6 Hz, *p*-C_6F_5), -166.84 (app. t, app. ^3J = 16.6 Hz, *m*-C_6F_5). ^{29}Si NMR (HMQC ^{1}H-observed, C_5D_5Br, 299.9 MHz, 293 K): -15.82 ($CH_2\underline{Si}Me_3$).

^{1}H and ^{13}C NMR characterising data for selected library compounds

Characterising data for [Ti(N-2,6-$C_6H_3{}^iPr_2$)(Me_3[9]aneN_3)Cl_2] (ID = 15)

Anal. found (calcd. for $C_{21}H_{38}Cl_2N_4Ti$): C, 53.9 (54.2); H, 8.4 (8.2); N, 12.0 (12.0) %. ^{1}H NMR ($CDCl_3$, 300.1 MHz, 298 K): 6.90 (d, ^3J = 7.6 Hz, 2 H, *m*-$C_6\underline{H}_3{}^iPr_2$), 6.72 (t, ^3J = 7.6 Hz, 1 H, *p*-$C_6\underline{H}_3{}^iPr_2$), 4.51 (sept, ^3J = 6.9 Hz, 2 H, C$\underline{H}Me_2$), 3.74 (m, 2 H, CH_2 ring), 3.33 (m, 2 H, CH_2 ring), 3.27 (s, 6 H, NMe cis), 3.16 (m, 2 H, CH_2 ring), 3.11 (m, 2 H, CH_2 ring), 2.77 (m, 2 H, CH_2 ring), 2.69 (s, 3 H, NMe trans), 2.56 (m, 2 H, CH_2 ring), 1.25 (d, ^3J = 6.9 Hz,12 H, CH$\underline{Me}_2$). ^{13}C-{^{1}H} NMR ($CDCl_3$, 75.5 MHz, 298 K): 155.7 (*i*-$\underline{C}_6H_3{}^iPr_2$), 145.0 (*o*-$\underline{C}_6H_3{}^iPr_2$), 122.8 (*m*-$\underline{C}_6H_3{}^iPr_2$), 121.3 (*p*-$\underline{C}_6H_3{}^iPr_2$), 58.3 ($CH_2$ ring), 57.3 (CH_2 ring), 54.4 (CH_2 ring), 54.0 (NMe cis), 49.1 (NMe trans), 27.4 ($\underline{C}HMe_2$), 25.3 (CH$\underline{Me}_2$). This compound has been crystallographically characterised and details will be reported in a subsequent full paper.

Characterising data for [Ti(NC_6F_5)(Me_3[9]aneN_3)Cl_2] (ID = 28)

Anal. found (calcd. for $C_{15}H_{21}Cl_2F_5N_4Ti$): C 38.3 (38.3); H 4.7 (4.5); N 11.7 (11.9) %. ^{1}H NMR (CD_2Cl_2, 300.1 MHz, 298 K): 3.56 (2 H, m, CH_2 ring), 3.21 (6 H, m, CH_2 ring), 3.15 (6 H, s, NMe cis), 3.01 (2 H, m, CH_2 ring), 2.75 (2 H, m, CH_2 ring), 2.74 (3 H, s, NMe trans). ^{19}F NMR (CD_2Cl_2, 282.4 MHz, 298K): -152.1 (2 F, m, *o*-C_6F_5), -167.6 (2 F, m, *m*-C_6F_5), -169.6 (1 F, m, *p*-C_6F_5). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 75.5 MHz, 298 K): 57.4 (NMe cis), 55.4 (2 signals overlapping, 2 x CH_2 ring), 53.5 (NMe trans), 49.7 (CH_2 ring), $\underline{C}_6F_5$ resonances too broad to be observed. This compound has been crystallographically characterised and details will be reported in a subsequent full paper.

