Supplementary Information

for

2-(N,N-Diethylaminomethyl)-6,7-trihydroquinolinyl-8-ylideneamine-Ni(II) chlorides: application in ethylene dimerization and trimerization

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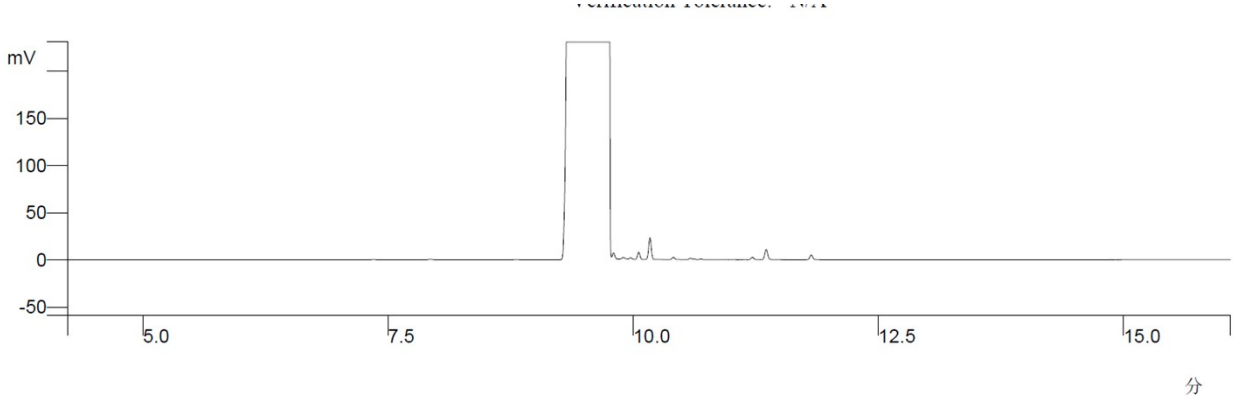
Table S1 Crystal data and structure refinement details for **Ni1** and **Ni3**

	Ni1	**Ni3**
Formula	$C_{22}H_{29}Cl_2N_3Ni$	$C_{26}H_{37}Cl_2N_3Ni$
Formula weight	465.09	521.19
T (K)	169.99(11)	170.00(11)
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	$P\bar{1}$
a (Å)	17.0468(2)	9.5112(2)
b (Å)	8.48720(10)	10.9618(3)
c (Å)	15.8299(2)	12.9408(2)
α/°	90	94.937(2)
β/°	107.7540(10)	95.5750(10)
γ/°	90	92.089(2)
Volume/Å^3	2181.19(5)	1336.48(5)
Z	4	2
D_{calc} (g cm^{-3})	1.416	1.295
μ/mm^{-1}	3.623	3.011
Crystal size/mm^3	0.50 × 0.20 × 0.150	0.5 × 0.3 × 0.25
θ Range (°)	5.444 - 150.814	8.014 – 151.
Limiting indices	$-21 \le h \le 21$	$-12 \le h \le 12$,
	$-10 \le k \le 10$	$-11 \le k \le 12$,
	$-14 \le l \le 19$	$-16 \le l \le 15$
No. of rflns collected	17597	16013
No. unique rflns [R(int)]	4381 (0.0300)	5313 (0.0198)
Data/restraints/parameters	4381/0/257	5313/0/295
Goodness of fit on F^2	1.145	1.112
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0328$	$R_1 = 0.0293$
	$wR_2 = 0.0880$	$wR_2 = 0.0782$
R indices (all data)	$R_1 = 0.0391$	$R_1 = 0.0339$
	$wR_2 = 0.1124$	$wR_2 = 0.0886$
Largest diff peak and hole (e Å^{-3})	0.31 and -0.51	0.28 and -0.36

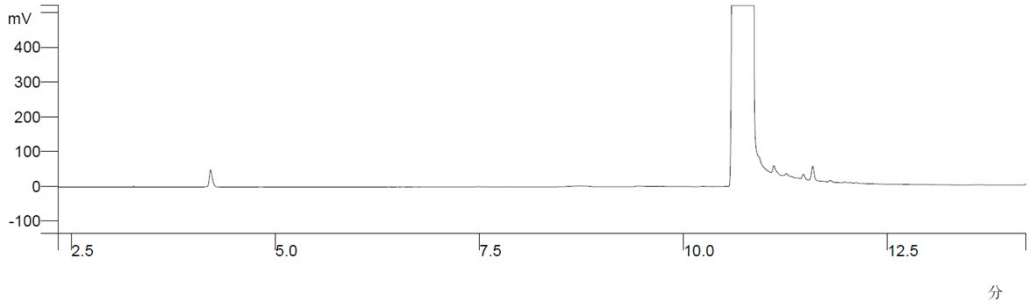
Table 2 Selected bond lengths (Å) and angles (°) for **Ni1** and **Ni3**

	Ni1	**Ni3**
	Bond lengths	
Ni1-N1	2.1669(17)	2.2040(14)
Ni1-N2	1.9752(17)	1.9868(13)
Ni1-N3	2.1804(18)	2.1905(13)
Ni1-Cl1	2.3234(6)	2.2893(5)
Ni1-Cl2	2.2445(6)	2.2434(4)
N2-C10	1.344(3)	1.344(2)
N2-C2	1.321(3)	1.325(2)
N3-C11	1.437(3)	1.445(2)
N3-C9	1.283(3)	1.285(2)
	Bond angles	
Cl1-Ni1-Cl2	108.40(2)	110.193(19)
N2-Ni1-Cl1	93.63(5)	94.28(4)
N2-Ni1-Cl2	157.91(6)	155.52(4)
N2-Ni1-N3	76.87(7)	77.02(5)
N2-Ni1-N1	79.92(7)	79.19(5)
N3-Ni1-Cl1	98.07(5)	99.47(4)
N3-Ni1-Cl2	97.95(5)	98.49(4)
N3-Ni1-N1	101.32(5)	151.97(5)
N1-Ni1-Cl1	96.74(5)	96.87(4)
N1-Ni1-Cl2	150.52(7)	97.02(4)



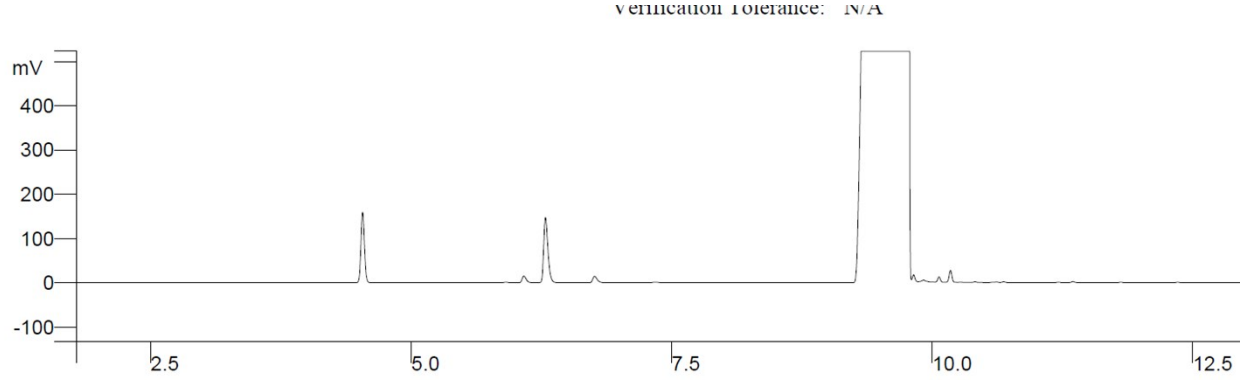
Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		100.0000	9.732	0.000	95378208	0.00	BB	9.1		0
	总数	**100.0000**		**0.000**	**95378208**					

Figure S1 Gas chromatograms of toluene



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		0.0814	4.207	0.000	130850	0.00	BB	2.3		0
2		99.9186	10.810	0.000	160540112	0.00	PB	8.4		0
	总数	**100.0000**		**0.000**	**160670960**					

Figure S2 Gas chromatograms of **Ni4**/MASC at 30 °C with toluene as the solvent (entry 3, Table 1)



