

# Supplementary Materials: Fine-Tuning Synthesis and Characterization of Mono-Sized H-Beta Zeolite-Supported Palladium-Iridium Nanoparticles and Application in the Selective Hydrogenation of Acetylene

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Table S1. Total amount of Si/(Al+SDA) ratio for synthesis of Beta-based catalysts.

Supports	NaAlO <sub>2</sub> (mM)	NaOH (mM)	TEOS (mM)	i (mM)	ii (mM)	iii (mM)	iv (mM)	$\frac{Si}{(Al + SDA)}$	BET (m <sup>2</sup> /g)
Beta(0)	70	95	2	---	---	---	---	28.57	1474.78
Beta(i)	50	95	1.45	20	---	---	---	20.71	---
Beta(i)	50	95	2	20	---	---	---	28.57	500
Beta(i)	50	95	3	20	---	---	---	42.86	---
Beta(i)	60	95	2	20	---	---	---	25.00	---
Beta(i)	70	95	2	20	---	---	---	22.22	950
Beta(i)	80	95	2	20	---	---	---	20.00	---
Beta(i)	70	95	2	35	---	---	---	19.05	1358.3
Beta(i)	70	95	2	40	---	---	---	18.18	---
Beta(i)	70	95	2	50	---	---	---	16.67	---
Beta(ii)	50	95	1.45	---	15.27	---	---	22.21	---
Beta(ii)	50	95	2	---	15.27	---	---	30.64	375
Beta(ii)	50	95	3	---	15.27	---	---	45.96	---
Beta(ii)	60	95	2	---	15.27	---	---	26.57	---
Beta(ii)	70	95	2	---	15.27	---	---	23.45	546
Beta(ii)	80	95	2	---	15.27	---	---	20.99	---
Beta(ii)	70	95	2	---	26.73	---	---	20.68	1054.2
Beta(ii)	70	95	2	---	30.55	---	---	19.89	---
Beta(ii)	70	95	2	---	38.19	---	---	18.49	---
Beta(iii)	50	95	1.45	---	---	46.68	---	15.00	---
Beta(iii)	50	95	2	---	---	46.68	---	20.69	257
Beta(iii)	50	95	3	---	---	46.68	---	31.03	---
Beta(iii)	60	95	2	---	---	46.68	---	18.75	---
Beta(iii)	70	95	2	---	---	46.68	---	17.14	348
Beta(iii)	80	95	2	---	---	46.68	---	15.79	---
Beta(iii)	70	95	2	---	---	81.70	---	13.18	745.9
Beta(iii)	70	95	2	---	---	93.37	---	12.24	---
Beta(iii)	70	95	2	---	---	116.71	---	10.71	---
Beta(iv)	50	95	1.45	---	---	---	55.61	13.73	---
Beta(iv)	50	95	2	---	---	---	55.61	18.94	110
Beta(iv)	50	95	3	---	---	---	55.61	28.41	---
Beta(iv)	60	95	2	---	---	---	55.61	17.30	---
Beta(iv)	70	95	2	---	---	---	55.61	15.92	250.3
Beta(iv)	80	95	2	---	---	---	55.61	14.75	---

Beta(iv)	70	95	2	---	---	---	97.31	11.95	587.4
Beta(iv)	70	95	2	---	---	---	111.22	11.04	---
Beta(iv)	70	95	2	---	---	---	139.02	9.57	---
i:TPAOH			ii:TPABr			iii: morpholine			iv:n-butylamine

Table S2. The amount value of metals loading on H-Beta(i)-based catalysts.

Catalysts	H <sub>2</sub> PdCl <sub>4</sub> (%mol)	AgNO <sub>3</sub> (%mol)	Ir.Cl <sub>3</sub> .H <sub>2</sub> O(%mol)	Ce(NO <sub>3</sub> ) <sub>3</sub> .6H <sub>2</sub> O(%mol)	BET(m <sup>2</sup> /gr)
1	0.009	---	---	---	
2	0.117	---	---	---	
3	0.235	---	---	---	
4	0.376	---	---	---	1248.1
5	0.399	---	---	---	
6	0.470	---	---	---	
7	0.376	0.927	---	---	
8	0.376	1.391	---	---	
9	0.376	1.669	---	---	
10	0.376	1.761	---	---	850.3
11	0.376	1.854	---	---	
12	0.376	2.781	---	---	
13	0.376	---	0.052	---	
14	0.376	---	0.104	---	
15	0.376	---	0.130	---	
16	0.376	---	0.151	---	1108.9
17	0.376	---	0.156	---	
18	0.376	---	0.208	---	
19	0.376	---	---	0.714	
20	0.376	---	---	1.427	
21	0.376	---	---	1.784	
22	0.376	---	---	1.998	
23	0.376	---	---	2.070	973.7
24	0.376	---	---	2.141	

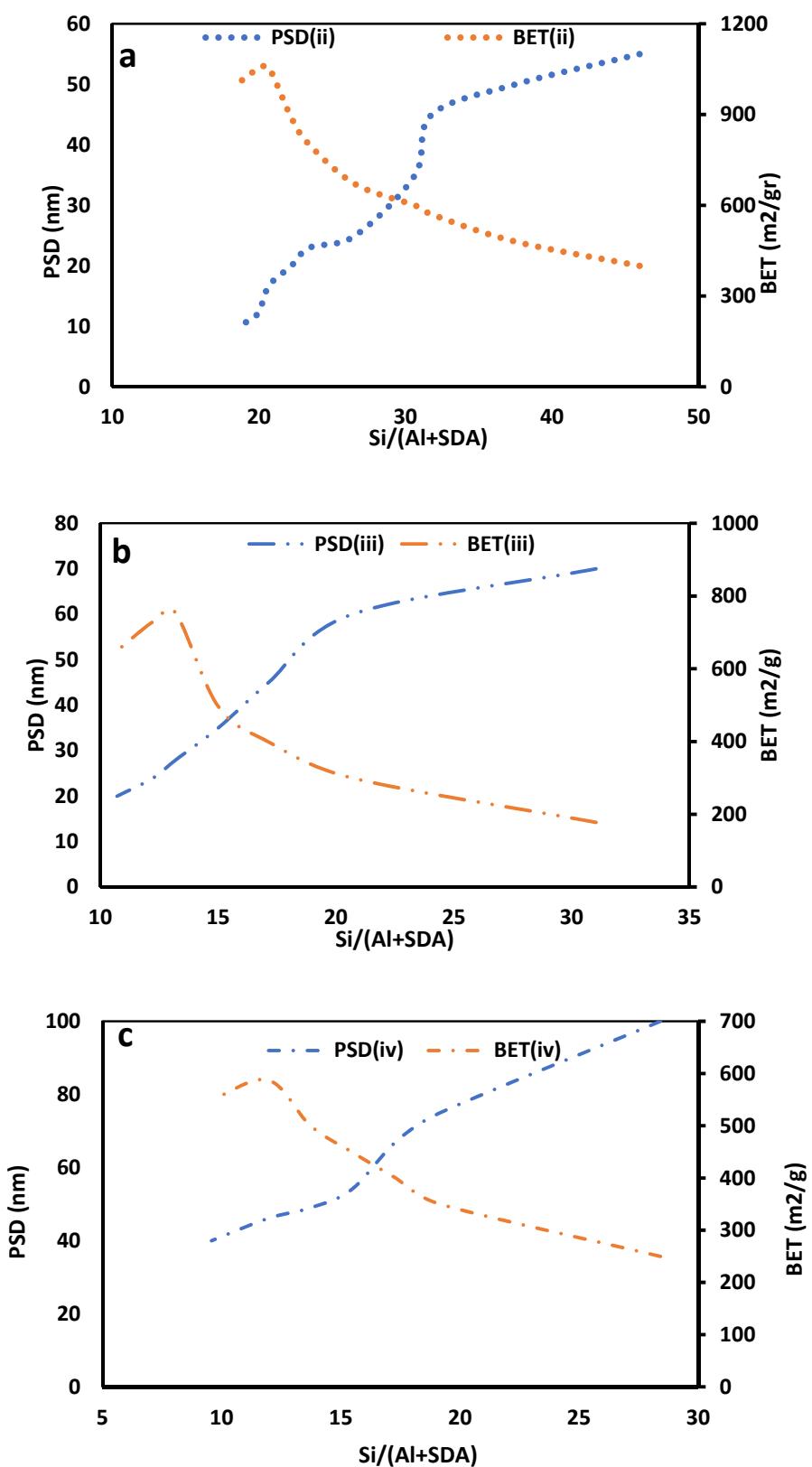


Figure S1. Effect of Si/(Al+SDA) ratio over PSD and BET of Beta-based catalyst for (a) TPABr, (b) morpholine and (c) n-butylamine as SDA.