Characterising data for [Ti(N-2,6-$C_6H_3Me_2$)(Me_3[9]aneN_3)Cl_2] (ID = 31)

Anal. found (calcd. for $C_{17}H_{30}Cl_2N_4Ti$): C 49.7 (49.9), H 7.5 (7.4), N 13.6 (13.7) %. ^{1}H NMR ($CDCl_3$, 300.1 MHz, 298 K): 6.76 (d, ^3J = 7.4 Hz, 2 H, *m*-$C_6\underline{H}_3Me_2$), 6.52 (t, ^3J = 7.4 Hz, 1 H, *p*$C_6\underline{H}_3Me_2$), 3.91 (m, 2 H, CH_2 ring), 3.34 (m, 2 H, CH_2 ring), 3.33 (s, 6 H, NMe cis), 3.12 (m, 2 H, CH_2 ring), 3.10 (m, 2 H, CH_2 ring), 2.78 (s, 6 H, $C_6H_3\underline{Me}_2$), 2.76 (m, 2 H, CH_2 ring), 2.70 (s, 3 H, NMe trans), 2.55 (m, 2 H, CH_2 ring). ^{13}C-{^{1}H} NMR ($CDCl_3$, 75.5 MHz, 298 K): 148.2 (*i*-$\underline{C}_6H_3Me_2$), 133.6 (*o*-$\underline{C}_6H_3Me_2$), 127.9 (*m*-$\underline{C}_6H_3Me_2$), 121.0 (*p*-$\underline{C}_6H_3Me_2$), 57.8 (CH_2 ring), 57.2 (CH_2 ring), 54.7 (CH_2 ring), 54.3 (NMe cis), 49.2 (NMe trans), 22.1 ($C_6H_3\underline{Me}_2$). This compound has been crystallographically characterised and details will be reported in a subsequent full paper.

Characterising data for [Ti(NCH$_2$Ph)(Me$_3$[9]aneN$_3$)Cl$_2$] (ID = 37)

Anal. found (calcd. for $C_{16}H_{28}N_4TiCl_2$): 48.5 (48.7); H 7.8 (7.2); N 13.5 (14.2) %. ^{1}H NMR data (CD_2Cl_2, 500.0 MHz, 298 K): 7.53 (2 H, d, ^{3}J = 7.3 Hz, *o*-C_6H_5), 7.30 (2 H, t, ^{3}J=7.8 Hz, *m*-C_6H_5), 7.17 (1 H, t, ^{3}J=7.3 Hz, *p*-C_6H_5), 4.53 (2 H, s, C$\underline{H}_2$Ph), 3.31 (2 H, m, CH_2 ring), 3.13 (2 H, m, CH_2 ring), 3.06 (6 H, s, NMe cis), 2.94 (4 H, m, CH_2 ring), 2.69 (2 H, m, CH_2 ring), 2.50 (2 H, m, CH_2 ring), 2.49 (3 H, s, NMe trans). ^{13}C-{^{1}H} NMR data (CD_2Cl_2, 125.7 MHz, 298 K): 142.0 (*i*-C_6H_5), 128.3 (*m*-C_6H_5), 127.6 (*o*-C_6H_5), 126.4 (*p*-C_6H_5), 68.6 ($\underline{C}H_2$Ph), 57.1 (CH_2 ring), 56.8 (CH_2 ring), 54.9 (CH_2 ring), 53.5 (NMe cis), 48.9 (NMe trans).

Characterising data for [Ti(N^{t}Bu)(Me$_3$[9]aneN$_3$)Cl$_2$] (1, ID =41)

Previously reported and crystallographically characterised: P. J. Wilson, A. J. Blake, P. Mountford and M Schr der, *Chem. Commun*., 1998, 1007.

Generic details for the synthesis of a library [Ti(NR)(Me$_3$[9]aneN$_3$)Cl$_2$]

[Ti(NMe$_2$)$_2$Cl$_2$][1] and Me$_3$[9]aneN$_3$[2] were prepared according to published literature procedures. A library of amines (1.94 mmol of amine per vial) was purchased in the shape of CombiKits from Aldrich and used as received. Dried solvents (benzene, toluene and hexanes) were purchased from Aldrich and used as received. Deuterated dichloromethane was dried over phosphorous pentoxide under a dinitrogen atmosphere, trap-to-trap distilled at room temperature and stored in ampoules fitted with J. Young Teflon valves. In preparation of the parallel synthesis procedure, stock solutions of [Ti(NMe$_2$)$_2$Cl$_2$] (0.32 M), Me$_3$[9]aneN$_3$ (1.06 M) and and the amine library (0.97 M) in benzene were prepared. ^{1}H NMR spectra were recorded on Bruker Avance 400 and a Varian Mercury-VX 300 spectrometers and mass spectra on a a Micromass GCT TOF Instrument using a solid probe inlet temperature program.