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Grou
1		0.3231	4.534	0.000	371333	0.00	BB	2.2		0
2		0.3582	6.290	0.000	411661	0.00	PB	2.5		0
3		99.3186	9.752	0.000	114127488	0.00	PB	13.7		0

Figure S3 Gas chromatograms of using **Ni4**/EASC at 30 °C with toluene as the solvent (entry 4, Table 1)

Figures S4 – S22 Gas chromatagrams for the MAO-promoted runs (Ni/MAO, Table 3):

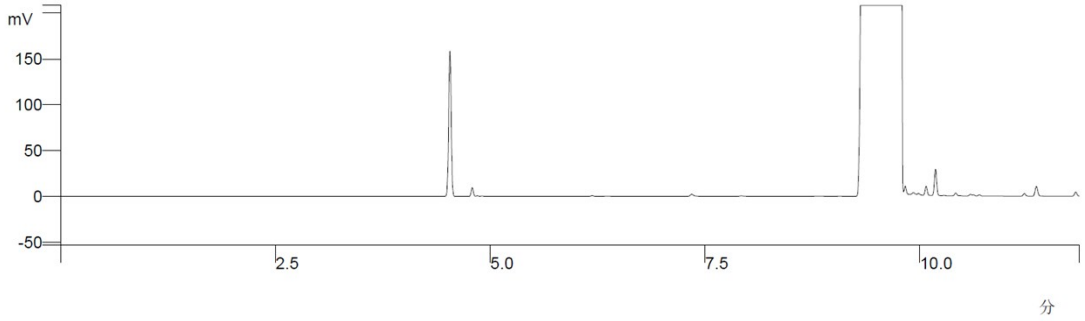


Figure S4 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; Al:Ni = 1000 (entry 1, Table 2).

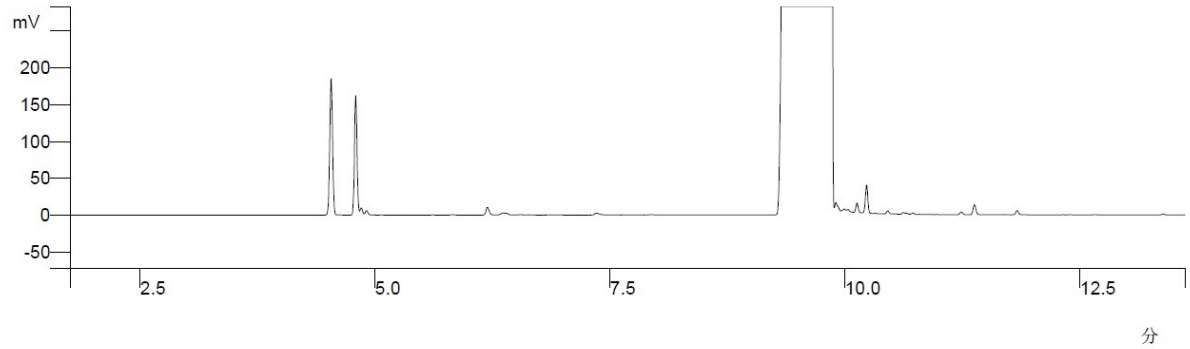


Figure S5 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; Al:Ni = 1250(entry 2, Table 3).

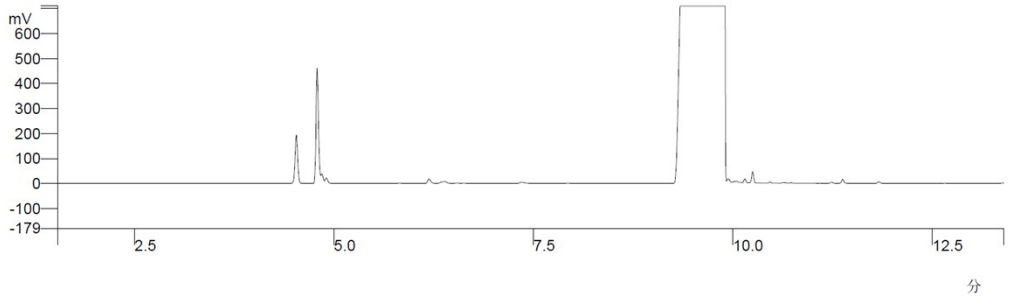


Figure S6 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; Al:Ni = 1500 (entry 3, Table 3).

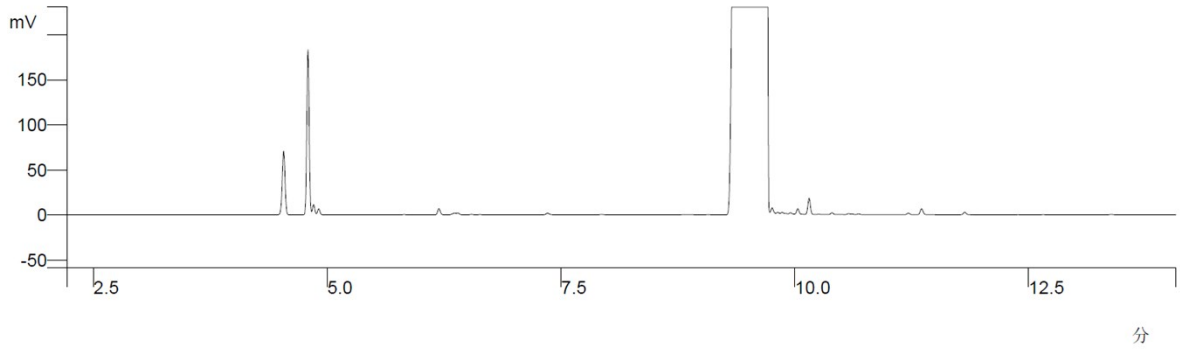


Figure S7 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; Al:Ni = 1750(entry 4, Table 3).

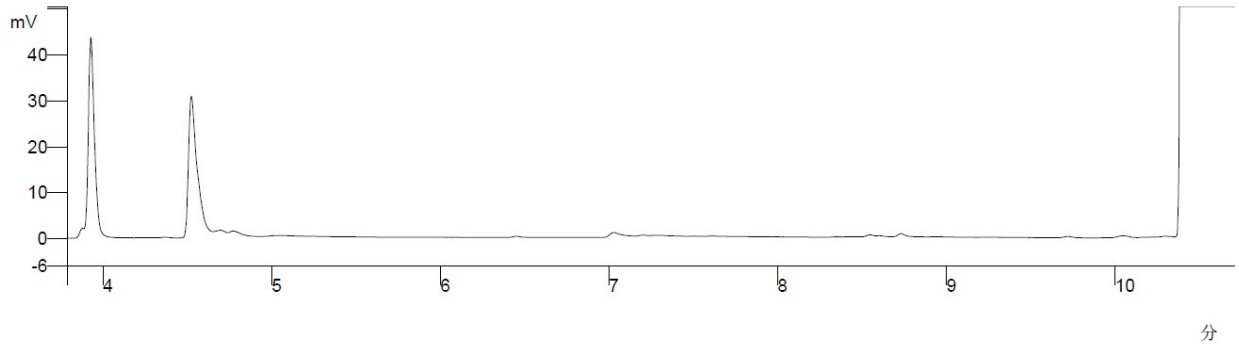


Figure S8 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; Al:Ni = 2000(entry 5, Table 3).

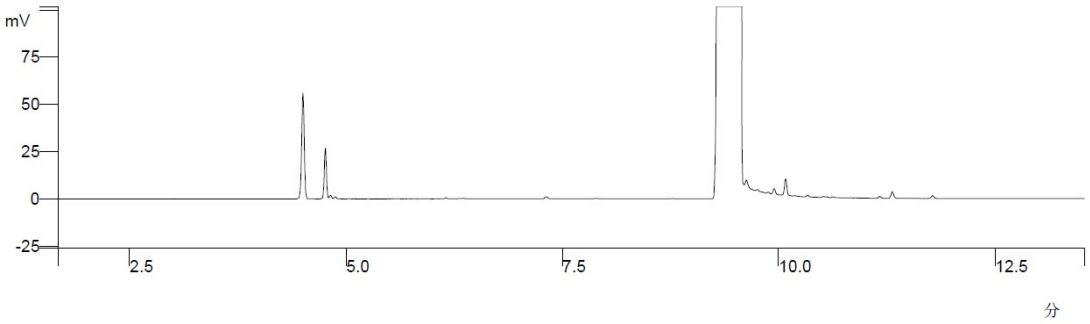


Figure S9 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; Al:Ni = 2500 (entry 6, Table 3).