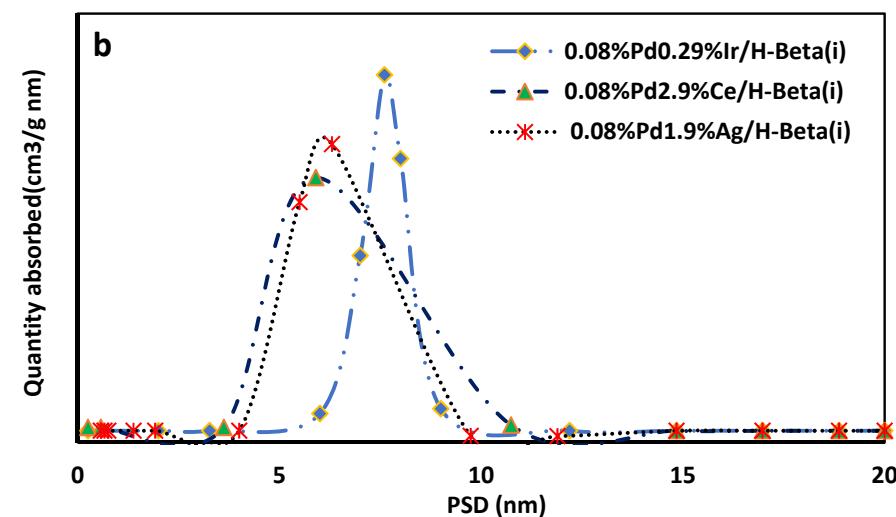
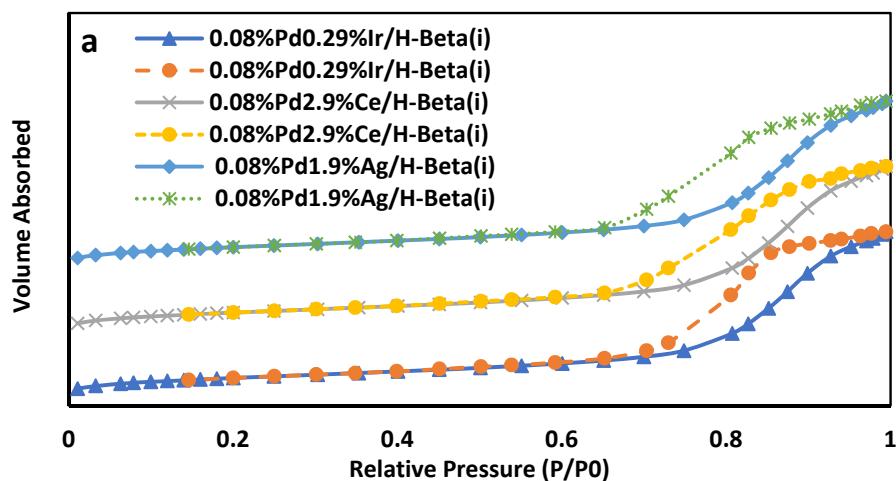


Figure S2.  $\text{N}_2$  adsorption-desorption isotherms (a) and BJH pore diameter distributions patterns (b) of the optimum catalysts.

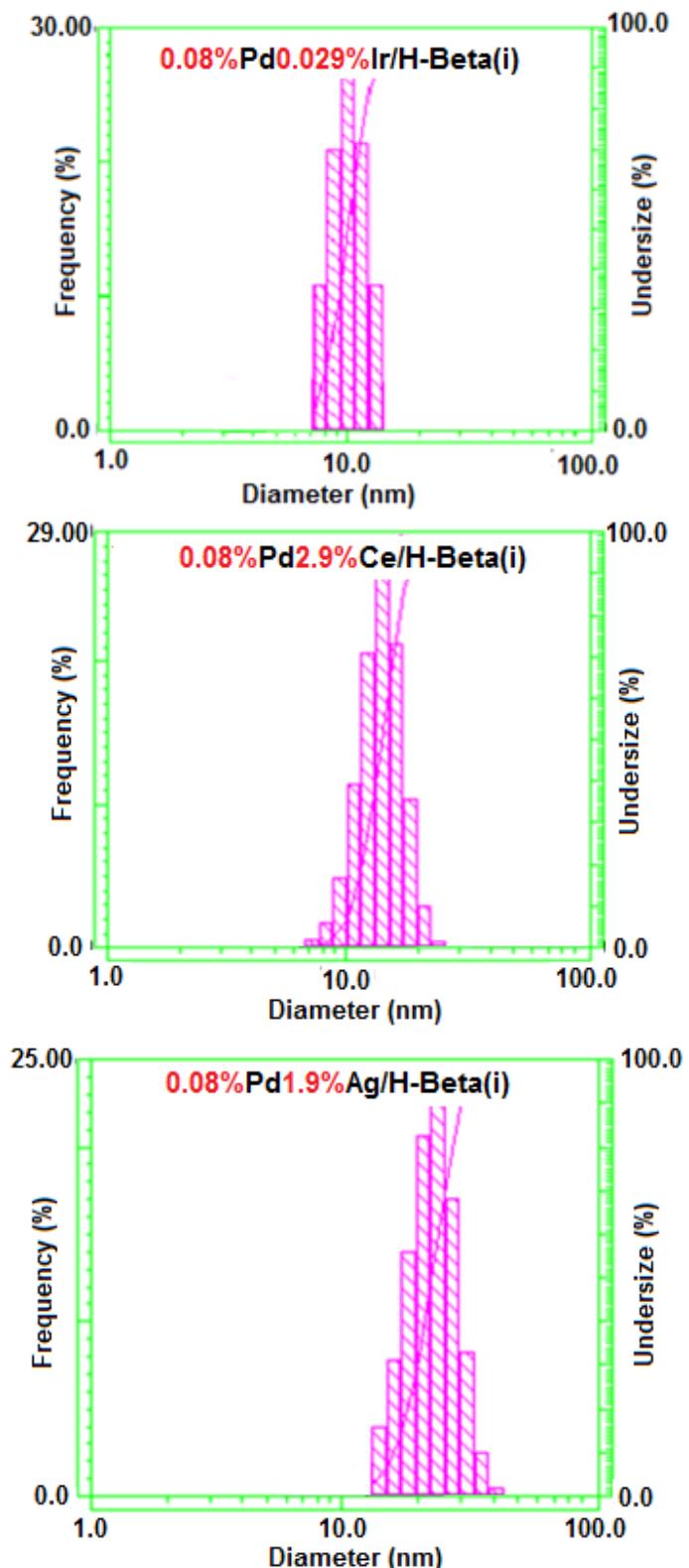
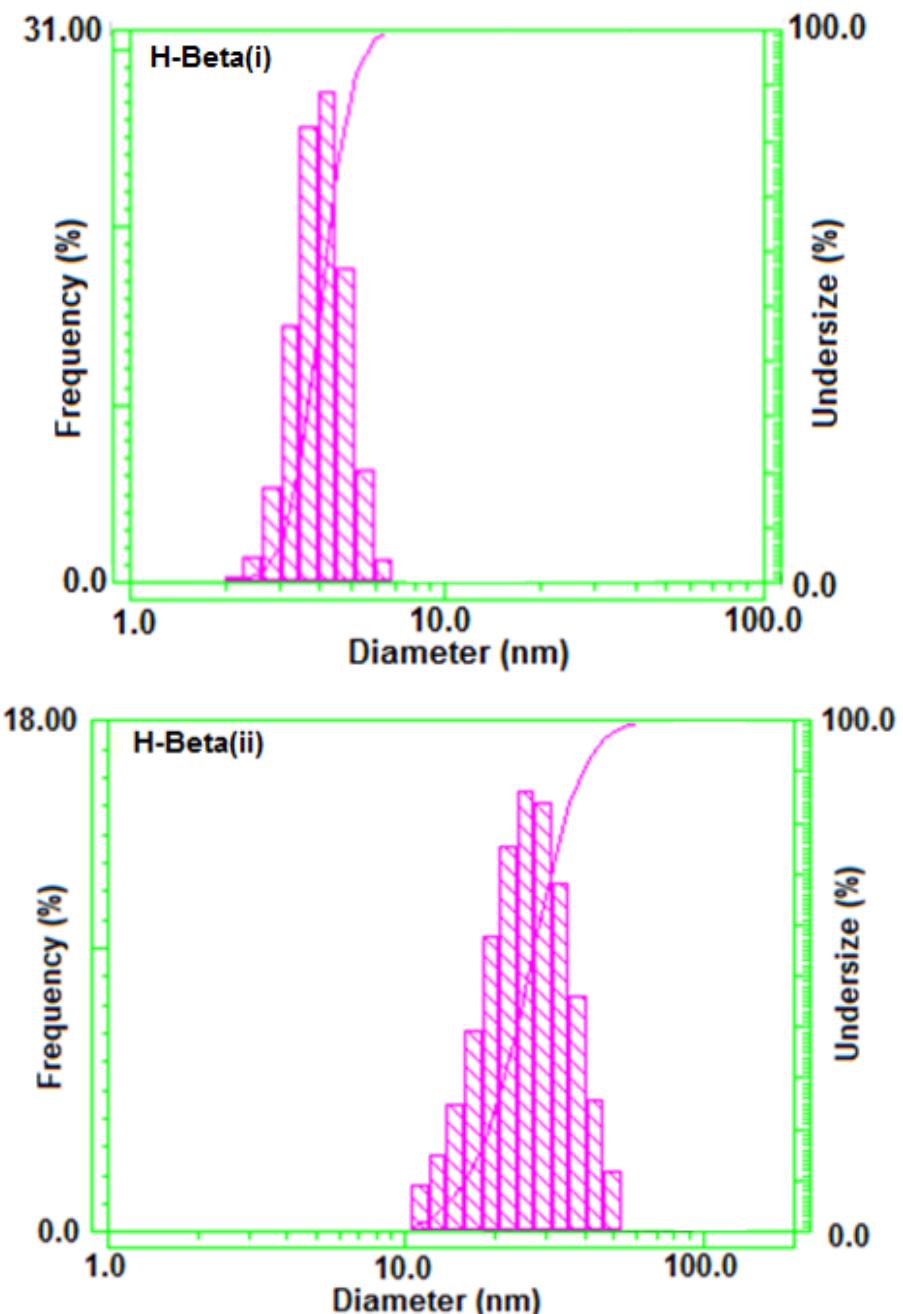


