Supplementary materials

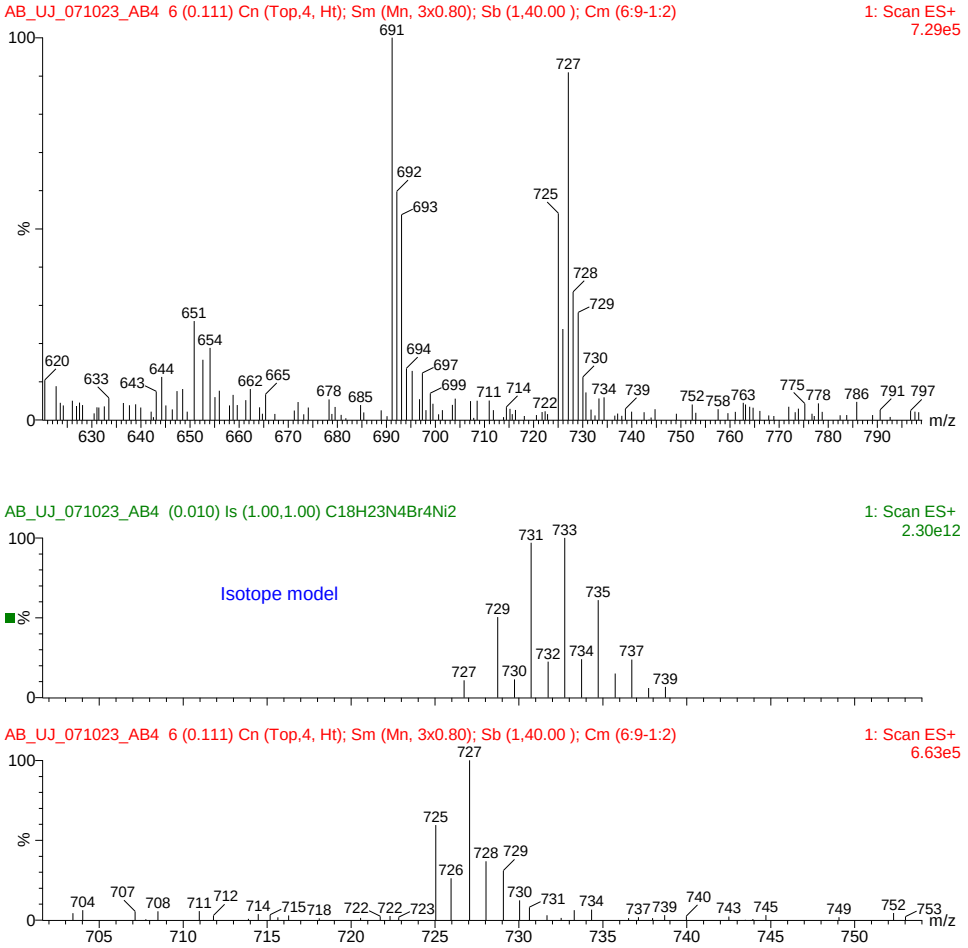


Figure S1: Parts of the mass spectrum of complex **5**, depicting the polymeric nature of this compound.