An M. Braun Labmaster Glovebox was equipped with a Tecan Miniprep liquid handling robot, two low-vortex flatbed shakers and a vacuum/N_2 connection. The protonolysis reaction was carried out in 24-well (6 x 4) plates, each well having a maximum volume capacity of 10 ml. In the first step, 3 ml of the titanium amide stock solution (corresponding to 200 mg of [Ti(NMe$_2$)$_2$Cl$_2$], 0.97 mmol/ well) were dispensed into each well, followed by 1 ml of the appropriate amine stock solution (corresponding to 0.97 mmol amine/well). The plate was sealed with a Teflon seal to prevent evaporation of the solvent and shaken for 16 h. After this time, the resulting solutions of [Ti(NR)Cl$_2$(NHMe$_2$)$_2$] were transferred to a 6 x 4 array of pre-weighed solid phase synthesis cartridges equipped with Teflon filter frits and housed in a specially constructed holder above a 24 well plate. The holder allows the application of either an overpressure or a vacuum from underneath the cartridges. After the solution transfer had been completed, the plates were manually checked for signs of crystallisation. If crystallisation had occurred, the crystals were gathered and

re-combined with the corresponding solution. During the solution transfer, an overpressure was applied from underneath the cartridges to keep the solutions above the frit. Subsequently, 1 ml of Me_3[9]aneN_3 stock solution (1.06 mmol/well) was dispensed into each cartridge under agitation. Addition of the macrocycle usually resulted in the formation of a thick precipitate of the corresponding [Ti(NR)(Me_3[9]aneN_3)Cl_2] complexes. The cartridges were shaken for 2 h, after which time the pressure underneath the cartridge was reversed to remove the reaction solvent, which was caught in the plate underneath. The resulting solids were washed with 3 x 1 ml of hexanes, the cartridges stoppered and the solids dried *in vacuo*. Subsequently, the cartridges were re-weighed to obtain the individual compound yields.

1. D. C. Bradley and Thomas, I. M. *J. Chem. Soc.* 1960, 3857.
2. Madison, S. A.; Batal, D. J.; *Improved synthesis of 1,4,7-triazacyclononane*; United States Patent; 5,284,944; 1994

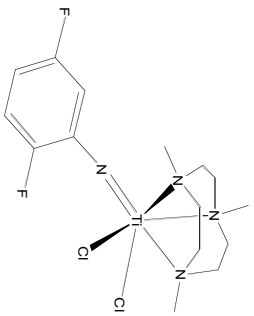
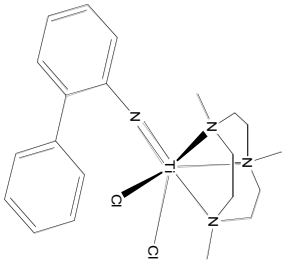
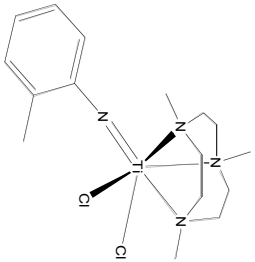
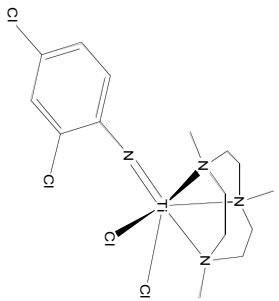
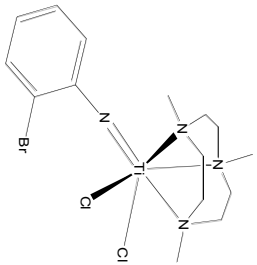
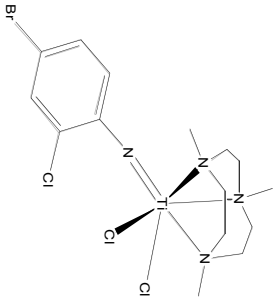
Further details of the polymer analysis