Figure S3. DLS pictures of the catalysts of optimum via TPAOH.



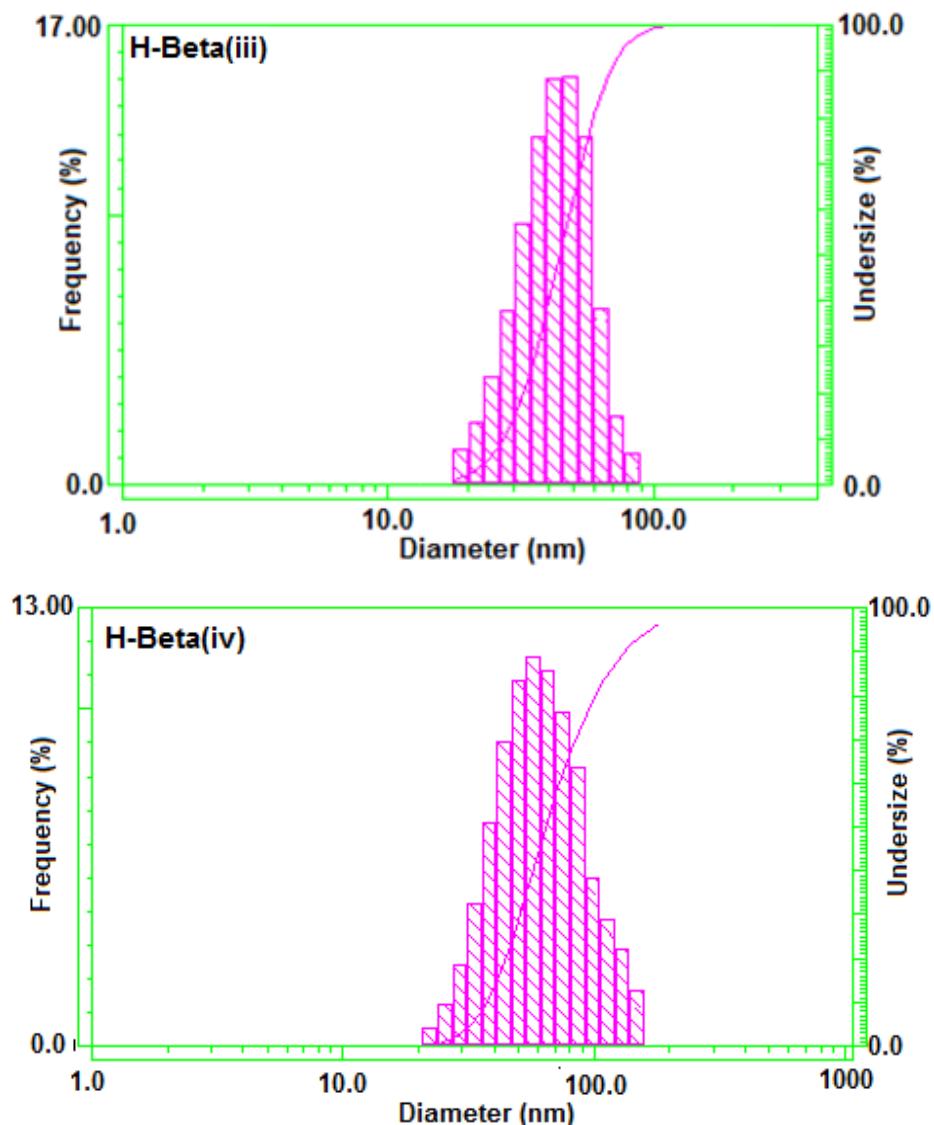
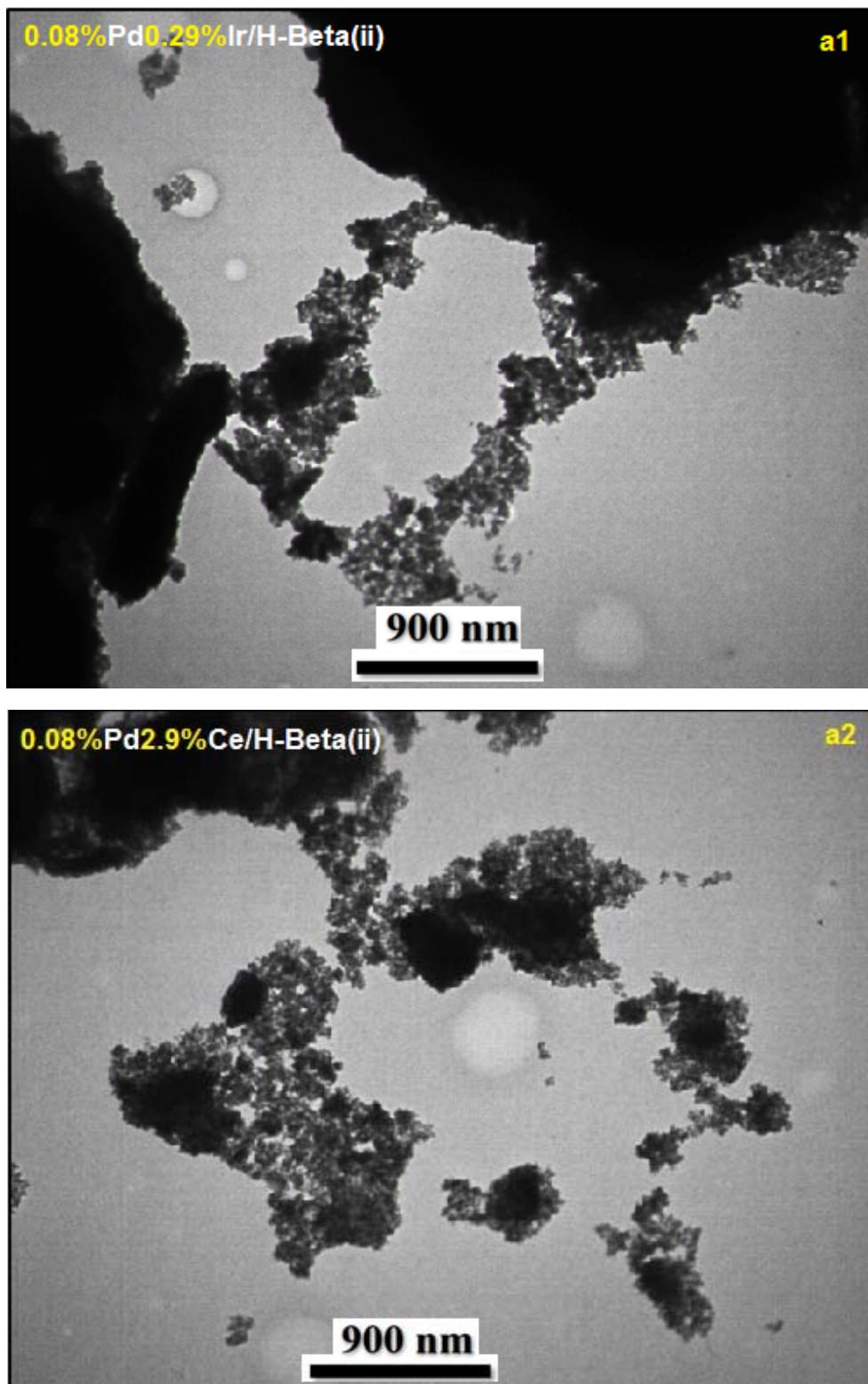