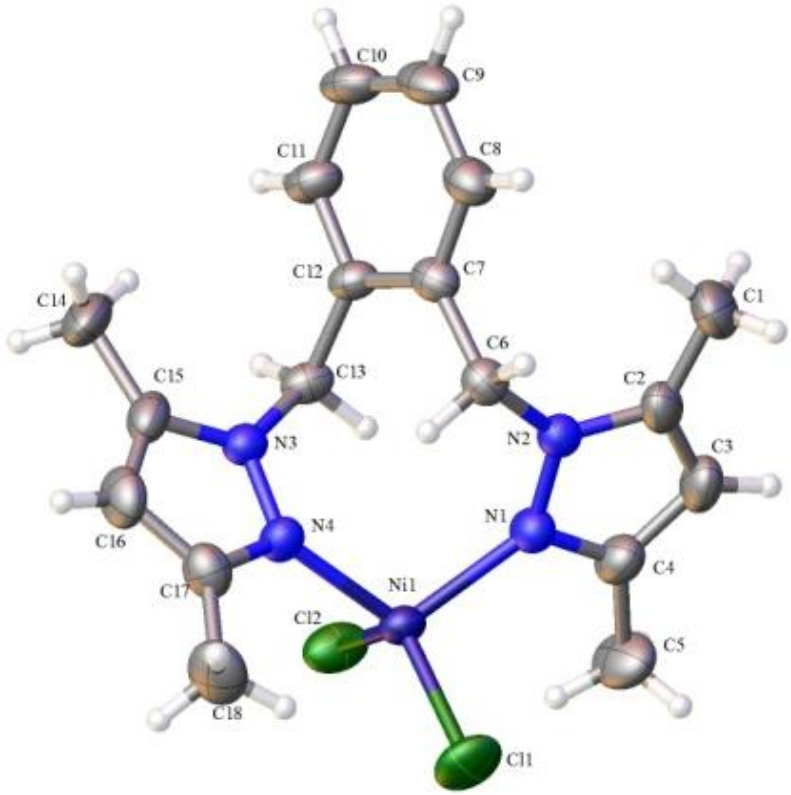


Figure S2: Molecular structure of complex **2**, with the ellipsoids drawn at 50% probability level. Selected bond lengths [Å] and angles [°]: N(1)-Ni(1), 2.019(2); N(4)-Ni(1), 2.003(2); Cl(1)-Ni(1), 2.2169(8); Cl(2)-Ni(1), 2.2569(7); N(3)-N(4), 1.372(3); N(1)-Ni(1)-N(4), 109.26(8); N(1)-Ni(1)-Cl(1), 102.01(7); N(4)-Ni(1)-Cl(1), 118.63(6); N(1)-Ni(1)-Cl(2), 105.86(7); N(4)-Ni(1)-Cl(2), 98.76(6); Cl(1)-Ni(1)-Cl(2), 121.60(3).

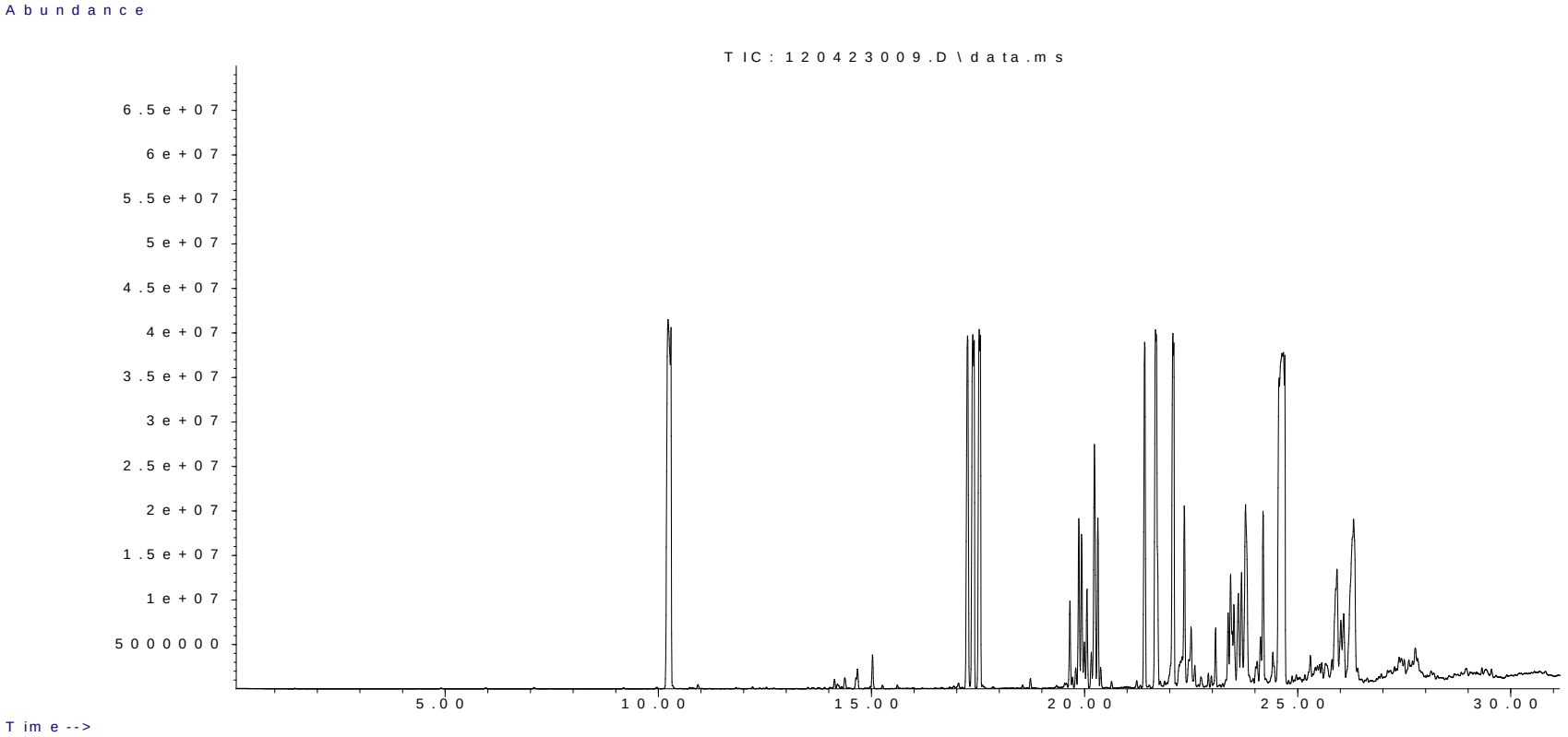
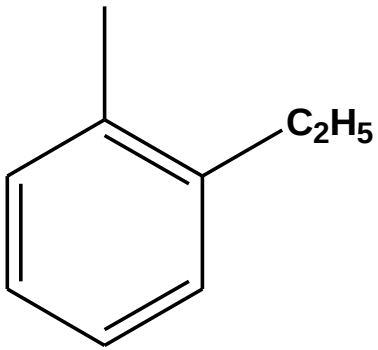