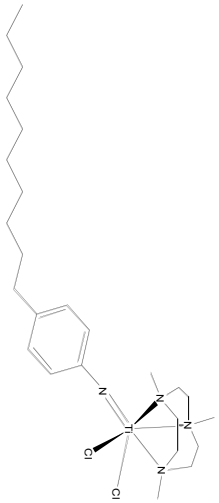
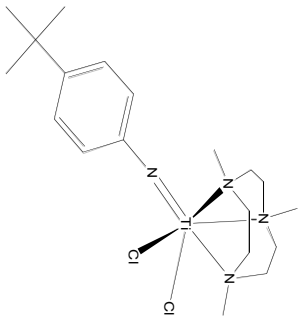
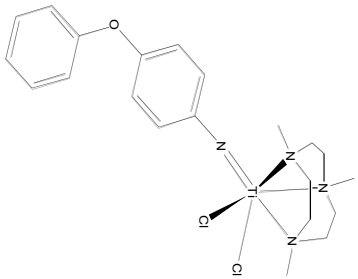
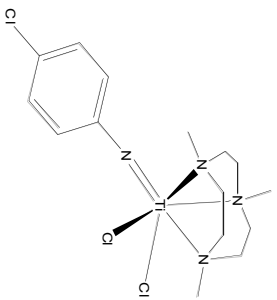
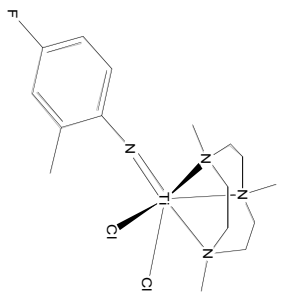
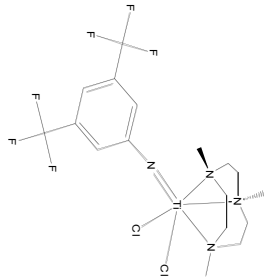
	GPC					°	FTIR CH3/1000C				FTIR C=C/100,000C-at		
ESI cmpd ID	**Mw**	**Mn**	**PD**	**Mp**	**Mz**	**Mz/Mw**	**Prop**	**But**	**Hex**	**Oct**	**main chain**	**end group**	**side chain**
16	1,501,900	391,200	3.8	1,218,200	2,739,700	1.8	0.1	0.2	0.2	0.2	0.0	5.9	4.0
45	145,950	24,450	6.0	60,700	524,600	3.8	0.6	0.8	0.9	1.1	0.5	33.1	22.6
41 (**1**)	273,850	39,500	7.0	117,900	1,101,900	4.0	1.3	2.0	2.1	2.5	4.4	21.9	14.9
34	190,700	33,000	5.8	75,300	782,800	4.1	0.7	1.0	1.1	1.3	1.5	22.7	15.5
2	119,400	19,400	6.2	57,500	546,700	4.6	1.3	1.9	2.1	2.4	2.8	43.3	29.5
32	152,700	15,200	10.0	38,800	1,266,500	8.3	1.5	2.1	2.3	2.6	3.5	53.4	36.4
7	50,300	10,400	4.8	30,700	216,000	4.3	0.9	1.4	1.5	1.7	2.5	90.6	61.7

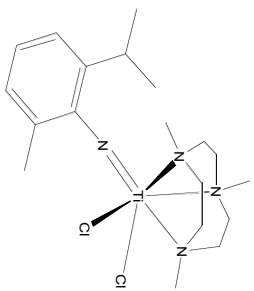
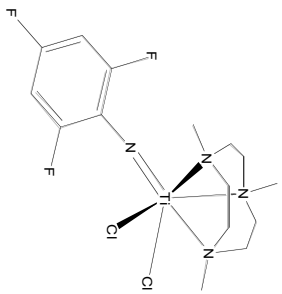
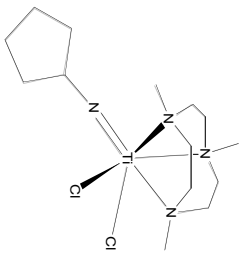
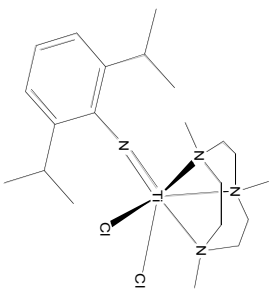
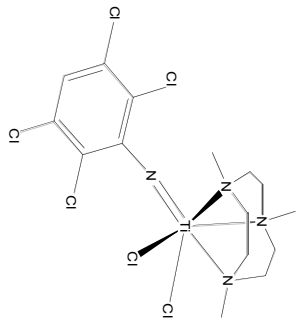
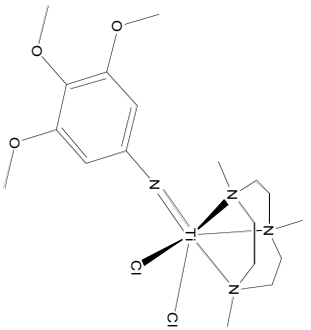
"Main chain" refers to RCH=CHR’