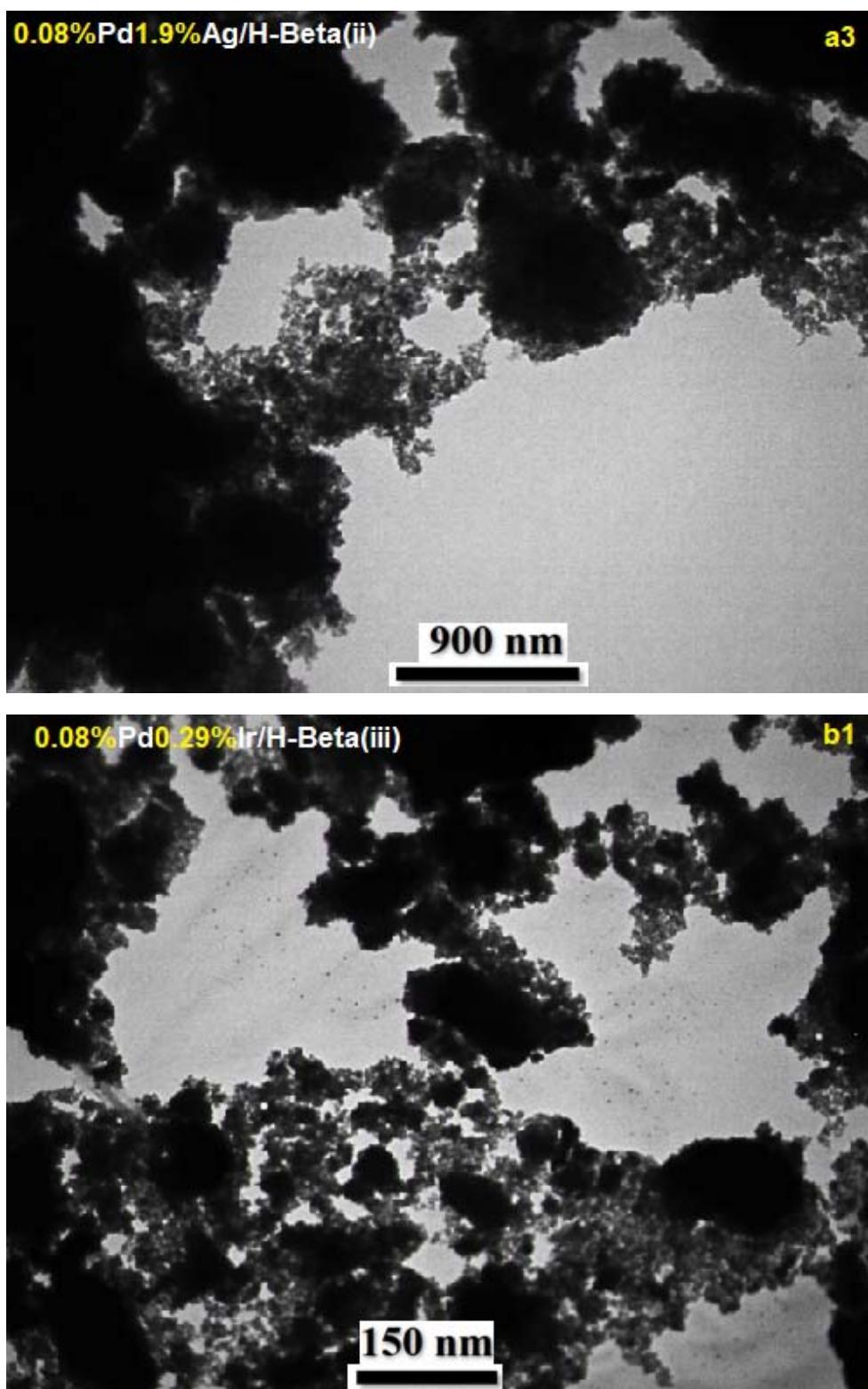
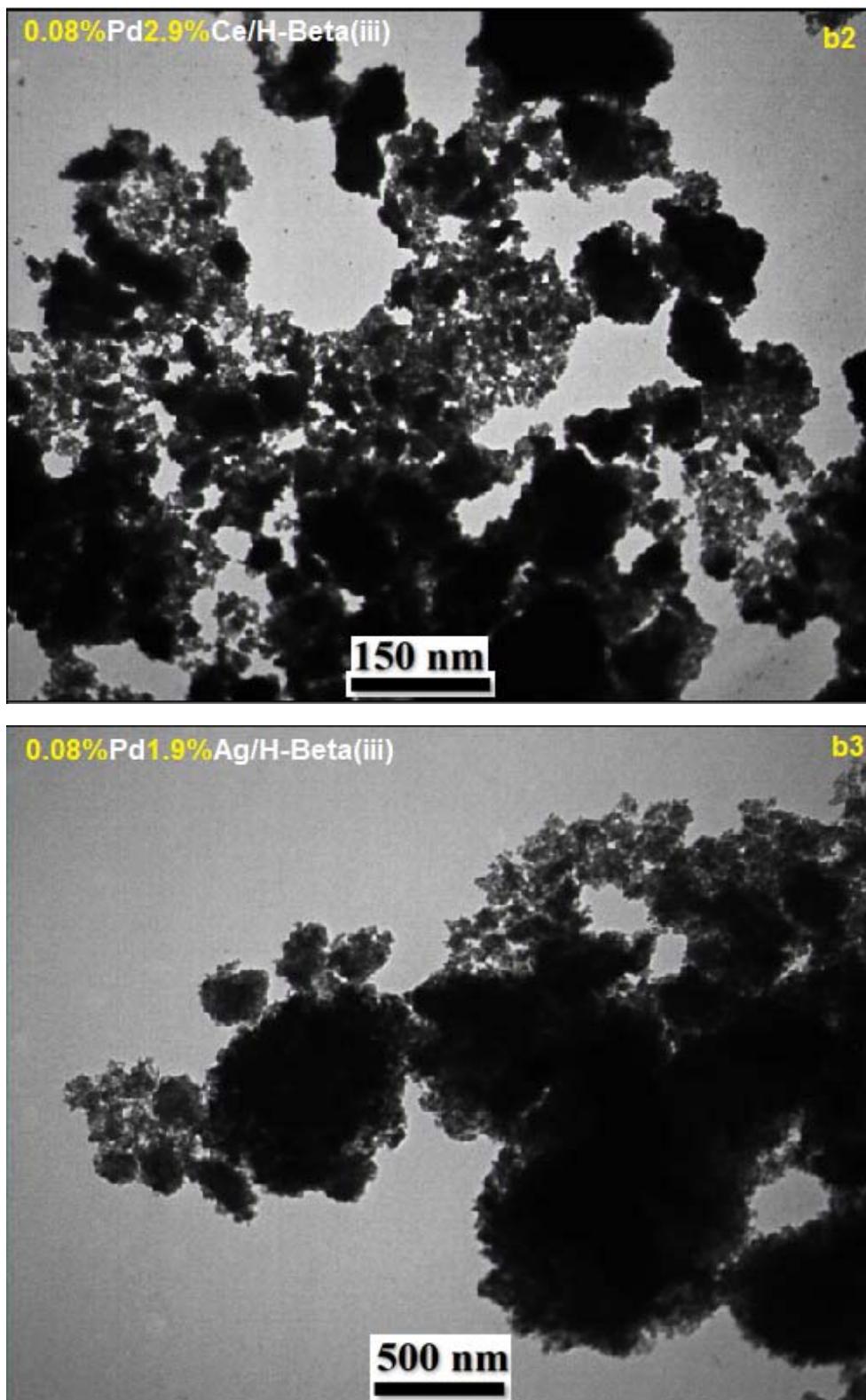
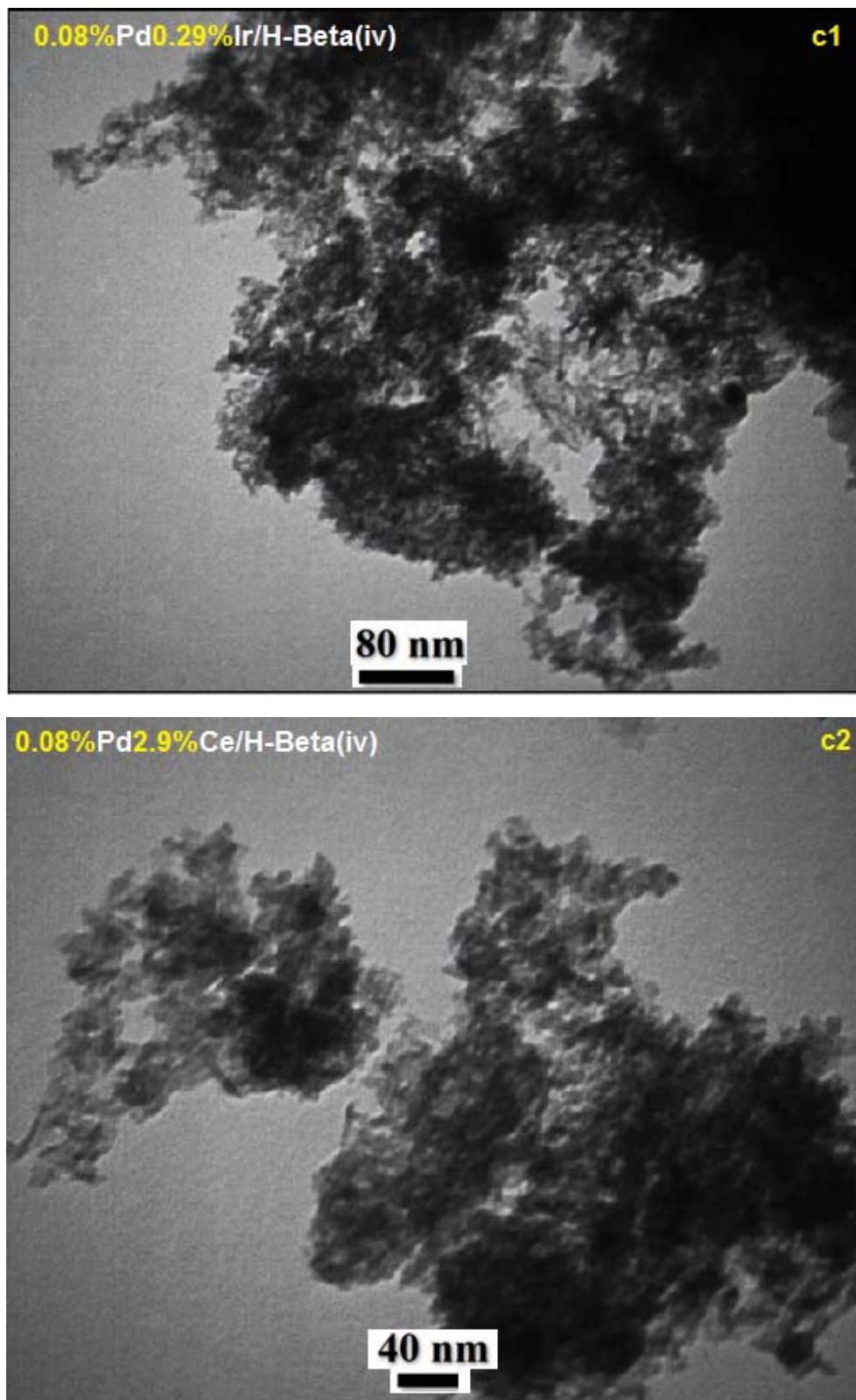


