

Chromium Complexes Supported by Bidentate Thioether-Imine [N,S] Ligands: Synthesis and Ethylene Oligomerization Studies

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Table S1. Energies of *fac* and *mer* isomers of compounds **2a–2d**. Energies are in kJ/mol, and zero values are defined as the most stable isomer.

Structure	2a		2b		2c		2d	
<i>isomer</i>	<i>fac</i>	<i>mer</i>	<i>fac</i>	<i>mer</i>	<i>fac</i>	<i>mer</i>	<i>fac</i>	<i>mer</i>
Energy (kJ/mol)	33.9	0	33.3	0	34.6	0	23.9	0

Table S2. Atomic charge values in Cr calculated via different methods.

	Mulliken	Löwdin	Hirshfeld	Voronoi
2a	0.076033	-1.051586	0.513244	0.527523
2b	0.076033	-1.096252	0.504983	0.527295
2c	0.015060	-1.059100	0.504993	0.527354
2d	0.096166	-1.059784	0.507759	0.528200

Table S3. Geometrical structures for complexes 2a**mer-Complex 2a**

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XYZ file generated by orca_plot on BaseName=Cr-struct2a_OPT

C	-12.724148	-1.829784	-0.400060
C	-12.205534	-1.983062	0.887325
C	-12.136299	-0.920907	-1.287992
C	-11.028686	-0.170542	-0.899956
C	-10.526016	-0.323052	0.397645
C	-11.106302	-1.223015	1.295825
S	-9.055352	0.515388	0.951885
C	-9.242390	2.161282	0.329335
C	-10.493311	2.760223	0.177510
C	-10.591803	4.090696	-0.231343
C	-9.436152	4.843558	-0.448890
C	-8.191301	4.256207	-0.248636
C	-8.059866	2.900828	0.112018
C	-6.677886	2.440444	0.265925
N	-6.127220	1.273280	0.195242
C	-4.600667	1.284123	0.298470
C	-4.069199	2.479012	1.114504
C	-4.081097	1.378799	-1.145589
C	-4.100896	0.013090	0.990827
H	-10.690390	-1.331817	2.297735
H	-12.659564	-2.690203	1.582345
H	-13.586463	-2.418867	-0.714347
H	-12.533895	-0.806703	-2.297354
H	-10.529913	0.505422	-1.595062
H	-9.505010	5.886278	-0.758197
H	-7.283354	4.842975	-0.399816
H	-11.394018	2.180404	0.373581
H	-11.576431	4.540995	-0.361834
H	-6.011539	3.293639	0.423248
H	-4.147647	3.444544	0.594738
H	-3.000008	2.308237	1.293175
H	-4.565745	2.553159	2.092860
H	-4.414876	2.317053	-1.612014
H	-2.982078	1.361546	-1.134749
H	-4.440671	0.538285	-1.749419
H	-4.461556	-0.038525	2.025233
H	-3.002078	0.041111	0.999479
H	-4.417979	-0.892786	0.468282
Cr	-7.208403	-0.461536	-0.389285
O	-8.551864	-2.013194	-0.946321
Cl	-5.639042	-1.660723	-1.527525
Cl	-7.867802	0.744834	-2.247838
Cl	-6.877434	-1.497591	1.660715
C	-8.480076	-3.332727	-0.323291
C	-9.637331	-4.090550	-0.956356
C	-9.726932	-3.510235	-2.388331
C	-8.822355	-2.271351	-2.364172
H	-9.273024	-1.361083	-2.763821
H	-7.853743	-2.436685	-2.856916
H	-9.373038	-4.224442	-3.142929
H	-10.762047	-3.243366	-2.636465
H	-8.554492	-3.180071	0.755339
H	-10.563840	-3.886414	-0.403923
H	-9.462413	-5.174021	-0.944842
H	-7.495396	-3.765563	-0.560468

fac-Complex 2a

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Coordinates from ORCA-job Cr-struc2a_fac_OPT

C	-12.89215170294304	-1.60175200894622	0.16556163259834
C	-12.40437808856082	-1.48194296381817	1.46775328572770
C	-12.14374964679929	-1.12111172704676	-0.91578318481490
C	-10.90122150921063	-0.52818020244705	-0.70651155128645
C	-10.42942987876156	-0.40455490749494	0.60523233629485
C	-11.16588580713851	-0.87355313578935	1.69390366732711
S	-8.84242711022601	0.33577657560275	0.93145146823987
C	-9.08155196631602	2.00202758417223	0.37933283033411
C	-10.36371250774538	2.54662775535143	0.28497353883990
C	-10.54220193124118	3.87035260887590	-0.11717974028546
C	-9.43607491584955	4.67555046552152	-0.39417419463215
C	-8.15990725655078	4.14161161848572	-0.26000405599837
C	-7.94835867775281	2.79413523291268	0.09649635075155
C	-6.54325970325502	2.40345953817211	0.17121190217604
N	-5.94964563513000	1.25721595481671	0.10769136885172
C	-4.42336759193953	1.35914492785415	0.15150609173110
C	-3.92968024420452	2.54976428062910	1.00021404069627
C	-3.96249117701961	1.53734647449101	-1.30412747093989
C	-3.81700572381400	0.09564148347338	0.76957337040222
H	-10.77565539033565	-0.75955487808129	2.70574053269269
H	-12.98548994691040	-1.85623593182741	2.31112880666318
H	-13.85861858867567	-2.07577855745365	-0.01066092542395
H	-12.51965207207395	-1.22946308709921	-1.93356646336348
H	-10.28577000885455	-0.17734546712481	-1.53590194448461
H	-9.56690009132859	5.71278883032131	-0.70163659230885
H	-7.28646513058181	4.76460212369566	-0.46171127948497
H	-11.22828062605126	1.92684197276172	0.51463309123534
H	-11.55272983267347	4.27155952640565	-0.20132297564296
H	-5.91090097294757	3.29325923823318	0.25836716993270
H	-4.06963468675079	3.52848844004530	0.52089456996174
H	-2.84905380601576	2.43009743792720	1.15089269217818
H	-4.40875621989407	2.56599099270062	1.99038417378493
H	-4.36934286923215	2.47000925074722	-1.72084294352465
H	-2.86467675273315	1.58813793120996	-1.33566866104659
H	-4.29776489770316	0.69802350447532	-1.92352981022234
H	-4.10260981033595	0.00074516491649	1.82599580914165
H	-2.72270279909467	0.18324160922097	0.72295600422607
H	-4.11453314693264	-0.80377832551629	0.22554580706846
Cr	-7.02745521126567	-0.57648334024599	-0.51939123526863
O	-6.25020749076236	-1.50667312760999	1.26556731544470
Cl	-5.36858439336846	-1.56276835289529	-1.71128066085538
Cl	-7.84571224652989	0.56937232200289	-2.28476672799848
Cl	-8.37847575826785	-2.39856548084929	-0.78503362043560
C	-6.51029078125178	-1.13317116715837	2.63788309041815
C	-7.48114564155730	-2.19942796764083	3.14235911034274
C	-7.10131190104093	-3.45720923860518	2.31366606199219
C	-6.04915187849386	-2.95200309501862	1.31792229159701
H	-6.16049591207743	-3.32905243999961	0.29913417404467
H	-5.01921901998559	-3.11749191874131	1.67425689081471
H	-6.69741855762581	-4.26185151316728	2.94170108543590
H	-7.97434786281128	-3.83698800234796	1.77072304218312
H	-6.89714362711025	-0.10965352338808	2.64665875947025
H	-8.51438610626319	-1.89736593914877	2.92377793377841
H	-7.39153239512149	-2.35191362887521	4.22582319256131
H	-5.55064400288331	-1.16352565668525	3.18281132907879