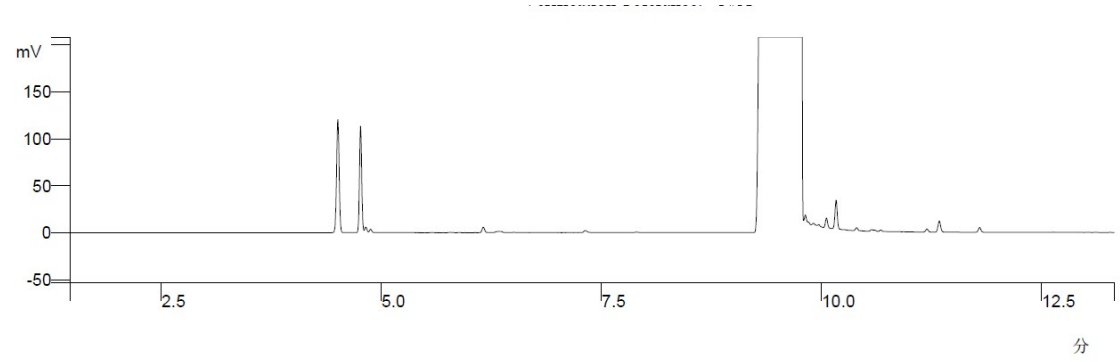


Figure S10 Gas chromatogram obtained using **Ni4**/MAO at 20 °C (entry 7, Table 3).

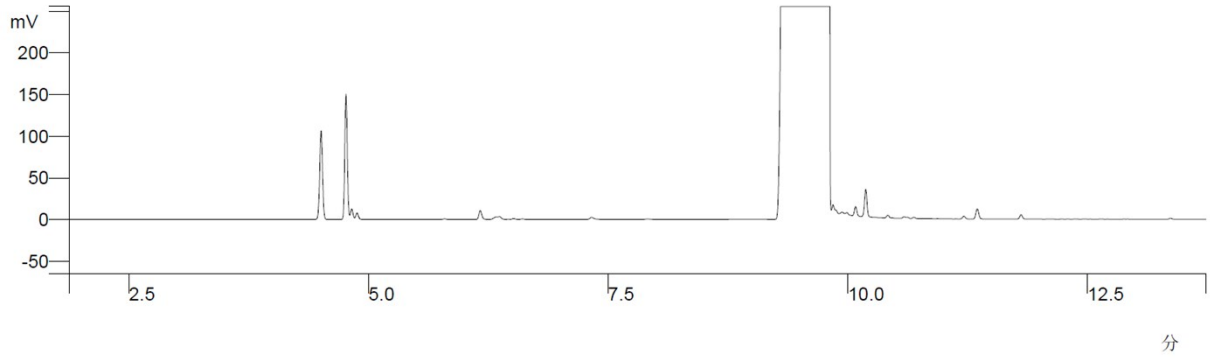


Figure S11 Gas chromatogram obtained using **Ni4**/MAO at 40 °C (entry 8, Table 3).

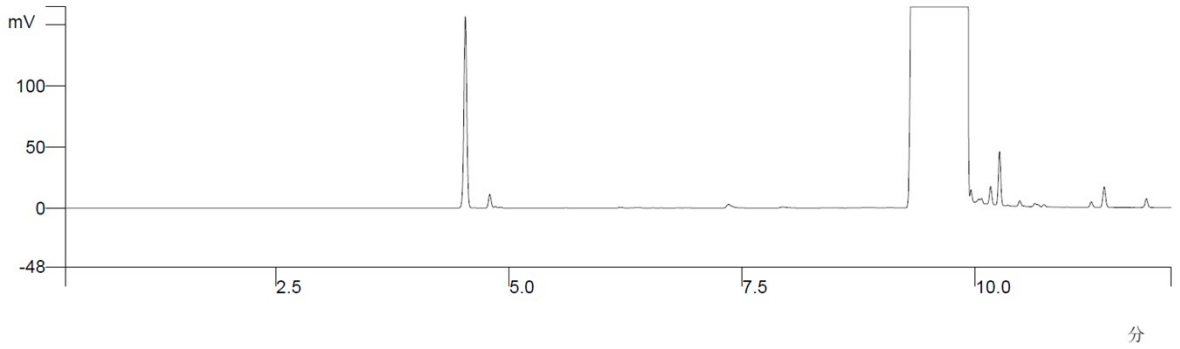


Figure S12 Gas chromatogram obtained using **Ni4**/MAO at 50 °C (entry 9, Table 3).

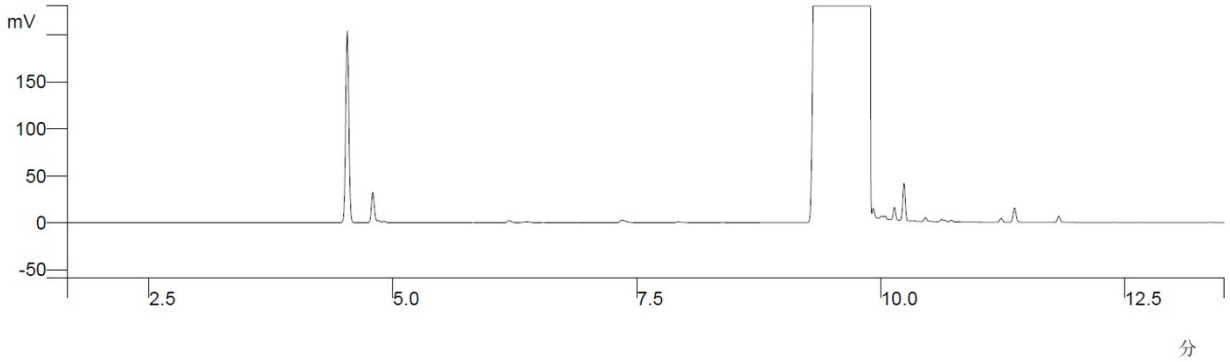


Figure S13 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; 5 min (entry 10, Table 3).

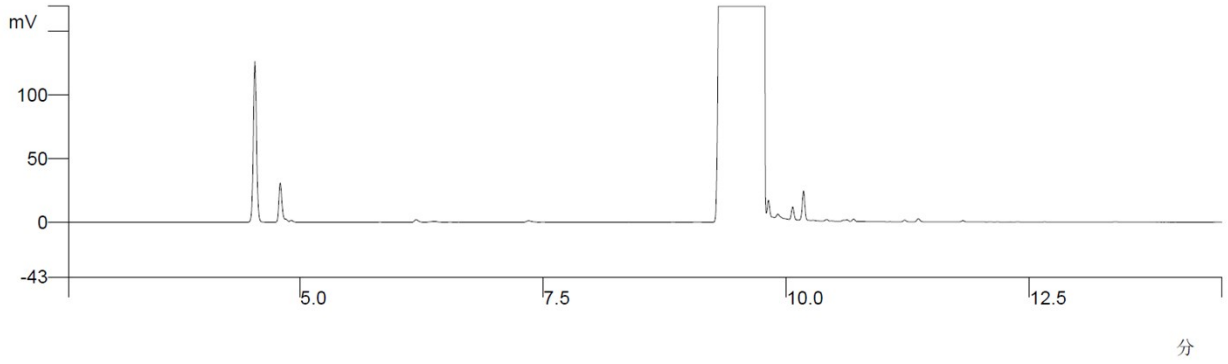


Figure S14 Gas chromatograms obtained using **Ni4**/MAO at 30 °C; 15 min (entry 11, Table 3).