Figure S4. DLS patterns of H-Beta-based catalyst with SDA.









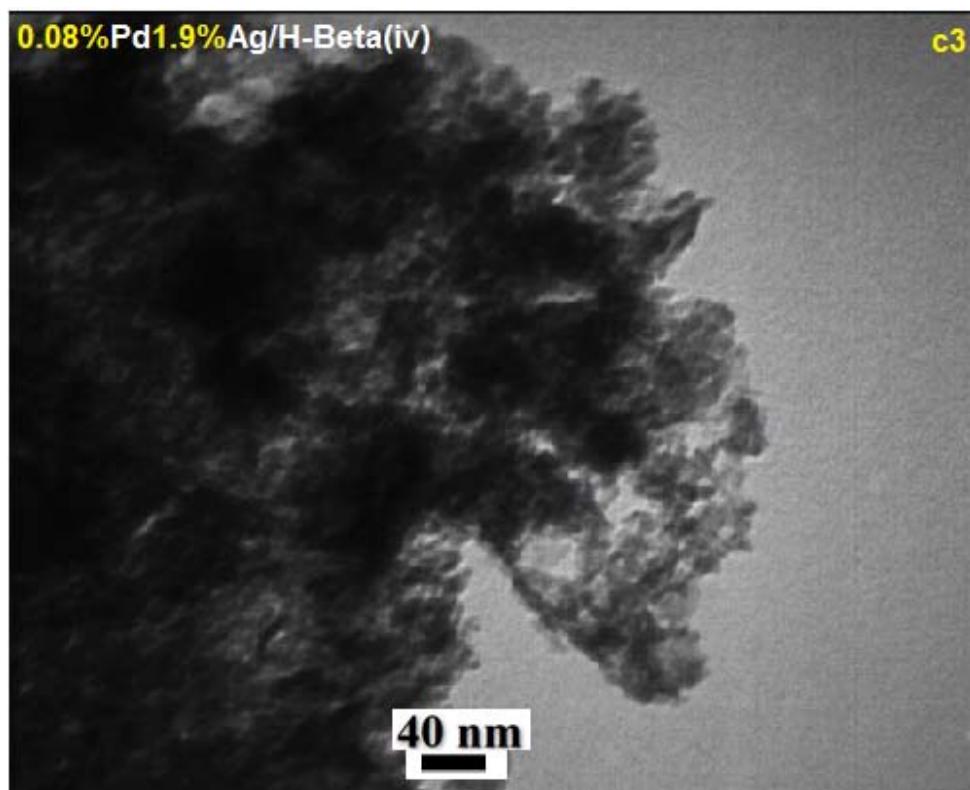
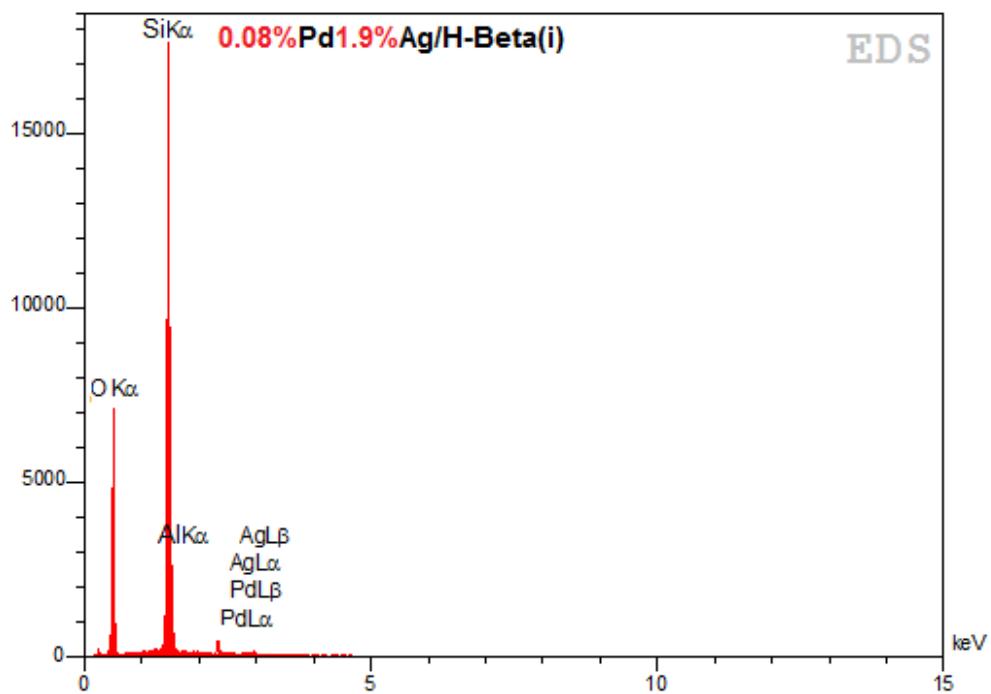


Figure S5. TEM patterns of different Beta-based catalysts, (a1) 0.08%Pd0.29%Ir/H-Beta(ii), (a2) 0.08%Pd2.9%Ce/H-Beta(ii), (a3) 0.08%Pd1.9%Ag/H-Beta(ii), (b1) 0.08%Pd0.29%Ir/H-Beta(iii), (b2) 0.08%Pd2.9%Ce/H-Beta(iii), (b3) 0.08%Pd1.9%Ag/H-Beta(iii), (c1) 0.08%Pd0.29%Ir/H-Beta(iv), (c2) 0.08%Pd2.9%Ce/H-Beta(iv), (c3) 0.08%Pd1.9%Ag/H-Beta(iv).