Table S4. Geometrical structures for complexes 2b**mer-Complex 2b**

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XYZ file generated by orca_plot on BaseName=Cr-struc2b_OPT3

C	-12.810577	-1.655308	-0.806465
C	-12.401133	-1.948490	0.496057
C	-12.130646	-0.684858	-1.551803
C	-11.037040	-0.013261	-1.009109
C	-10.643064	-0.308104	0.301213
C	-11.319138	-1.268355	1.060316
S	-9.180509	0.386768	1.043494
C	-9.200894	2.093466	0.566593
C	-10.403892	2.786468	0.424081
C	-10.405029	4.158750	0.172405
C	-9.198279	4.858817	0.102977
C	-8.001338	4.174573	0.279951
C	-7.964890	2.779383	0.484981
C	-6.629559	2.210390	0.597668
N	-6.218136	0.986854	0.449462
C	-4.795570	0.816031	0.442228
C	-4.177900	-0.111995	1.281710
H	-10.988635	-1.485949	2.076397
H	-12.929020	-2.701530	1.082244
H	-13.660162	-2.181890	-1.242808
H	-12.442837	-0.461094	-2.572821
H	-10.462932	0.702261	-1.597318
H	-9.191468	5.933117	-0.080165
H	-7.053928	4.714291	0.231668
H	-11.345804	2.246036	0.508570
H	-11.354236	4.681234	0.048941
H	-5.850649	2.959519	0.793285
Cr	-7.312649	-0.642694	-0.221145
O	-8.634465	-2.129374	-0.913642
Cl	-5.630052	-1.741912	-1.253213
Cl	-7.829607	0.675060	-2.057747
Cl	-7.078317	-1.750012	1.811867
C	-8.654786	-3.461342	-0.313174
C	-9.754825	-4.198323	-1.073942
C	-9.817564	-3.486470	-2.450508
C	-8.782391	-2.366255	-2.351209
H	-9.076859	-1.413466	-2.795990
H	-7.793654	-2.654902	-2.738530
H	-9.580086	-4.160815	-3.283214
H	-10.820157	-3.075036	-2.622345
H	-8.836465	-3.326271	0.755243
H	-10.714196	-4.099742	-0.549932
H	-9.522883	-5.267562	-1.160093
H	-7.657993	-3.906945	-0.454543
C	-4.024402	1.570424	-0.455957
C	-2.647529	1.405648	-0.503317
C	-2.021324	0.489062	0.355826
C	-2.793949	-0.266014	1.251826
O	-0.663775	0.392929	0.236021
C	0.000855	-0.574627	1.047626
H	-0.126307	-0.354696	2.120437
H	-0.366124	-1.592320	0.837596
H	1.061889	-0.505809	0.784522
H	-2.038022	1.958617	-1.217816
H	-4.525023	2.234489	-1.161265
H	-2.331091	-0.989797	1.919610
H	-4.791717	-0.719039	1.944842

fac-Complex 2b

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Coordinates from ORCA-job Cr-struct2b_fac_OPT

C	-13.07794720409436	-1.21147849653792	0.82758267986579
C	-12.37805755903013	-1.13094310050697	2.03290696466382
C	-12.47771780832622	-0.79568481210331	-0.36655930389340
C	-11.17346727765855	-0.30621570039911	-0.36866777400276
C	-10.48844294238409	-0.21771045505051	0.84843129203461
C	-11.07480677267174	-0.62577483495923	2.04848932276246
S	-8.80679056798919	0.36184589836222	0.90536056481876
C	-8.94479050038813	2.05882063807090	0.38985479580068
C	-10.16888422184099	2.72555249840261	0.42052727871098
C	-10.24535225144390	4.07254462923943	0.06130373026976
C	-9.09295738497916	4.77765181743130	-0.29266602887666
C	-7.86687578999483	4.12231160323987	-0.28467555516148
C	-7.76841581211533	2.75150536589433	0.01983345355902
C	-6.43395500605450	2.17766969995747	0.00112921740026
N	-6.08246935766259	0.94251479661053	-0.21113609323039
C	-4.71539081694279	0.65846942446251	0.11845872088457
C	-4.28344200433810	0.87726330603690	1.43067514707250
H	-10.51632676834284	-0.54664855843478	2.98169597167059
H	-12.84344800989831	-1.45660694084625	2.96374078850359
H	-14.09520034559994	-1.60512231864735	0.81593898626801
H	-13.02027705140841	-0.87444893016512	-1.30909447317101
H	-10.67357550304831	-0.00634470381698	-1.29064971765123
H	-9.14972627659827	5.83171814434432	-0.56319005108869
H	-6.95488326808867	4.66084227095834	-0.54874187461210
H	-11.06837253791672	2.18790960449947	0.71441735150175
H	-11.21443518138383	4.57256927534992	0.07322700248998
H	-5.62752733174890	2.89791999284252	0.19727496928682
Cr	-7.36393059667153	-0.66165963876087	-0.86102748724739
O	-6.25331294700877	-1.77008838207319	0.63836024815843
Cl	-5.96954848780818	-1.53979569637770	-2.41162141378533
Cl	-8.38461978905838	0.66570505983779	-2.38191368104729
Cl	-8.84627412926171	-2.38377280614369	-0.96984109363880
C	-6.43811055995874	-1.62784250108945	2.06781099320542
C	-7.38342589061939	-2.76505308774933	2.43464686385039
C	-6.94724549695859	-3.90265931553749	1.47704489020137
C	-6.04669587744017	-3.20720058228693	0.44113716692702
H	-6.29377515557409	-3.42290744205002	-0.60015511371095
H	-4.97663134180566	-3.39579642316459	0.61861670485046
H	-6.39430505195032	-4.68998534268428	2.00664863749743
H	-7.81892616631942	-4.35163632051599	0.98833032979085
H	-6.82479546633045	-0.62347313964293	2.26446389364210
H	-8.41949788868904	-2.46922246168703	2.21886733589274
H	-7.31152212214020	-3.03944667915319	3.49536497995591
H	-5.44942368701628	-1.73507345073461	2.54574339353651
C	-3.80631385011779	0.17728364686413	-0.83461829282389
C	-2.49522167175584	-0.08514985083224	-0.46724571250658
C	-2.06674954604495	0.11022497969814	0.85727095624771
C	-2.96883843920979	0.59747470079404	1.81245442980812
O	-0.76168471325479	-0.20075242580331	1.11381974442446
C	-0.28744855672854	-0.00307412713491	2.44425794804534
H	-0.36452121016461	1.05493757320893	2.74469452919852
H	-0.84105817976770	-0.62819490674884	3.16444960184704
H	0.76547009511680	-0.30411635165605	2.43414058824925
H	-1.77554617751409	-0.44915521097816	-1.20056809903670
H	-4.14452869522605	0.00849533939309	-1.85374166649922
H	-2.66717165632386	0.75879830254864	2.84558004290962
H	-4.99606579244901	1.23985644622497	2.17315307618116