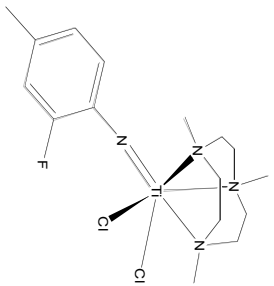
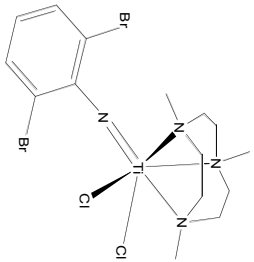
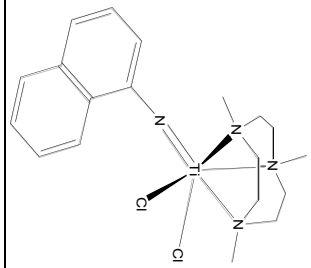
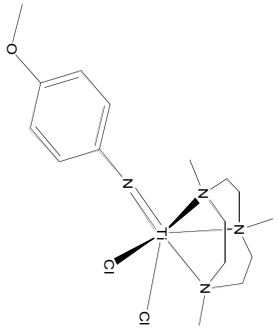
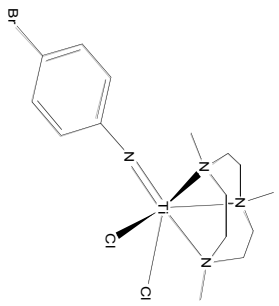
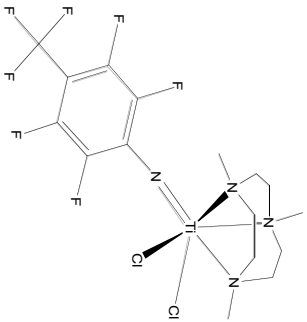
"End group" refers to $RCH=CH_2$

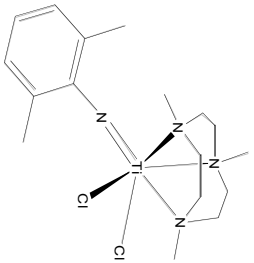
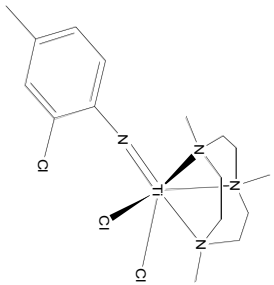
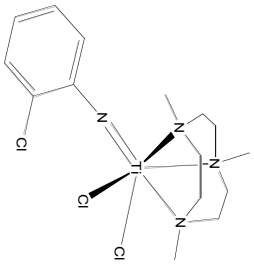
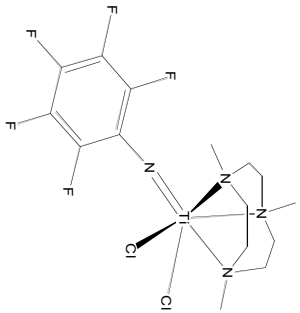
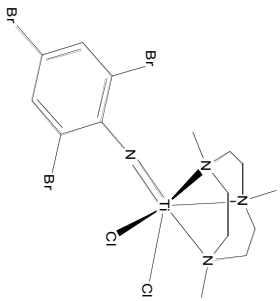
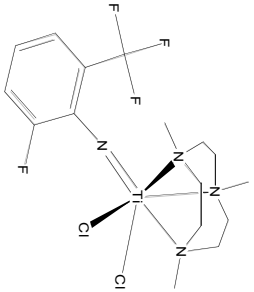
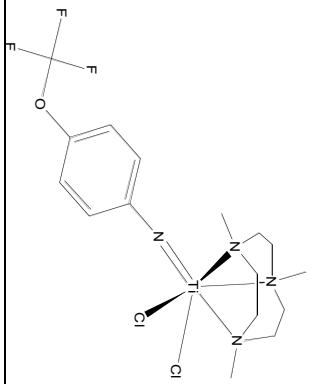
"Side chain" refers to $RCH(CH=CH_2)CH_2R$’