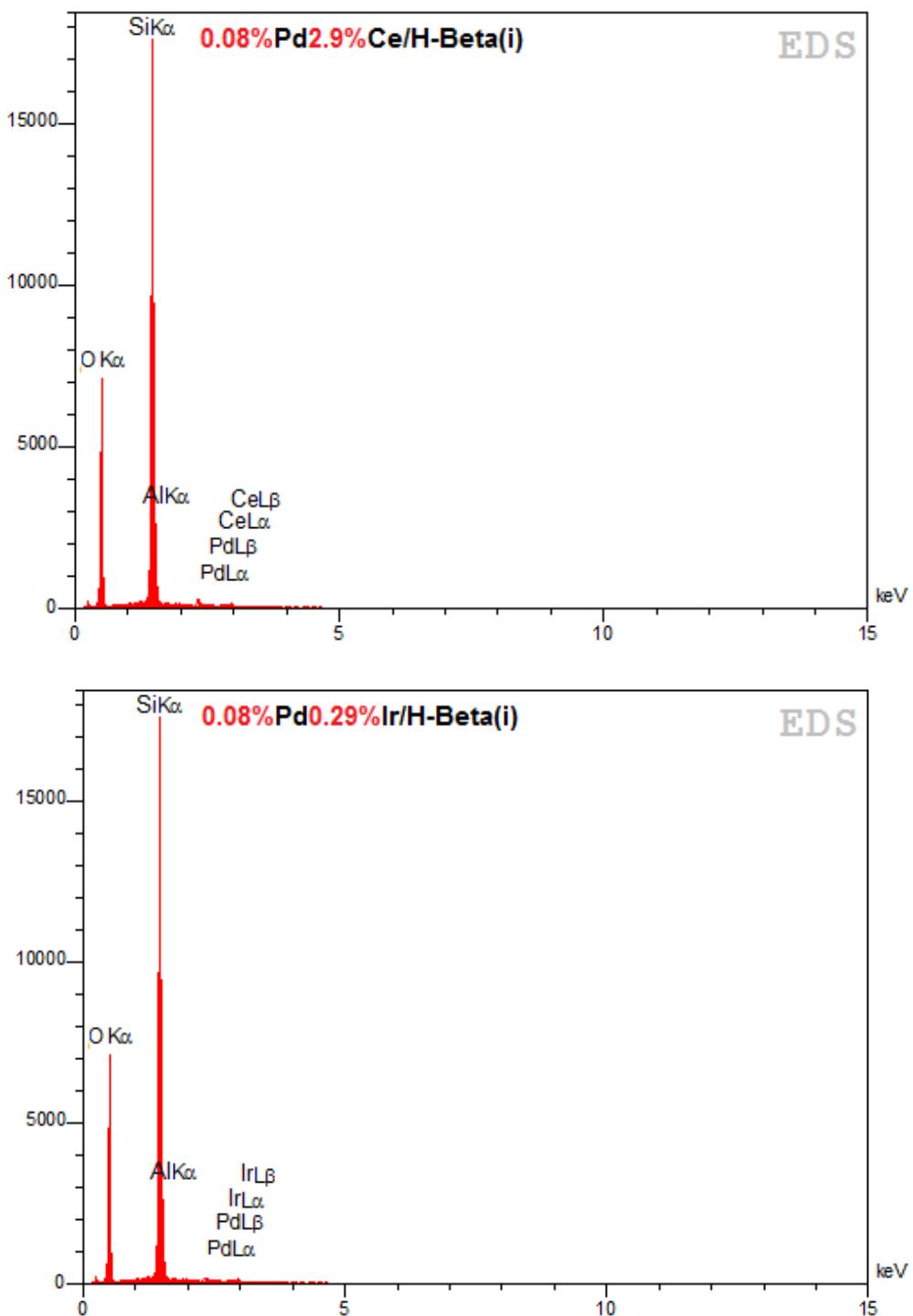
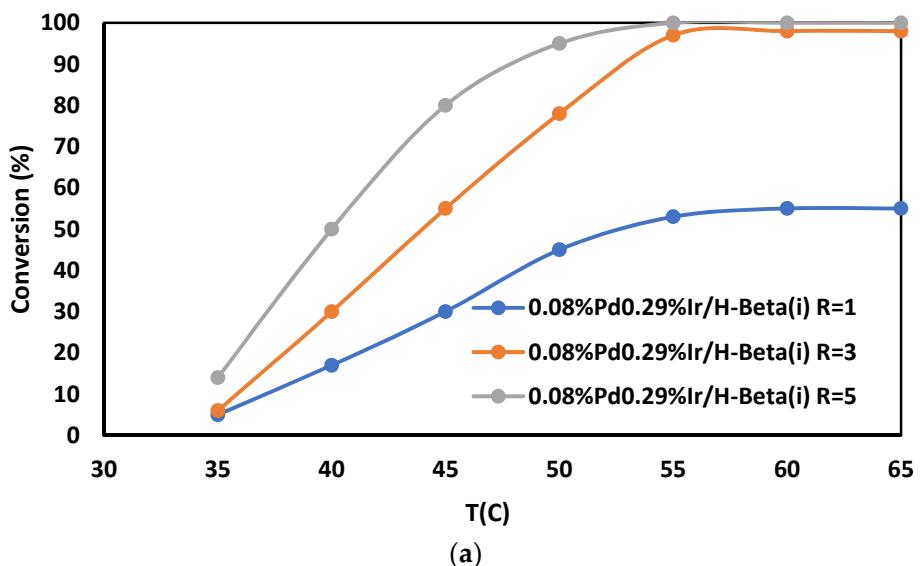
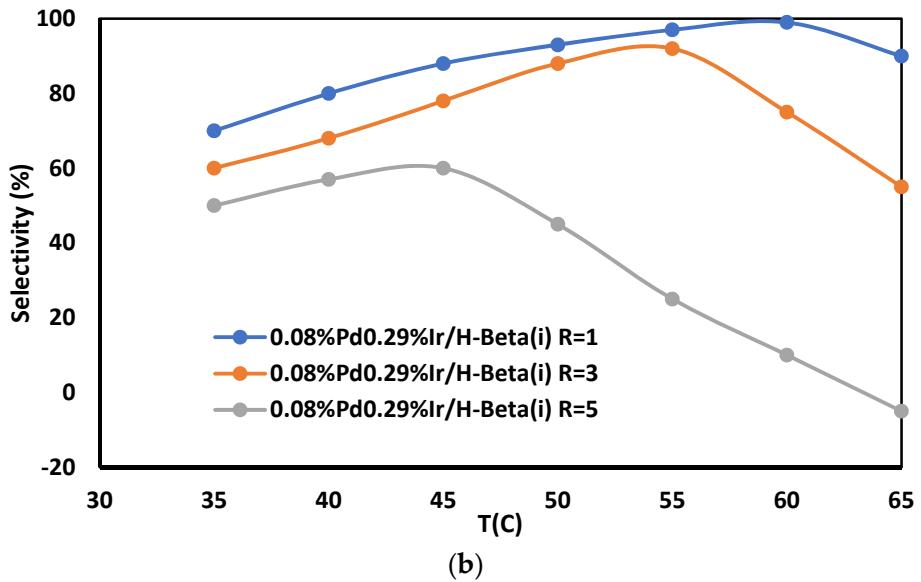