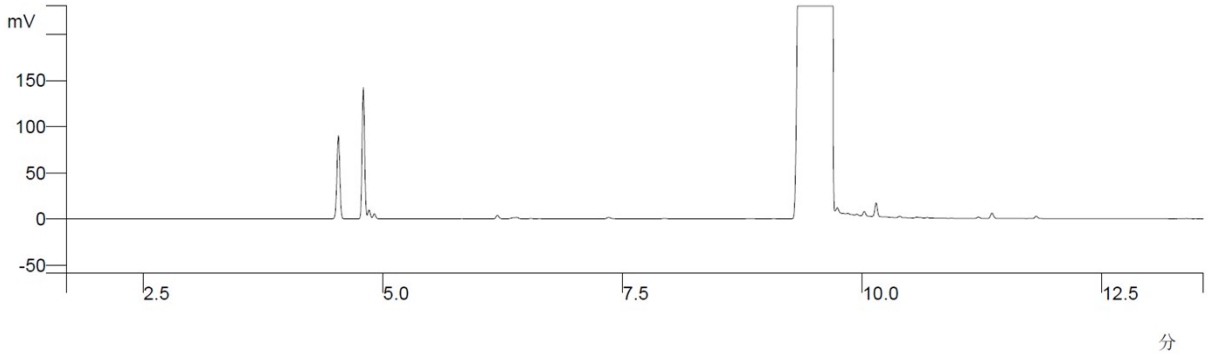


Figure S15 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; 45 min (entry 12, Table 3).

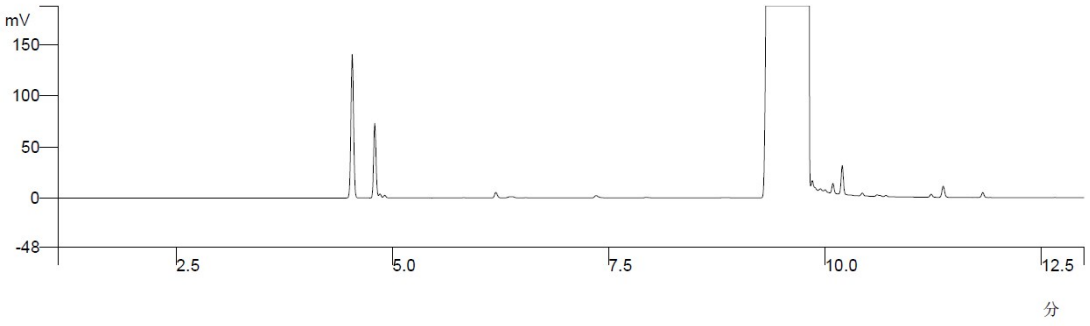


Figure S16 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; 60 min (entry 13, Table 3).

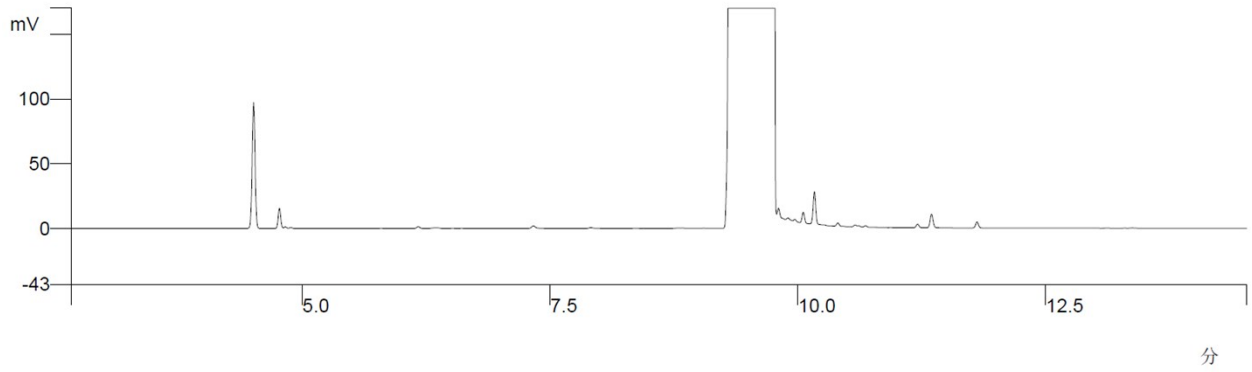


Figure S17 Gas chromatogram obtained using **Ni4**/MAO at 30 °C; 5 atm C_2H_4 (entry 14, Table 3).

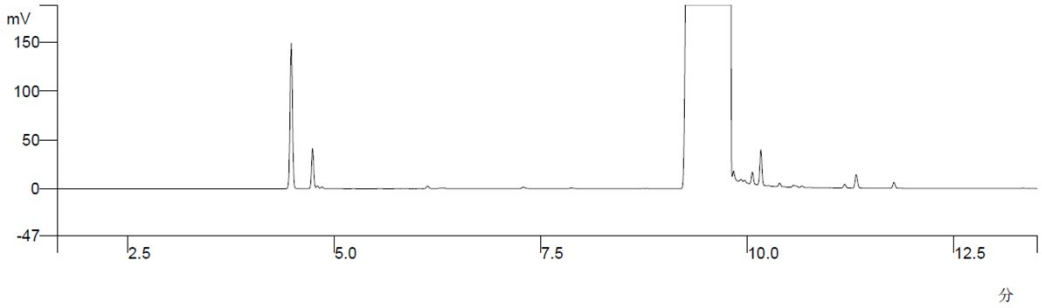


Figure S18 Gas chromatogram obtained using **Ni1**/MAO at 30 °C (entry 15, Table 3).

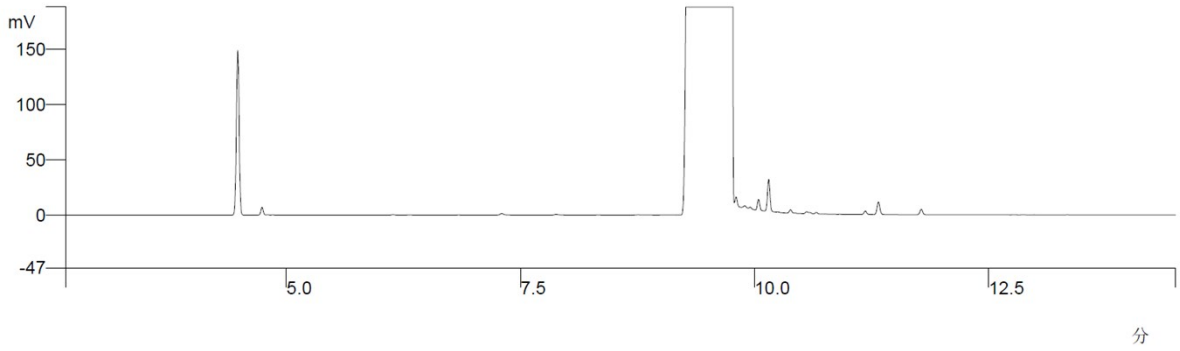


Figure S19 Gas chromatogram obtained using **Ni2**/MAO at 30 °C (entry 16, Table 3).

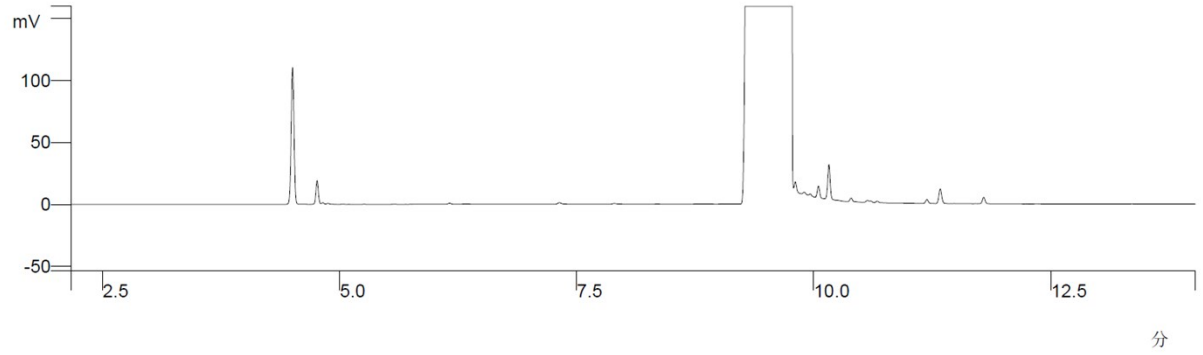


Figure S20 Gas chromatogram obtained using **Ni3**/MAO at 30 °C (entry 17, Table 3).