Table S5. Geometrical structures for complexes 2c

***mer*-Complex 2c**

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XYZ file generated by orca_plot on BaseName=Cr-struc2c_OPT4

C	-12.905810	-1.485510	-0.783322
C	-12.470155	-1.814724	0.502224
C	-12.224398	-0.513929	-1.525160
C	-11.104557	0.125349	-0.995190
C	-10.685048	-0.204286	0.298535
C	-11.362089	-1.168206	1.053484
S	-9.197702	0.449026	1.028559
C	-9.156898	2.150653	0.535036
C	-10.333385	2.889916	0.401823
C	-10.284092	4.258440	0.135019
C	-9.052558	4.910480	0.040209
C	-7.881034	4.181797	0.210398
C	-7.897212	2.789231	0.431693
C	-6.582498	2.170352	0.538849
N	-6.227444	0.929551	0.412340
C	-4.808456	0.695861	0.429259
C	-4.234609	-0.125943	1.402056
H	-11.011429	-1.413331	2.056514
H	-12.997695	-2.570539	1.085012
H	-13.776683	-1.985091	-1.209269
H	-12.555919	-0.263206	-2.533666
H	-10.532976	0.843261	-1.582731
H	-9.006770	5.981581	-0.155238
H	-6.913878	4.683391	0.145794
H	-11.294839	2.388837	0.506045
H	-11.213976	4.816403	0.019854
Cr	-7.374114	-0.670505	-0.224651
O	-8.708378	-2.147910	-0.871322
Cl	-5.723268	-1.828564	-1.240034
Cl	-7.861464	0.628191	-2.081759
Cl	-7.174633	-1.735942	1.831613
C	-8.678826	-3.491818	-0.260520
C	-9.219056	-4.448360	-1.326417
C	-9.912837	-3.519990	-2.333377
C	-9.021865	-2.295175	-2.294380
H	-9.491961	-1.361926	-2.610878
H	-8.075795	-2.431338	-2.840268
H	-9.978113	-3.950653	-3.341058
H	-10.926375	-3.256874	-1.996445
H	-9.308677	-3.427377	0.634539
H	-9.895692	-5.196665	-0.894137
H	-8.388609	-4.978887	-1.812435
H	-7.646962	-3.703777	0.037102
C	-4.023631	1.291885	-0.564366
C	-2.647332	1.066646	-0.578411
C	-2.060059	0.259924	0.398719
C	-2.856032	-0.330483	1.385133
H	-2.036576	1.511924	-1.364632
H	-4.510019	1.873297	-1.348126
H	-2.402087	-0.967536	2.145061
H	-4.876046	-0.607412	2.137709
H	-0.984477	0.079989	0.384182
H	-5.771316	2.890400	0.712251

fac-Complex 2c

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Coordinates from ORCA-job Cr-struct2c_fac_OPT

C	-12.53401153832755	-0.29096246616154	-2.58010310529115
C	-12.56393854761625	-1.28643580767154	-1.60115261106248
C	-11.55647840299072	0.70801091280745	-2.53481379886913
C	-10.60493437941829	0.71377805281077	-1.51693068590975
C	-10.65804747199962	-0.27709080292312	-0.53245761798754
C	-11.62740332887224	-1.28211766299388	-0.56579836389266
S	-9.44358756079164	-0.35344874705843	0.77239011174190
C	-9.27037040495054	1.36909639093330	1.17212987998386
C	-10.42286530192003	2.02164359039861	1.63021067502709
C	-10.38643614105767	3.35350062222171	2.03079866686757
C	-9.17716737768427	4.05642652148854	1.98850747247476
C	-8.03440894448669	3.41756286504091	1.53135596090277
C	-8.04111048252675	2.06438013821970	1.10690824511313
C	-6.75637797919046	1.60830435530080	0.59587141913389
N	-6.33807308196539	0.45402225236182	0.17032058693831
C	-4.95061067976613	0.45758482276615	-0.22346359134818
C	-3.98236042382607	0.91350127325925	0.68159488463534
H	-11.62640101539061	-2.06110893201406	0.19491851093159
H	-13.31779540298590	-2.07330923759845	-1.63977802658083
H	-13.26832104179708	-0.29739520065539	-3.38645332750547
H	-11.51822020430759	1.47418780748131	-3.30985751997008
H	-9.81794619931826	1.46559656849598	-1.49632278746446
H	-9.13086345326235	5.09866501620301	2.30408036909694
H	-7.09310816015124	3.96780272051972	1.47953656556934
H	-11.35932269287361	1.46414552904391	1.66342094035647
H	-11.29761733154161	3.83902040030555	2.38150256493768
Cr	-7.37997392352871	-1.39354789641754	0.02098445664186
O	-7.14829658365723	-1.48226186536876	2.17144819764162
Cl	-5.52139721722980	-2.66800937430420	-0.15611407001292
Cl	-7.76511724294932	-0.89613746909988	-2.14693702457717
Cl	-8.79804775422901	-3.19353605555183	0.01321201068794
C	-5.85326756625872	-1.13128153991755	2.76752885308873
C	-5.64722376156950	-2.11045440181332	3.91732928007742
C	-7.08410089223539	-2.49060503377105	4.30069851153082
C	-7.74996531139756	-2.57960716118546	2.93933096231917
H	-8.83268199821339	-2.41509839449297	2.93189934367930
H	-7.52716600304796	-3.52130957791365	2.42019462483538
H	-7.14723024719095	-3.43995411809630	4.84794911552947
H	-7.54832927908484	-1.70324179839560	4.91389039666085
H	-5.93768745779801	-0.08887600025984	3.11089128382213
H	-5.07813398655515	-1.66275169909044	4.74219430273015
H	-5.10329318409290	-2.99575511482309	3.55884465142343
H	-5.08994075404203	-1.21825309037589	1.98607335831606
C	-4.57101355913127	0.01551016798423	-1.49555237292039
C	-3.22618548803209	0.05106722432799	-1.85606452834630
C	-2.25378100591427	0.49642704376457	-0.95520423153593
C	-2.63482046454589	0.92415315603384	0.31746228919355
H	-2.93543921933091	-0.28816761671401	-2.85075178685547
H	-5.33696237079081	-0.34524953177786	-2.17974062394833
H	-1.88493112408941	1.26047915393390	1.03453683338270
H	-4.28502862786902	1.22596188325825	1.68204873237874
H	-1.20159110934428	0.50186470036676	-1.24191587791630
H	-6.02261676885298	2.42479480711759	0.55187166434457

Table S6. Geometrical structures for complexes 2d

mer-Complex 2d

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XYZ file generated by orca_plot on BaseName=Cr-struct2d_OPT3