Figure S3: Total ion chromatogram showing C4-, C8-, and C12- toluenes as major products. Thus addition of butene may be the most facile process which leads to alkyltoluenes.

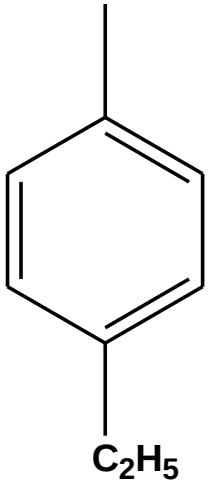
(A)

(i) Toluene + C_2

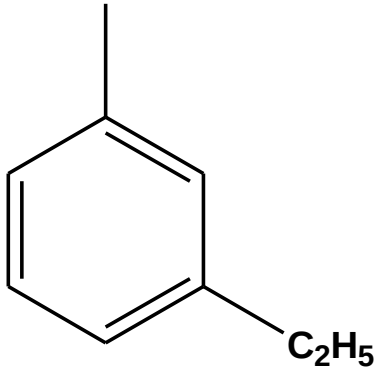
(MW = 120)



2-ethyltoluene



4-ethyltoluene

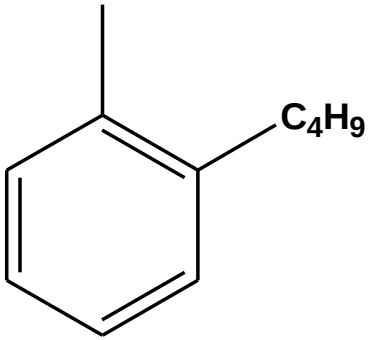


3-ethyltoluene

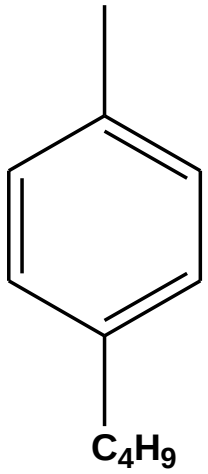
Figure S4: Retention time = 15 min

(B)

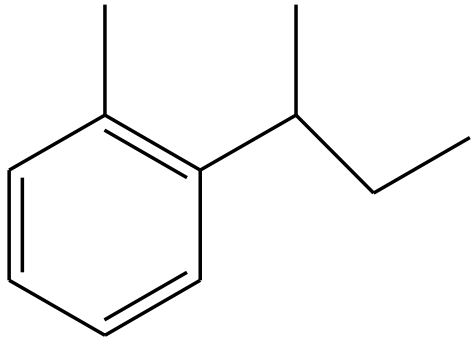
(ii) Toluene + C_4 **(MW = 148)**



2-butyltoluene



4-butyltoluene

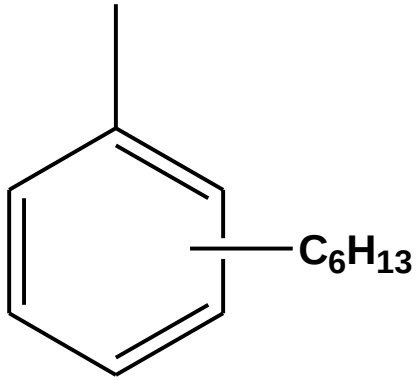


2-isopropyltoluene

Figure S5: Retention time = 17.00 – 18.00 min

(C)