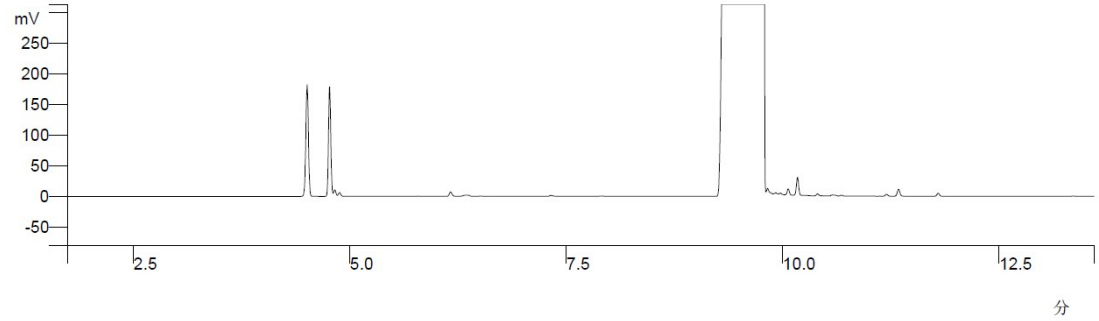


Figure S21 Gas chromatogram obtained using **Ni5**/MAO at 30 °C (entry 18, Table 3).

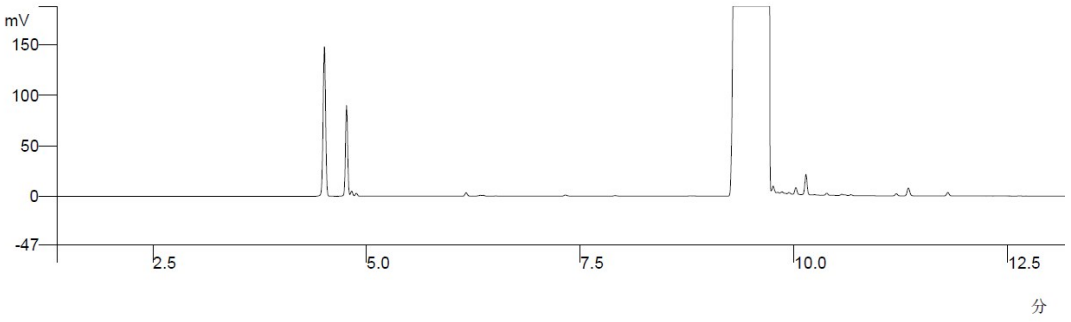


Figure S22 Gas chromatogram obtained using **Ni6**/MAO at 30 °C (entry 19, Table 3).

Figures S23 – S43 Gas chromatograms for the MMAO-promoted runs (Ni/MMAO, Table 2):

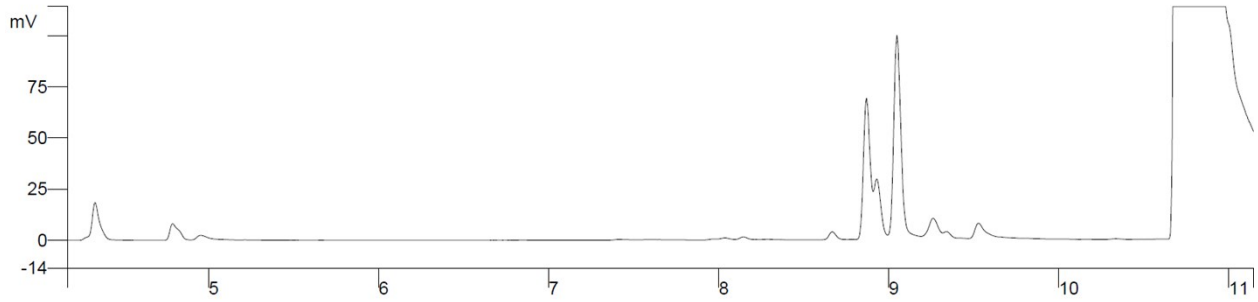


Figure S23 Gas chromatogram obtained using **Ni4**/MMAO at 30 °C; Al:Ni = 1500 (entry 1,T Table 2).

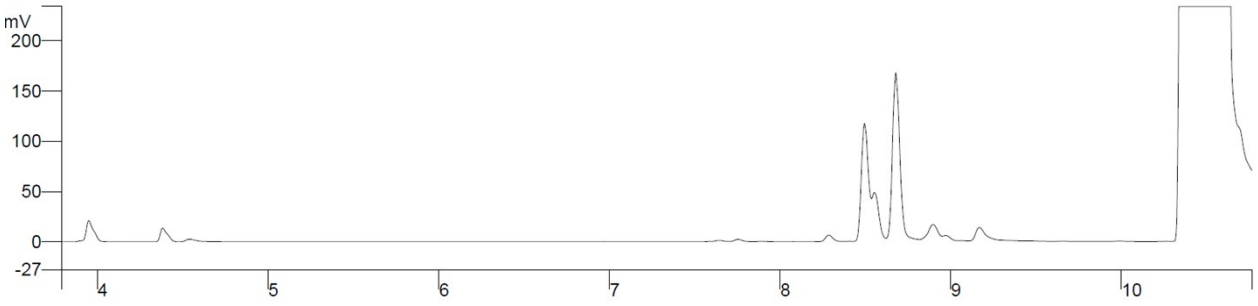


Figure S24 Gas chromatogram obtaiined using **Ni4**/MMAO at 30 °C; Al:Ni = 2000 (entry 2, Table 2).

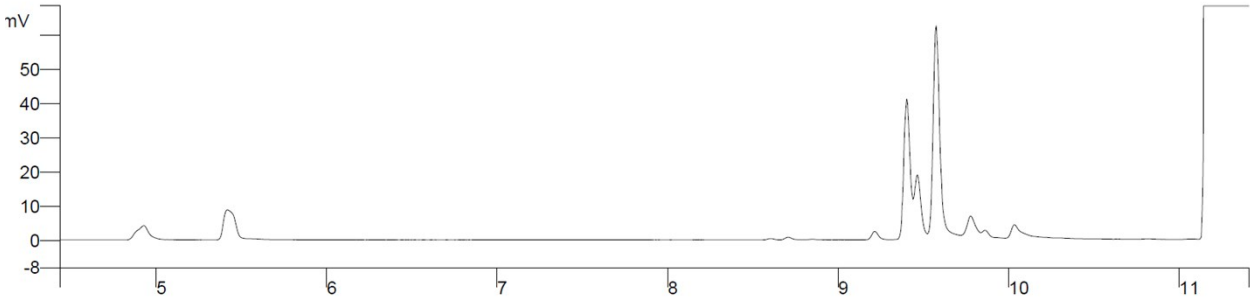


Figure S25 Gas chromatogram obtained using **Ni4**/MMAO at 30 °C; Al:Ni = 2250 (entry 3, Table 2).

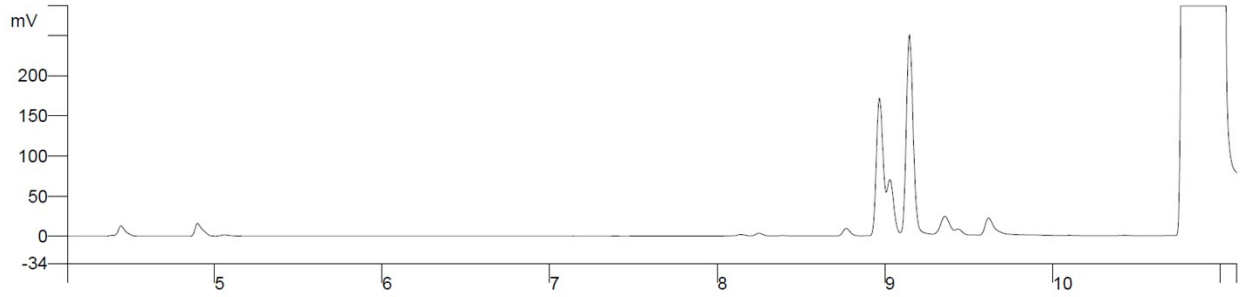


Figure S26 Gas chromatogram obtained using **Ni4**/MMAO at 30 °C; Al:Ni = 2500 (entry 4, Table 2).