C	-11.306624	-0.526850	-1.201249
C	-10.974572	-0.525157	0.290112
S	-9.323046	0.294254	0.640542
C	-9.352191	1.959162	0.031365
C	-10.489990	2.638403	-0.409175
C	-10.435103	3.989119	-0.760046
C	-9.244082	4.703955	-0.642801
C	-8.106869	4.041109	-0.195566
C	-8.121807	2.666849	0.107184
C	-6.823864	2.108562	0.449401
N	-6.397153	0.888777	0.340049
C	-4.996577	0.714089	0.633946
C	-4.587342	-0.043099	1.732285
H	-10.522483	-1.048659	-1.759582
H	-9.201100	5.762560	-0.896958
H	-7.160628	4.578000	-0.108005
H	-11.438970	2.121411	-0.492459
H	-11.341197	4.482178	-1.114283
Cr	-7.351356	-0.718548	-0.560980
O	-8.370391	-2.327169	-1.517399
Cl	-5.449187	-1.564736	-1.447933
Cl	-7.793045	0.635788	-2.371802
Cl	-7.275531	-1.960481	1.401180
C	-8.029940	-3.705860	-1.142258
C	-8.911670	-4.566441	-2.043620
C	-9.167004	-3.678237	-3.290486
C	-8.436230	-2.371279	-2.982505
H	-8.941051	-1.459256	-3.308236
H	-7.401292	-2.357174	-3.355531
H	-8.781368	-4.128814	-4.213814
H	-10.241985	-3.502864	-3.428747
H	-8.212127	-3.798714	-0.069227
H	-9.857478	-4.813629	-1.543526
H	-8.409771	-5.509890	-2.293234
H	-6.954854	-3.838285	-1.334697
C	-4.061291	1.322025	-0.210366
C	-2.700222	1.168217	0.049979
C	-2.277810	0.418415	1.150456
C	-3.222820	-0.180836	1.987669
H	-1.969235	1.624907	-0.618241
H	-4.411645	1.860312	-1.091320
H	-2.897780	-0.769125	2.846619
H	-5.335752	-0.529274	2.354185
H	-1.212922	0.293521	1.350194
C	-10.752885	-1.965382	0.774800
C	-12.053520	0.119440	1.170181
H	-11.408580	0.476114	-1.628612
H	-12.258111	-1.061320	-1.349048
H	-11.769133	0.064198	2.229287
H	-12.990334	-0.443613	1.037778
H	-12.257144	1.167678	0.929369
H	-10.023050	-2.484543	0.147871
H	-10.401349	-1.998529	1.813795
H	-11.715290	-2.495244	0.711591
H	-6.090758	2.851544	0.791396

fac-Complex 2d

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Coordinates from ORCA-job Cr-struc2d_fac_OPT

C	-11.62024697722361	-0.40207590955092	-0.46574098616950
C	-11.05117769661907	-0.14604621670486	0.93043505117838
S	-9.26610493164493	0.47266462111144	0.85149835106462
C	-9.27644259131193	2.04347013089896	0.01102167325805
C	-10.43191208931522	2.70018193564176	-0.42259469740707
C	-10.37395387270092	3.97545326106087	-0.98687159303868
C	-9.15980086935467	4.65058778062678	-1.10210084089937
C	-8.00306885325443	4.01094911615536	-0.67520304719026
C	-8.03126916042546	2.70050215614327	-0.16447230728533
C	-6.73139991290746	2.12597087873870	0.12211501492896
N	-6.37827277391865	0.88215865692298	0.04401951620225
C	-5.03338460685815	0.63068905153550	0.48799208861188
C	-4.76964057595091	0.62480241640138	1.86188898134425
H	-11.00302027416381	-1.13923592217353	-0.99375939382064
H	-9.11485955808622	5.65442156408774	-1.52304620865055
H	-7.03473666705861	4.50570401608979	-0.77044993624924
H	-11.39821534953133	2.21937144033655	-0.34947427833667
H	-11.29861566692035	4.44222506885540	-1.32837071263475
Cr	-7.55281888001599	-0.80072651890247	-0.60329653715683
O	-6.68167089173458	-1.67602687806746	1.21900671765639
Cl	-5.89959938745461	-1.68479062504878	-1.86564459715664
Cl	-8.40247085204571	0.30825477348835	-2.36989033668438
Cl	-8.87324959769692	-2.64201526663880	-0.81853289532079
C	-7.52416814674435	-2.35086739180782	2.19339827674863
C	-7.26686025586607	-3.85764338804426	2.02094188799095
C	-5.99647338404205	-3.91752397653707	1.13673034507690
C	-5.46721156588385	-2.49326011458870	1.18257703783325
H	-4.89357693352076	-2.18900062734752	0.30494248663332
H	-4.90440105153669	-2.27726280304891	2.10571591371333
H	-5.25710979269727	-4.64357022974071	1.49905493093029
H	-6.26318696923011	-4.16464709308073	0.10128224013210
H	-8.55331845460795	-2.05639259063422	1.99309570240992
H	-8.11321000606923	-4.34065522859937	1.51961248737835
H	-7.11448273726956	-4.33799672547831	2.99689493485479
H	-7.22218513318939	-1.98941832520356	3.19047591251977
C	-4.00866432746534	0.40828764942773	-0.43538995699417
C	-2.71580412186788	0.16190244395026	0.03020327714386
C	-2.44638544597997	0.13302532583981	1.40151123282598
C	-3.47471620450929	0.37153352347550	2.31689805175504
H	-1.91450269294251	-0.01239371219103	-0.68861527436515
H	-4.23814631499132	0.41292937863088	-1.49817643628868
H	-3.27170547533176	0.35914042679531	3.38854459923069
H	-5.59057999011292	0.79043263576074	2.55992619785593
H	-1.43505807262987	-0.06927605326107	1.75582682398294
C	-10.95387302413227	-1.47735221408069	1.68758983229754
C	-11.87281492079358	0.81738341413890	1.79970014705106
H	-11.67732949838984	0.49259022115316	-1.09289456850103
H	-12.63835976355892	-0.80696890701251	-0.35307425850613
H	-11.43150736591783	0.90042384507143	2.80214852588729
H	-12.88458868273647	0.39688211991977	1.90712414157227
H	-11.97297935538807	1.82737692993101	1.39308803847360
H	-10.39145839085413	-2.22207580848262	1.11132027667078
H	-10.50909422381941	-1.34473075312547	2.68398926470397
H	-11.97785798131174	-1.85472863993094	1.82740196057713
H	-5.95289269041602	2.85431788709302	0.39025895216139