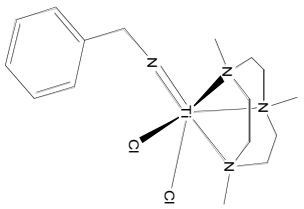
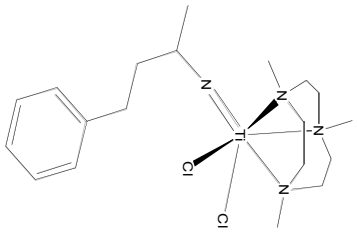
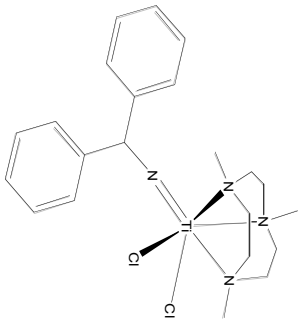
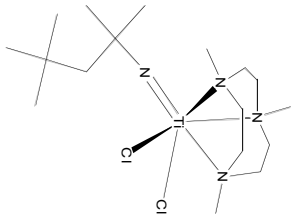
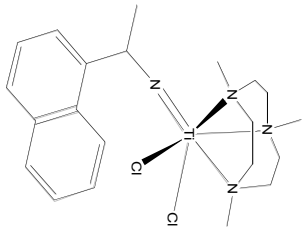
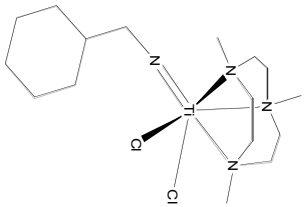
						**Structure**
6	5	4	3	2	1	**ESI compound ID**
0.188	0.216	0.296	0.258	0.247	0.191	**Yield (g)**
47	49	78	59	56	40	**Yield (%)**
416.0826	456.1327	394.1170	448.0235	458.0119	491.9729	**EI-HRMS (calcd)**
416.0828	456.1324	394.1151	448.0229	458.0136	491.9743	**EI-HRMS found)**
0.03	0.03	0.02	0.01	0.90	0.02	**Yield PE (g)**
161	161	107	54	4,821	107	**Activity (kg/mol/h/bar)**
				119,400		**Mw**
				19,400		**Mn**
				6.2		**Mw/Mn**

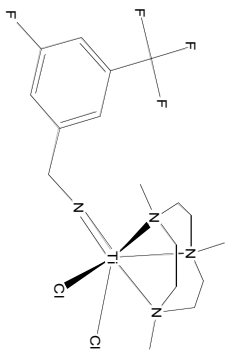
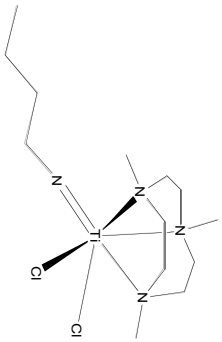
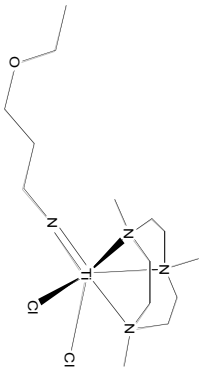
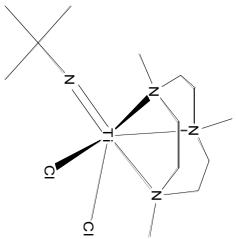
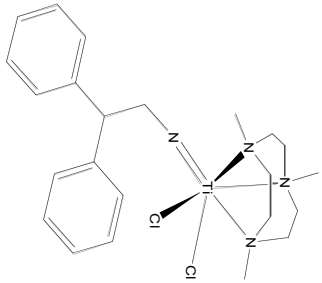
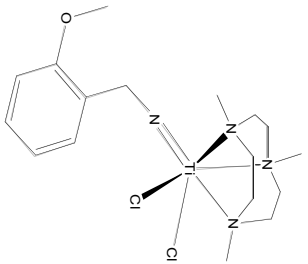
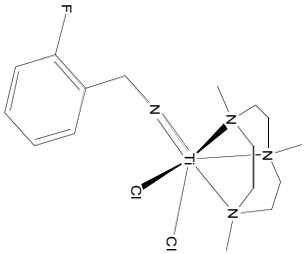
					