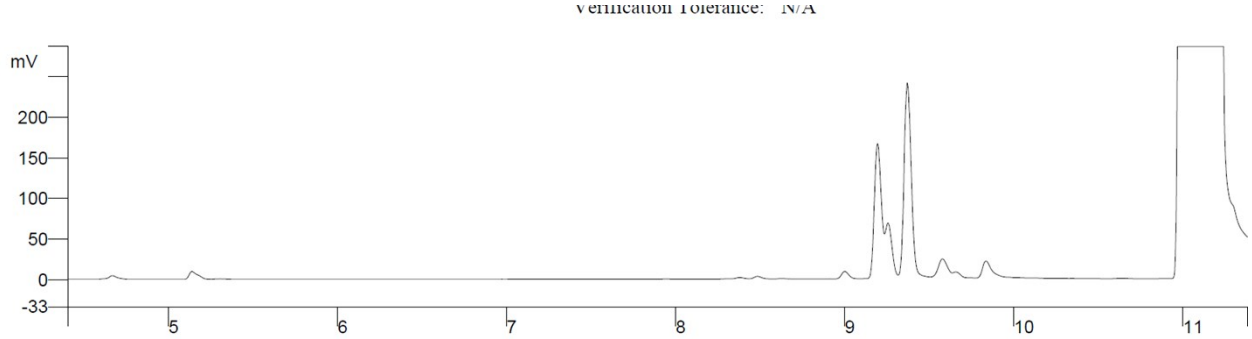


Figure S27 Gas chromatogram obtained using using **Ni4**/MMAO at 30 °C; Al:Ni = 2750 (entry 5, Table 2).

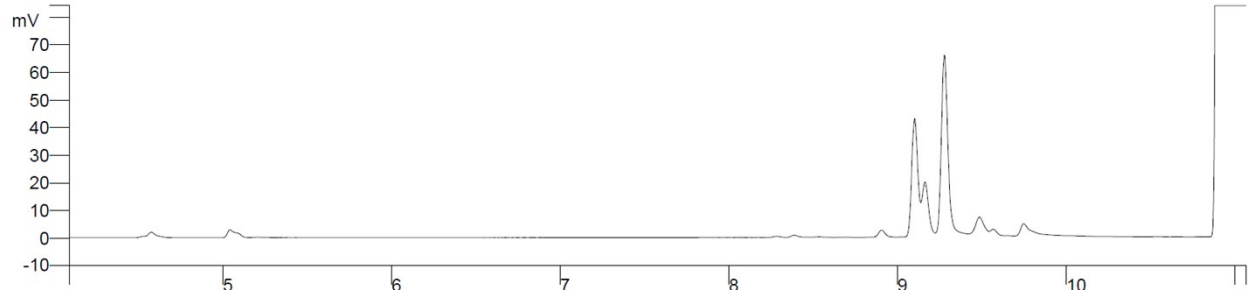


Figure S28 Gas chromatogram obtained using **Ni4**/MMAO at 30 °C; Al:Ni =3000 (entry 6, Table 2).

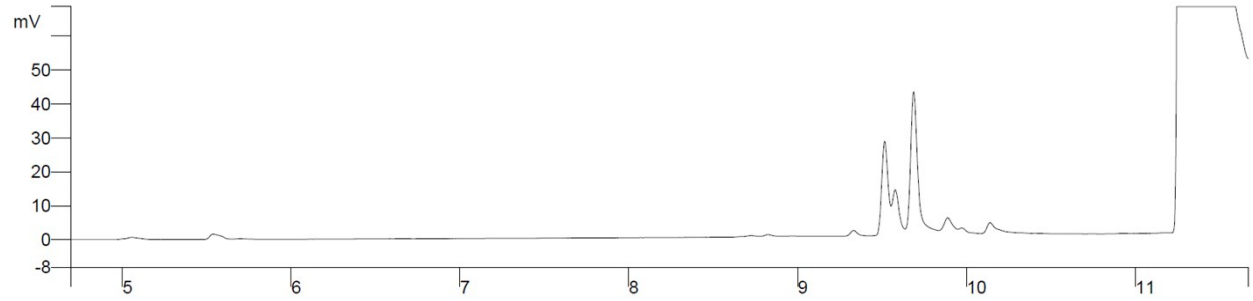


Figure S29 Gas chromatogram obtained using **Ni4**/MMAO at 20 °C (entry 7, Table 2).

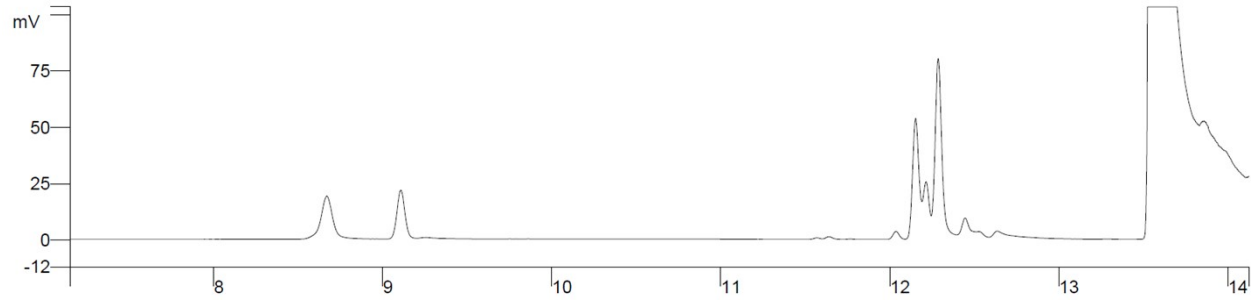


Figure S30 Gas chromatogram obtained using **Ni4**/MMAO at 40 °C (entry 8, Table 2).

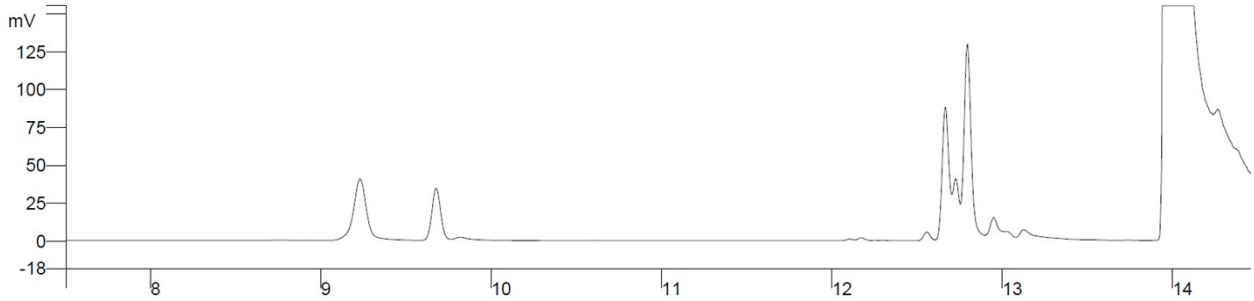


Figure S31 Gas chromatogram obtained using **Ni4**/MMAO at 50 °C (entry 9, Table 2).

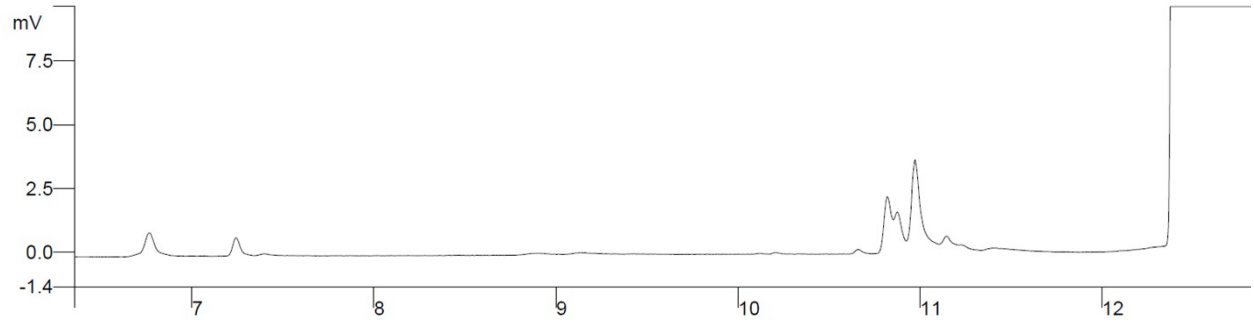


Figure S32 Gas chromatogram obtained using **Ni4**/MMAO at 60 ºC (entry 10, Table 2).