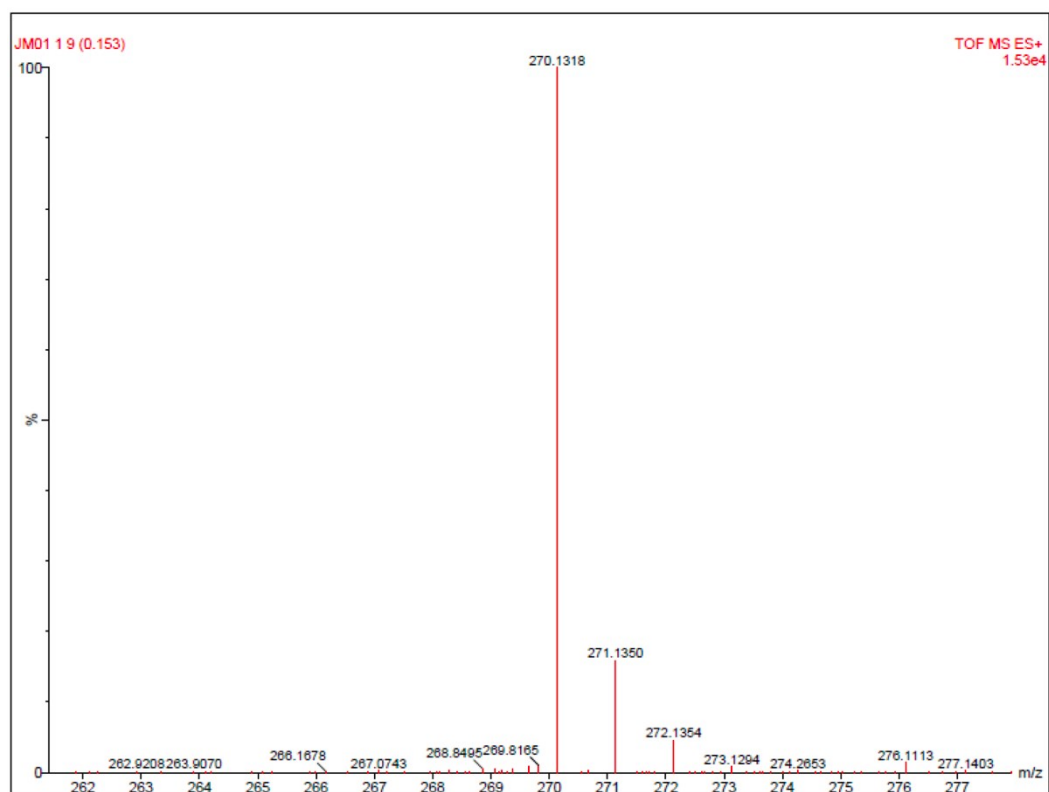


Figure S1. ESI-HRMS(+) for **1a**

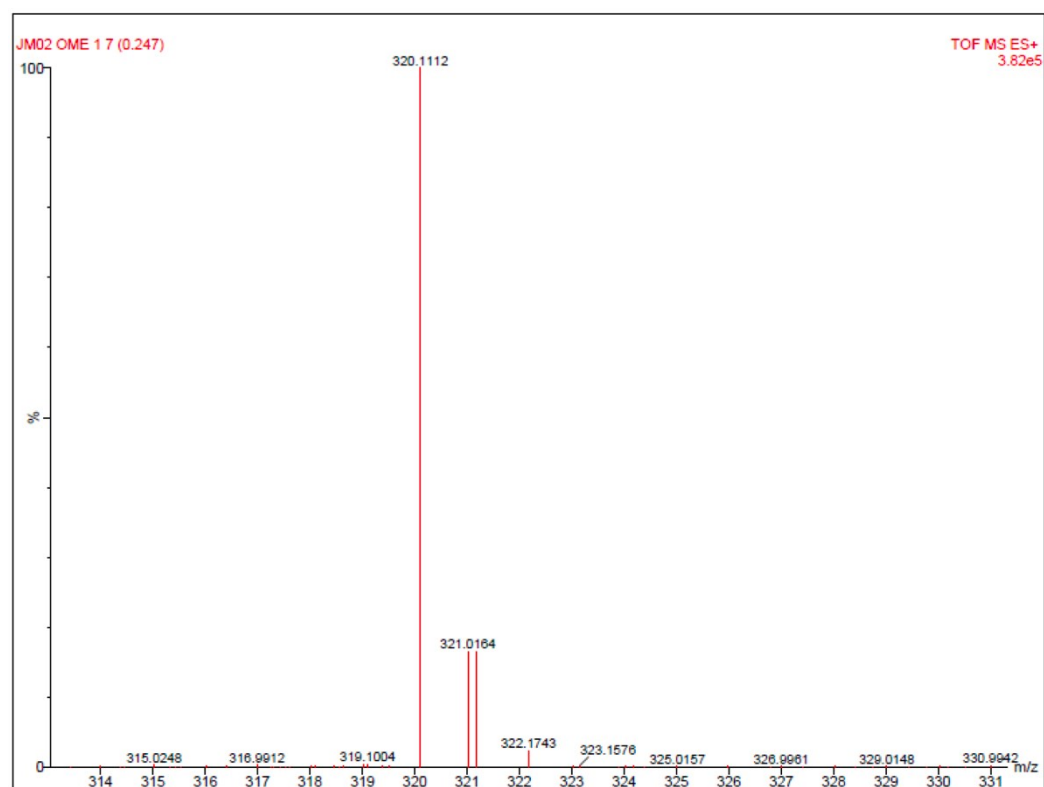


Figure S2. ESI-HRMS(+) for **1b**

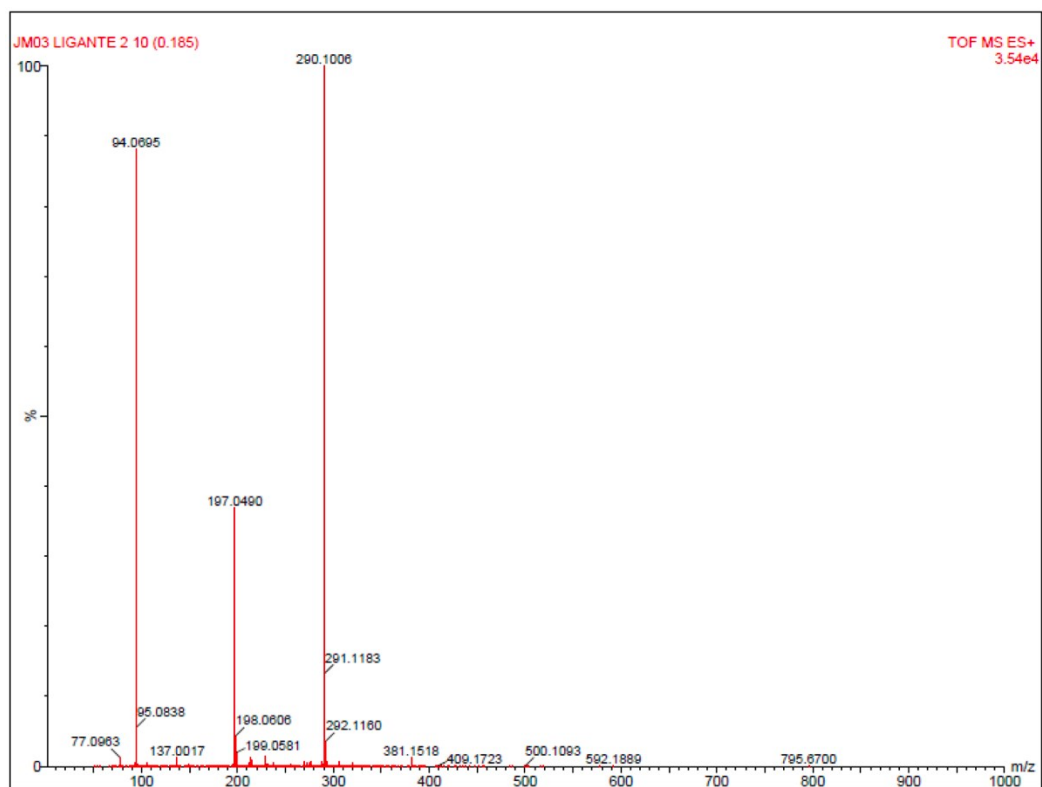


Figure S3. ESI-HRMS(+) for 1c

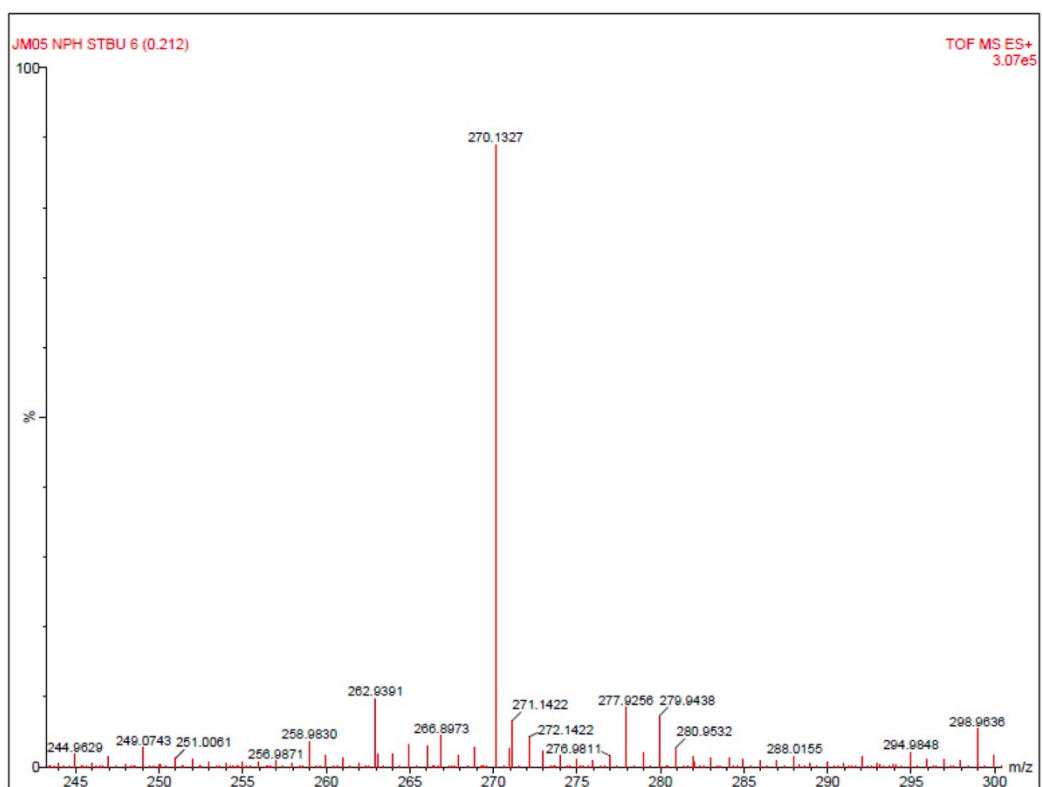