(iii) Toluene + C_6 **(MW = 176)**



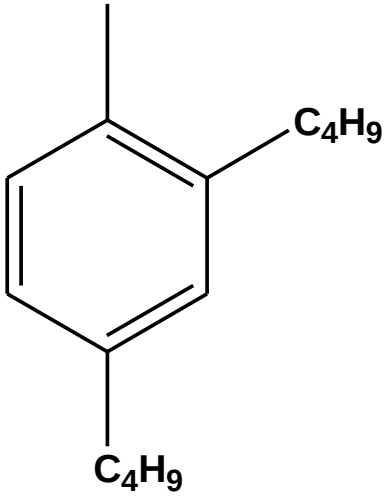
hexyltoluene

Figure S6: Retention time = 19.50 – 20.50 min

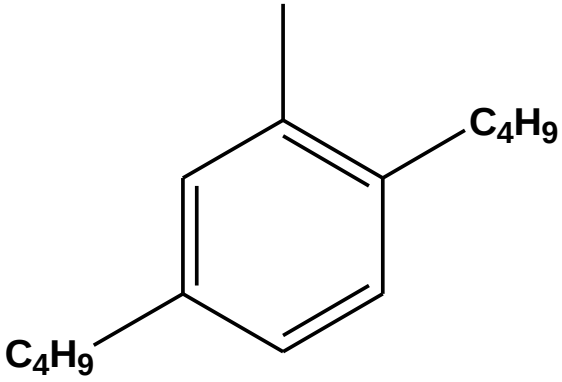
(Comments: 2-n-hexyl; 4-n-hexyl- and several isomers of C6 on toluene)

(D)

(iv) Toluene + 2 x C_4 **(MW = 204)**



2,4-dibutyltoluene



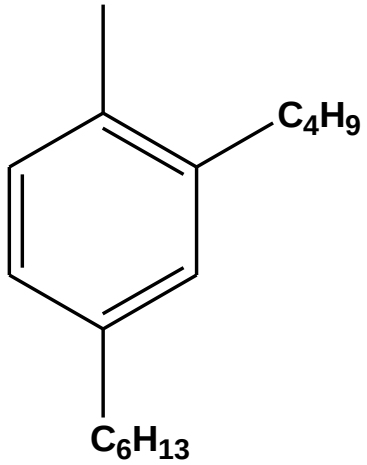
2,5-dibutyltoluene

Figure S7: Retention time = 21.20 – 23.70 min

(Comments: 2 x C4 alkylation of toluene, with isomerization of C4 chain)

(E)

(v) Toluene + C_4 + C_6 **(MW = 232)**



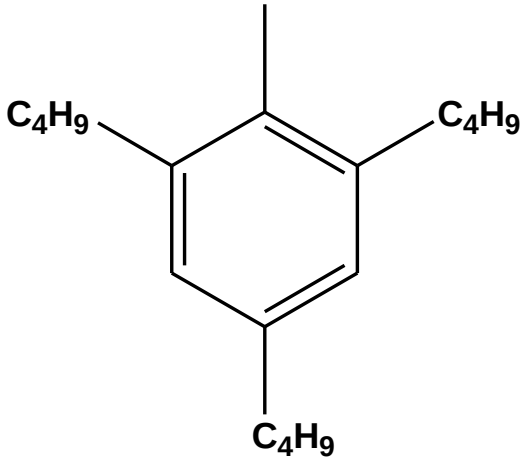
2-ethyl-6-hexyltoluene

Figure S8: Retention time = 22.90 – 24.30

(Comments: Unlikely to have 2 x C4 + C2; sine there is very little of C2 alkylation; hence most likely is C4 + C6. Product as above, with isomers from the isomerization of the alkyl chain)

(F)

(vi) Toluene + 3 x C_4 **(MW = 260)**



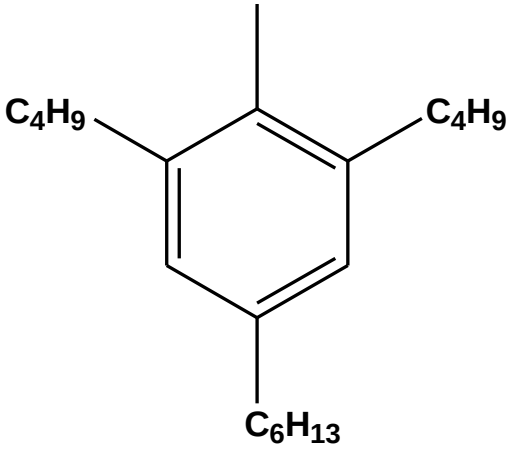
2,4,6-tributyltoluene

Figure S9: Retention time = 24.60

(Comments: Unlikely to have other combination since GC shows one dominant peak at this retention time)

(G)

(vii) Toluene + 2 x C_4 + C_6 **(MW = 288)**



2,6-dibutyl-4-hexyltoluene

Figure S10: Retention time = 25.80 – 26.50 min

(Comments: Unlikely to be C_8 + C_6 alkylation of toluene since there is very little amount of C_8 formed in the hexane and no evidence of C_8 alkylation of toluene. Most likely is a 2 x C_4 + C_6 alkylation of toluene)