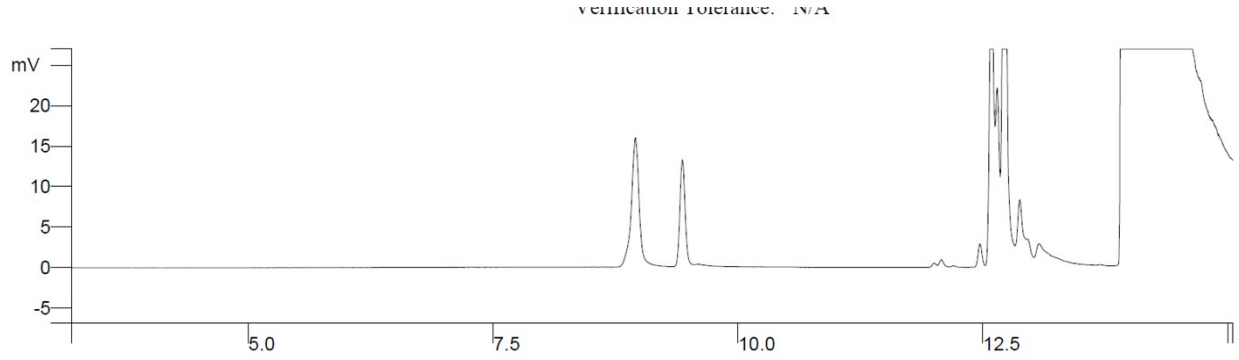


Figure S33 Gas chromatogram obtained using **Ni4**/MMAO at 30 ºC; 5 min (entry 11, Table 2).

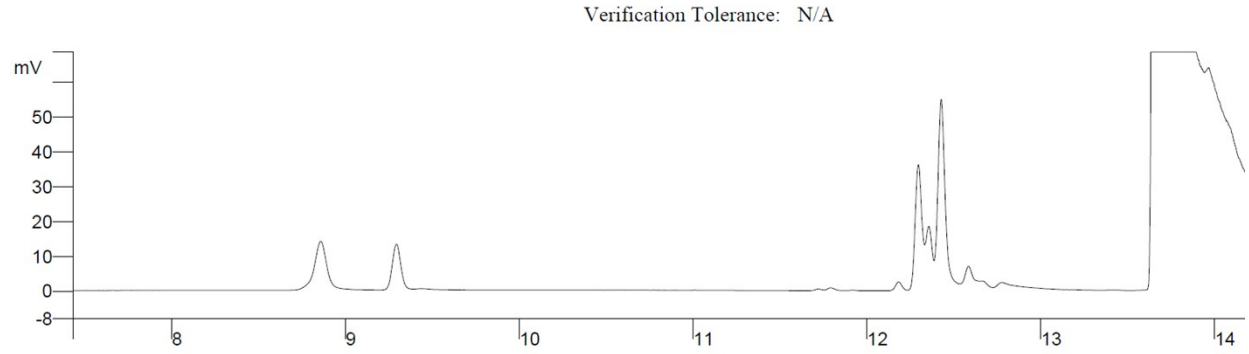


Figure S34 Gas chromatogram obtained using **Ni4**/MMAO at 30 ºC; 15 min (entry 12, Table 2).

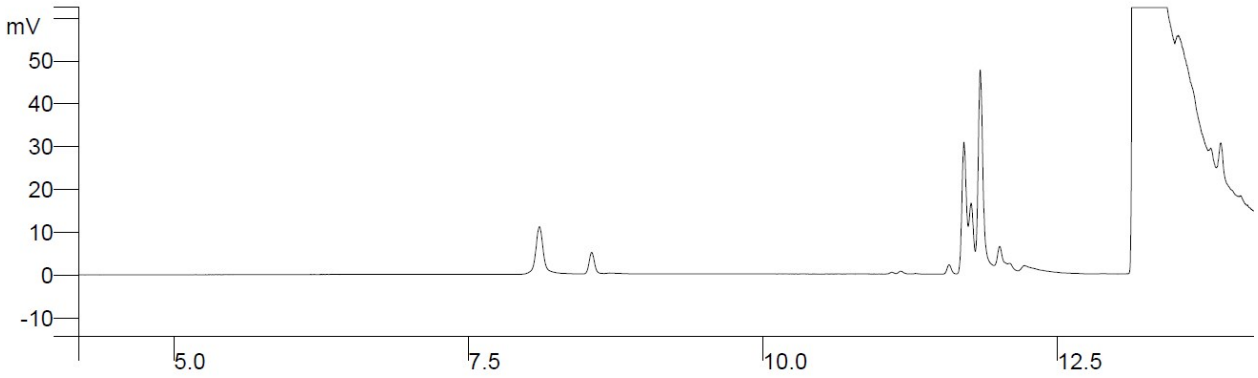


Figure S35 Gas chromatogram obtained using **Ni4**/MMAO at 30 ºC; 45 min (entry 13, Table 2).

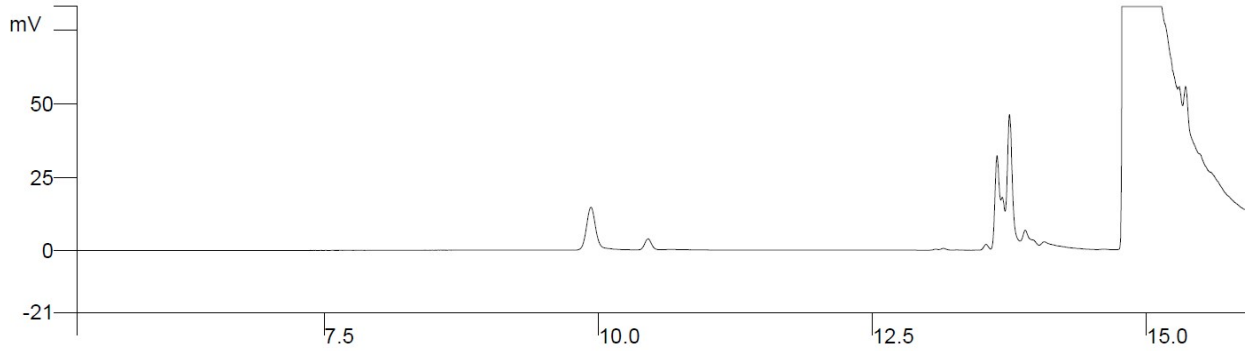


Figure S36 Gas chromatogram obtained using **Ni4**/MMAO at 30 °C; 60 min (entry 14, Table 2).

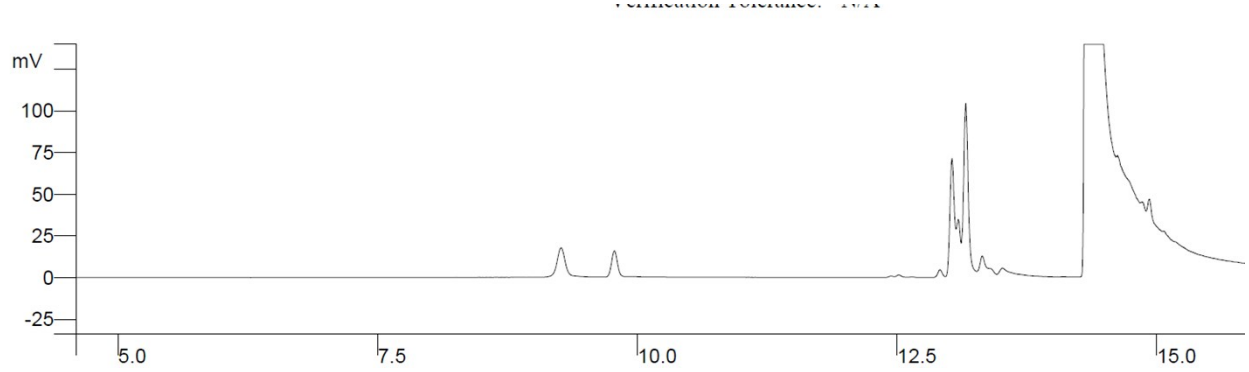


Figure S37 Gas chromatogram obtained using **Ni4**/MMAO at 30 °C; 5 atm C_2H_4 (entry 15, Table 2).