Figure S3. ESI-HRMS(+) for 1d

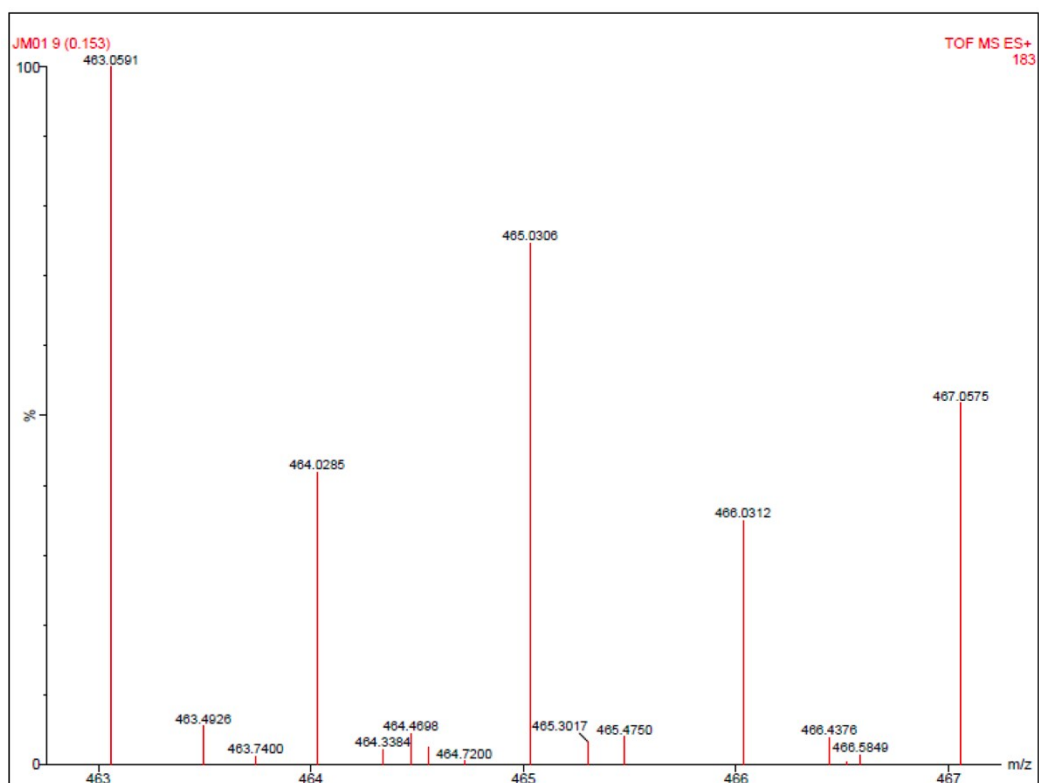


Figure S5. ESI-HRMS(+) for **2a**

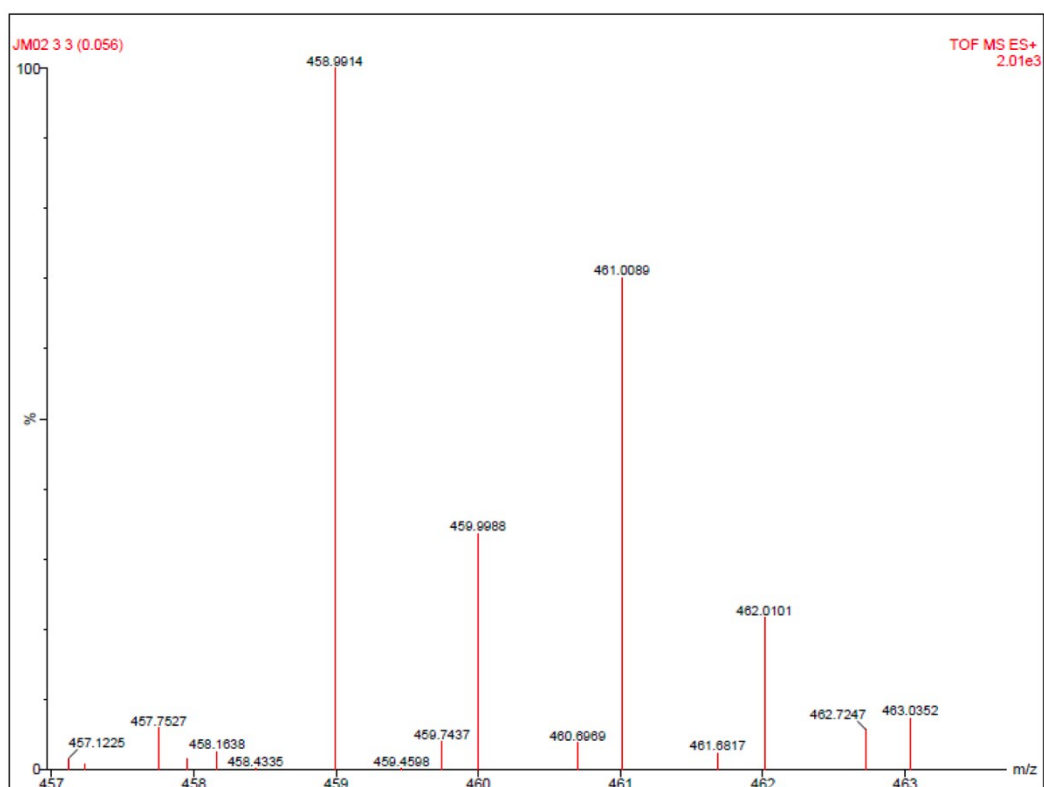


Figure S6. ESI-HRMS(+) for **2b**

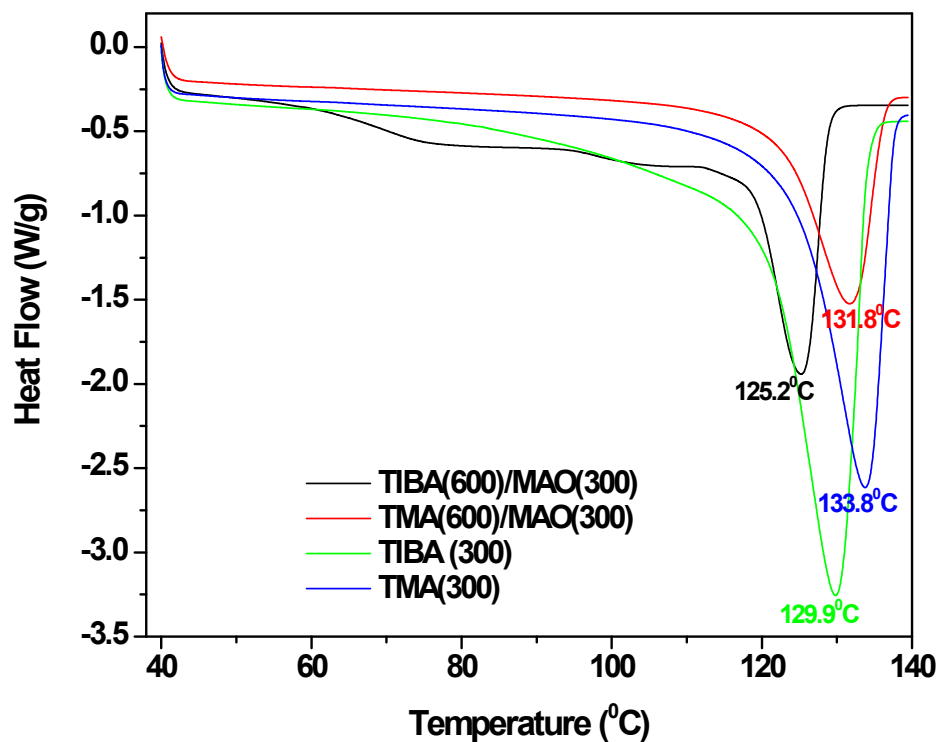


Figure S7. DSC curve of polyethylene produced by **2a** varying