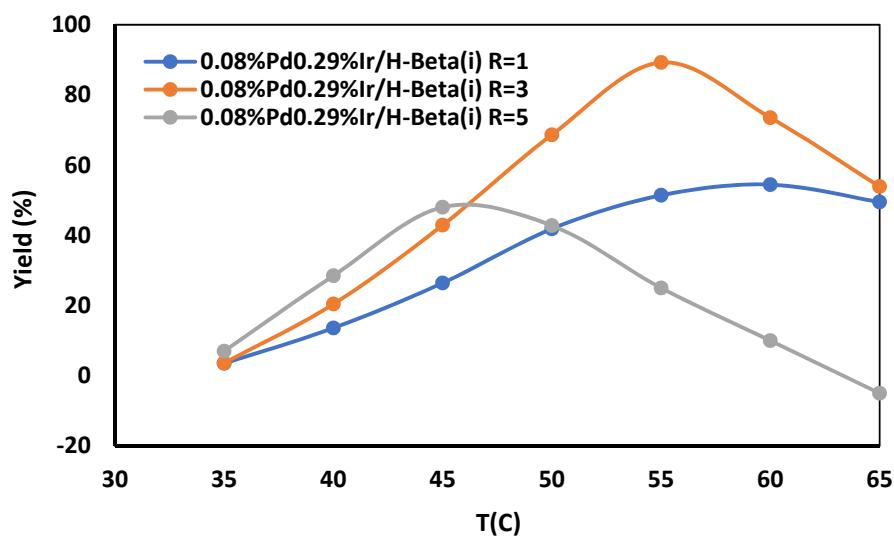
Figure S6. EDX analyses of the optimum catalysts.



(a)

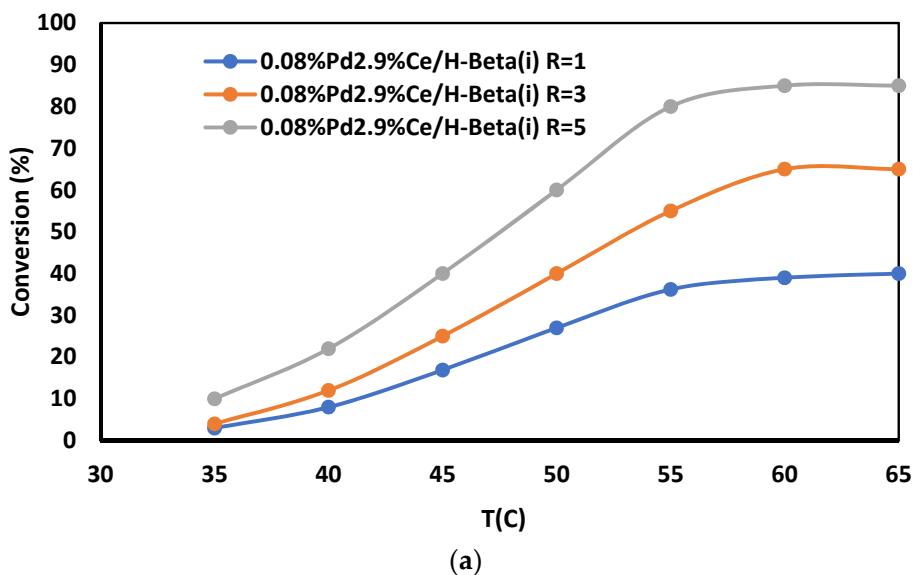


(b)



(c)

Figure S7. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd 0.29%Ir/H-Beta(i) catalysts under different H<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> ratios, GHSV=4030 h<sup>-1</sup>, and P=20 bar.



(a)

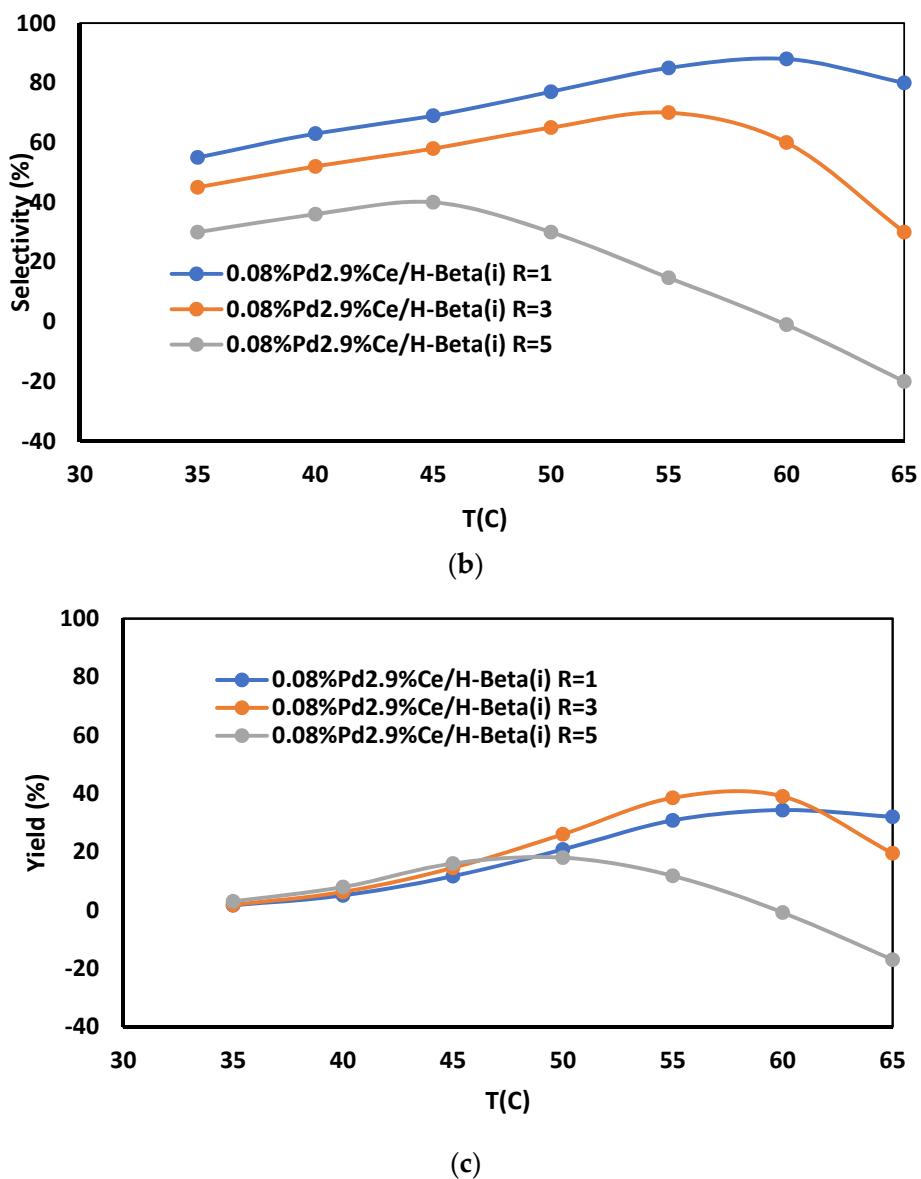
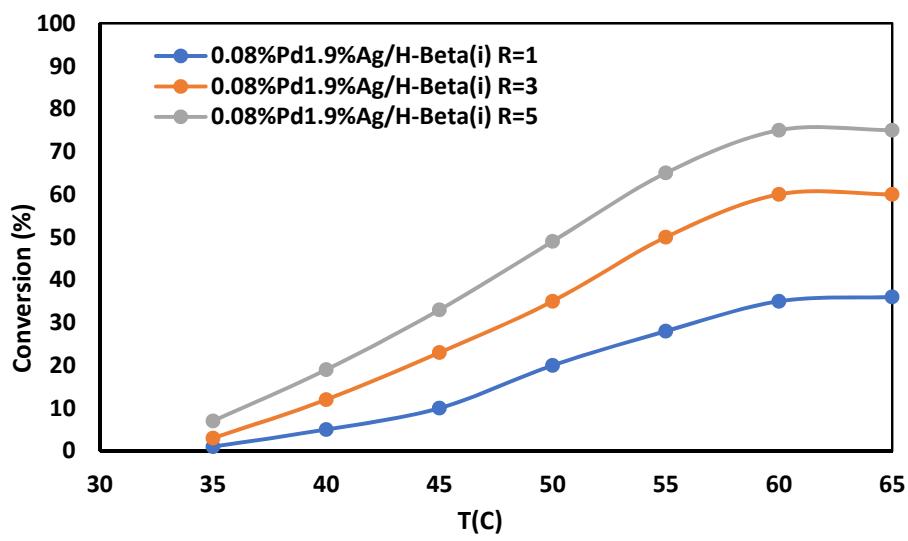
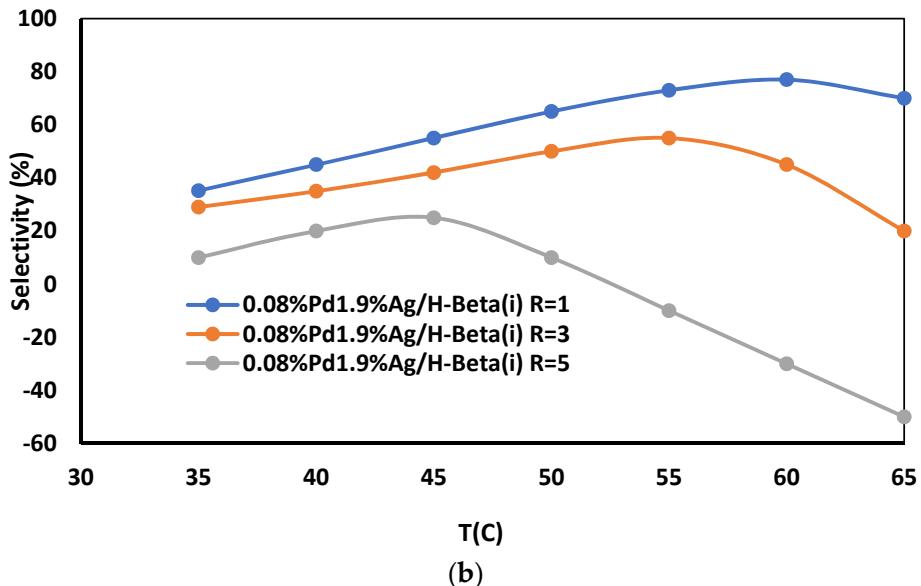