12	11	10	9	8	7
0.263	0.217	0.433	0.194	0.328	0.259
52	51	95	48	82	52
	436.1640	472.1276	414.0624	412.1076	516.0762
not observed	436.1649	472.1292	414.0625	412.1081	516.0761
0.00	0.00	0.00	0.07	0.01	0.63
0	0	0	375	54	3,375
					50,300
					10,400
					4.8

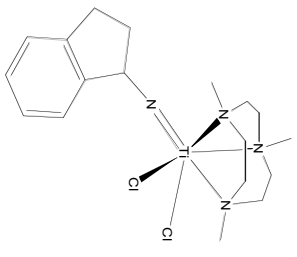
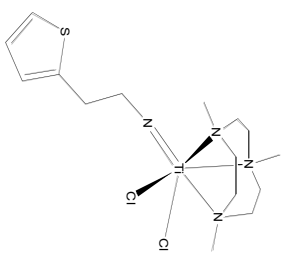
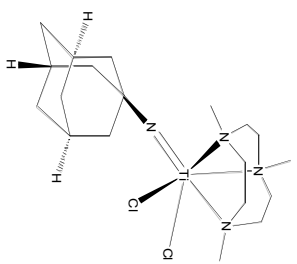
					
18	17	16	15	14	13
0.332	0.354	0.24	0.375	0	0.447
79	84	67	83	0	97
436.1640	434.0731	337.1638 [M-Cl]	464.1953	515.9455	470.1331
436.1625	434.0719	337.1631	464.1966	515.9455	470.1343
0.01	0.01	0.90	0.00	0.01	0.05
54	54	4,821	0	54	268
		1,501,900			
		391,200			
		3.8			

					
24	23	22	21	20	19
0.132	0.341	0.341	0.334	0.345	0.42
33	66	82	84	78	83
412.1076	535.9224	430.1170	410.1120	458.0119	520.0511
412.1082	535.9214	430.1154	410.1120	458.0127	520.0497
0.00	0.01	0.09	0.01	0.01	0.01
0	54	482	54	54	54

						
31	30	29	28	27	26	25
0.221	0.175	0.259	0.233	0.153	0.153	0.127
56	42	65	51	26	34	28
408.1327	428.0781	414.0624	470.0543	613.8329	466.0794	464.0837
408.1310	428.0786	414.0613	470.0544	613.8321	466.0793	464.0836
0.00	0.01	0.01	0.04	0.01	0.00	0.00
0	54	54	214	54	0	0

					
37	36	35	34	33	32
0.264	0.282	0.316	0.233	0.299	0.265
69	67	69	58	67	68
394.1170	421.1405 [M-Me]	434.1717 [M-H-Cl]	401.1718 [M-Me]	443.1249 [M-Me]	365.195 [M-Cl]
394.1160	421.1400	434.1583	401.1710	443.1249	365.1961
0.01	0.00	0.01	1.63	0.10	1.10
54	0	54	8,732	536	5,893
			190,700		152,700
			33,000		15,200
			5.8		10.0

						
44	43	42	41	40	39	38
0.281	0.228	0.21	0.113	0.276	0.285	0.279
60	65	56	32	59	69	70
480.0950	317.0779 [M - C3H7]	390.1433	345.1092 [M-Me]		424.1276	412.1076
480.0928	317.0774	390.1417	345.1082	not recognisable fragment	424.1264	412.1077
0.02	0.00	0.00	1.88	0.01	0.00	0.00
107	0	0	10,071	54	0	0
			273,850			
			39,500			
			6.9			

		
47	46	45
0.247	0.251	0.238
61	63	56
420.1330	414.0891	438.1796
420.1320	414.0890	438.1798
0.01	0.00	1.93
54	0	10,339
		145,950
		24,450
		6.0