the cocatalyst composition and cocatalyst type (80°C, 20 bar, time = 15 min).

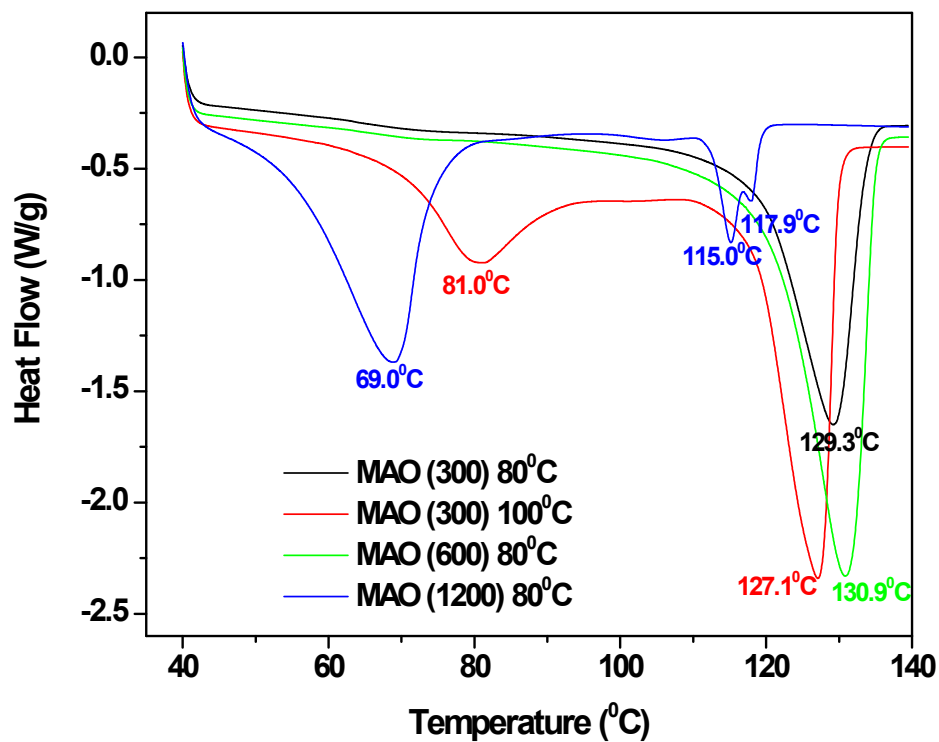


Figure S8. DSC curve of polyethylene produced by **2a**/MAO systems varying the temperature and [Al]/[Cr] molar ratio (20 bar, time = 15 min, [Al]/[Cr] = 300).