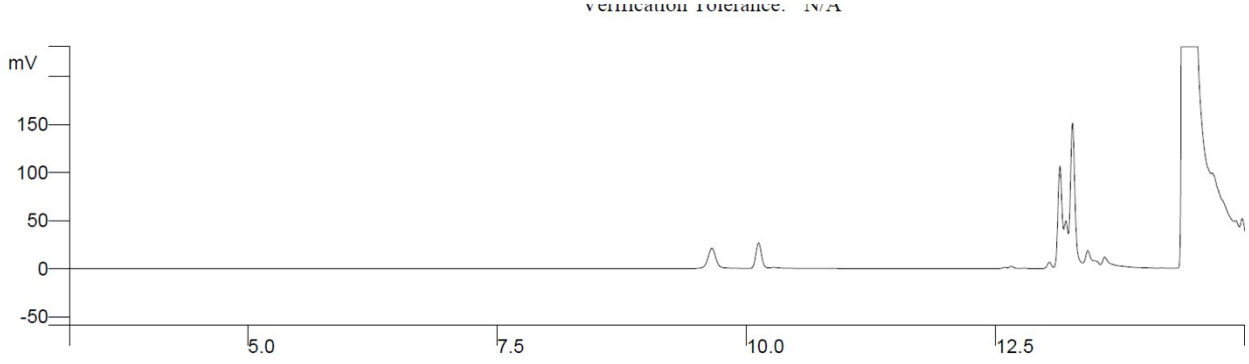


Figure S38 Gas chromatogram obtained using **Ni1**/MMAO at 30 °C (entry 16, Table 2).

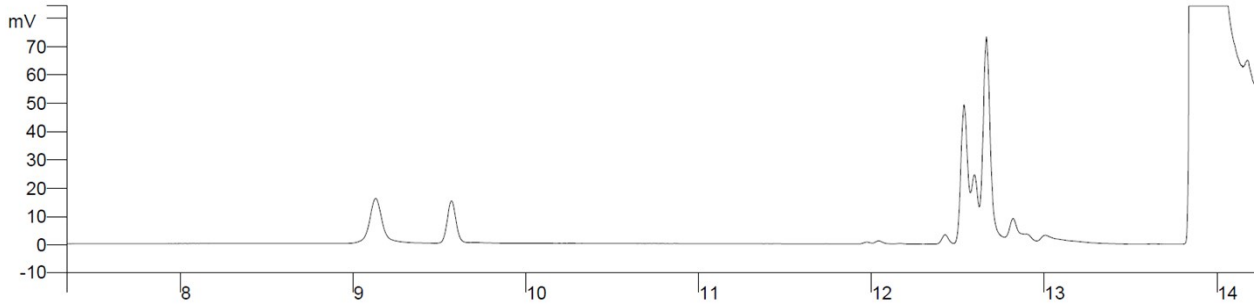


Figure S39 Gas chromatogram obtained using **Ni2**/MMAO at 30 °C (entry 17, Table 2).

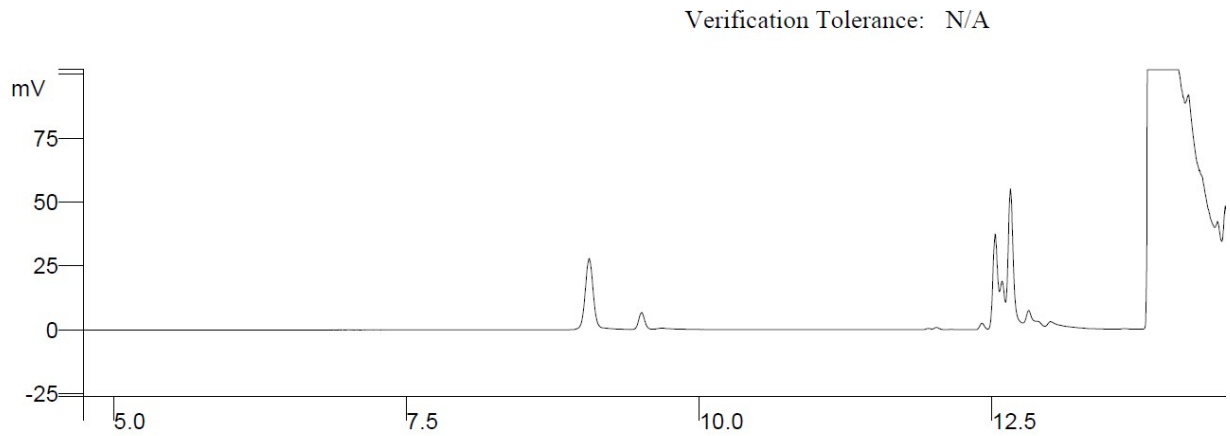


Figure S40 Gas chromatogram obtained using **Ni3**/MMAO at 30 °C (entry 18, Table 2).

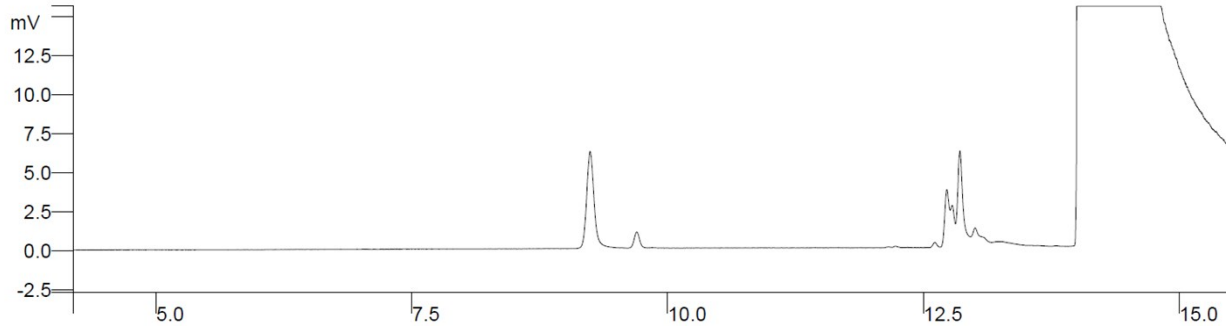


Figure S41 Gas chromatogram obtained using **Ni5**/MMAO at 30 °C (entry 19, Table 2).

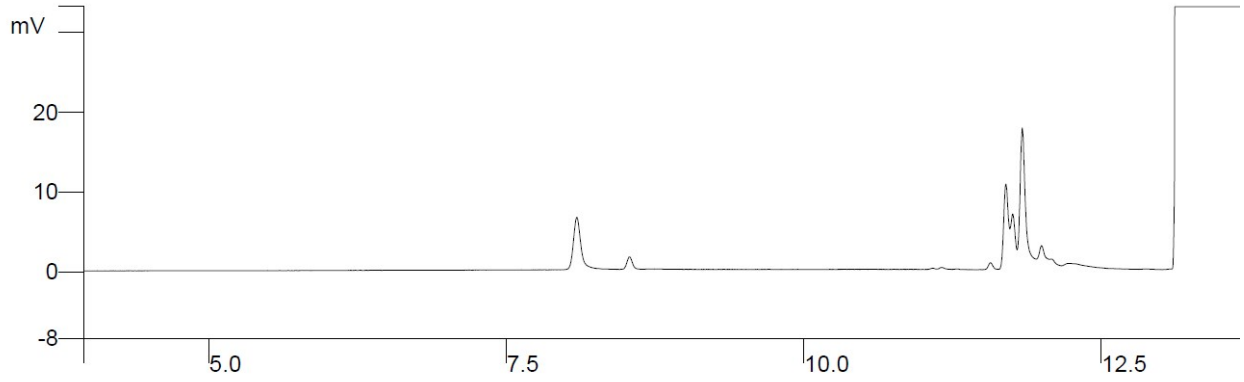


Figure S42 Gas chromatogram obtained using **Ni6**/MMAO at 30 °C (entry 20, Table 2).