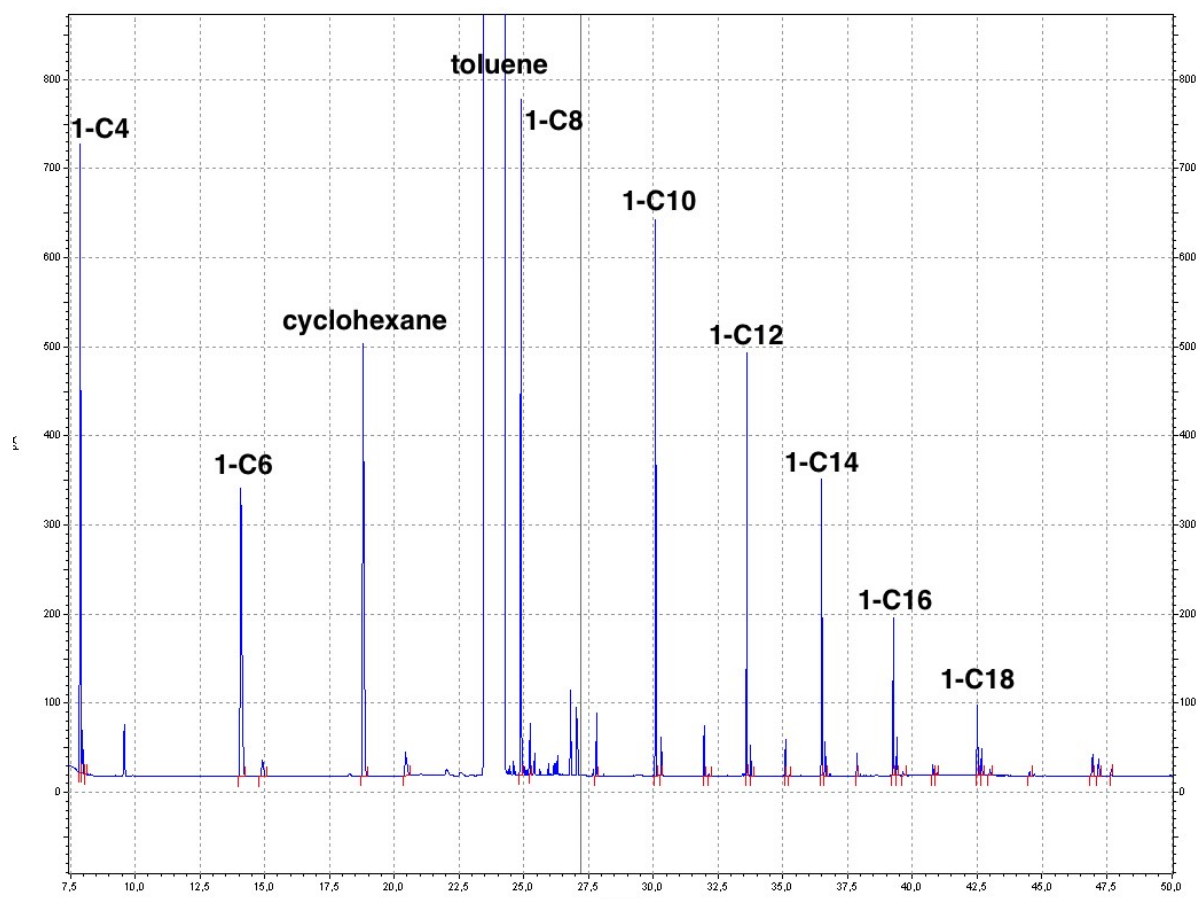


Figure S9. Typical GC trace for the toluene soluble fraction using **2a**/MAO (Table 2, entry 1, [Al]/[Cr] = 300, oligomerization time = 15 min, P(ethylene) = 20 bar, T = 80°C).

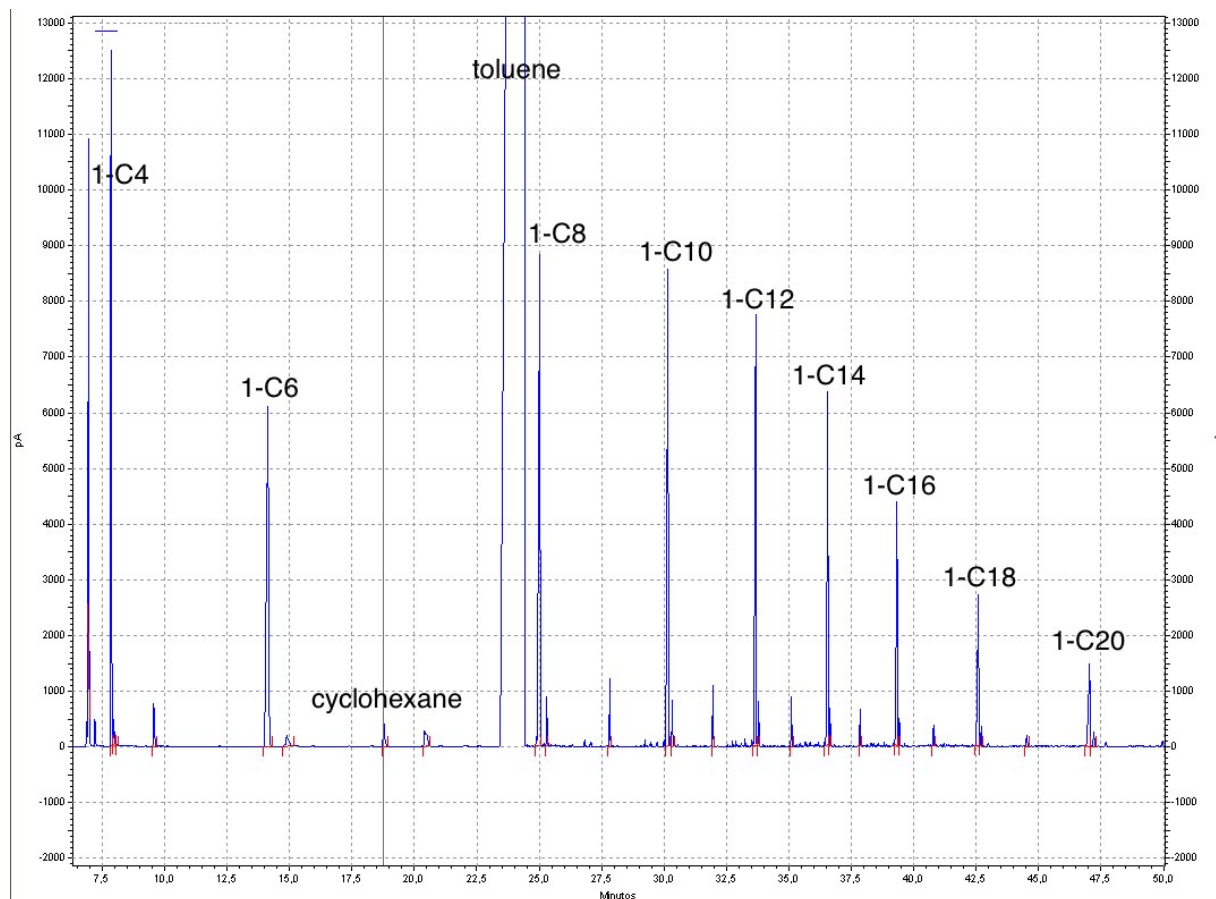


Figure S10. Typical GC trace for the toluene soluble fraction using **2a**/MAO (Table 2, entry 7, $[Al]/[Cr] = 2000$, oligomerization time = 15 min, $P(\text{ethylene}) = 20$ bar, $T = 80^\circ\text{C}$).