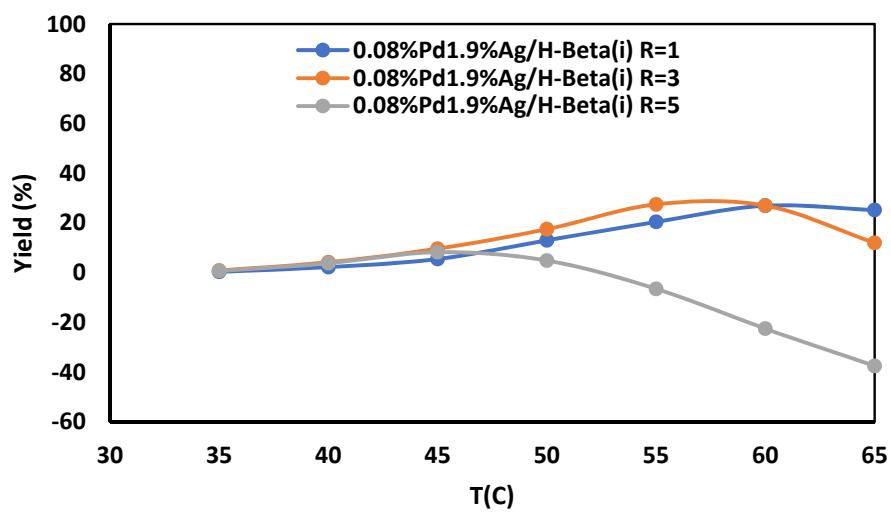
Figure S8. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd 2.9%Ce/H-Beta(i) catalysts under different H<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> ratios GHSV=4030 h<sup>-1</sup>, and P=20 bar.



(a)

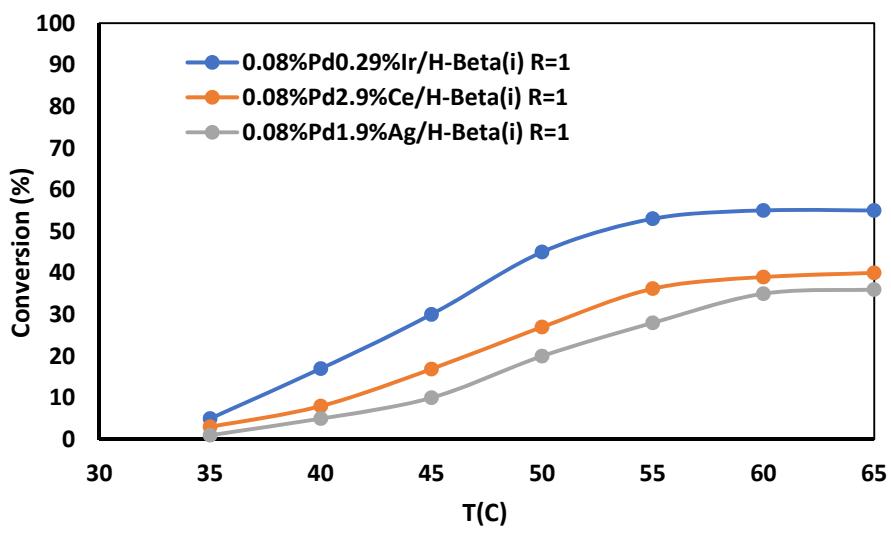


(b)

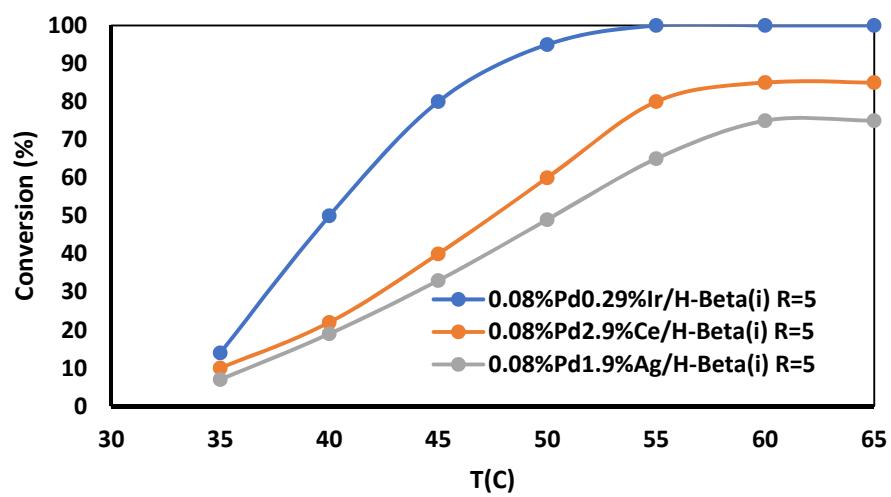


(c)

Figure S9. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd 1.9%Ag/H-Beta(i) catalysts under different H<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> ratios GHSV=4030 h<sup>-1</sup>, and P=20 bar.

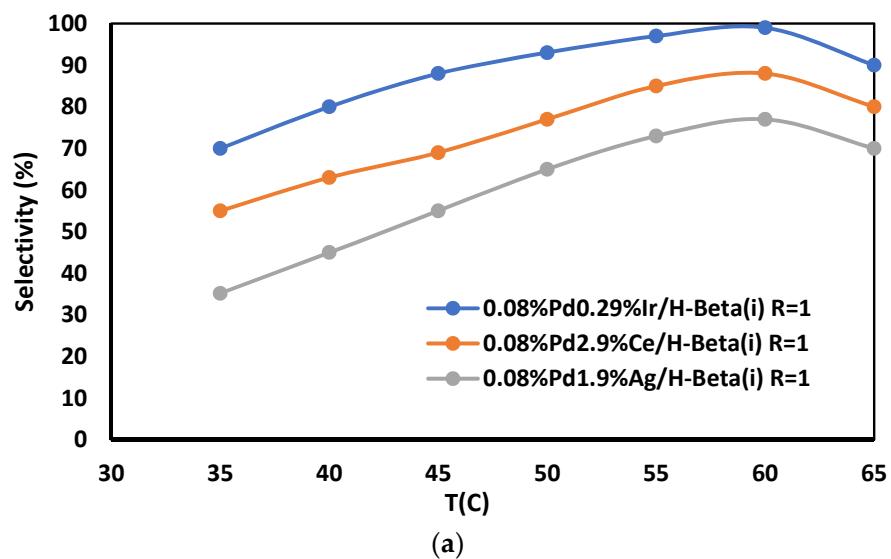


(a)



(b)

Figure S10. Acetylene conversion over optimum catalysts under  $P=20$  bar and  $GHSV = 4030 \text{ h}^{-1}$  (a)  $R=1$  and (b)  $R=5$ .



(a)

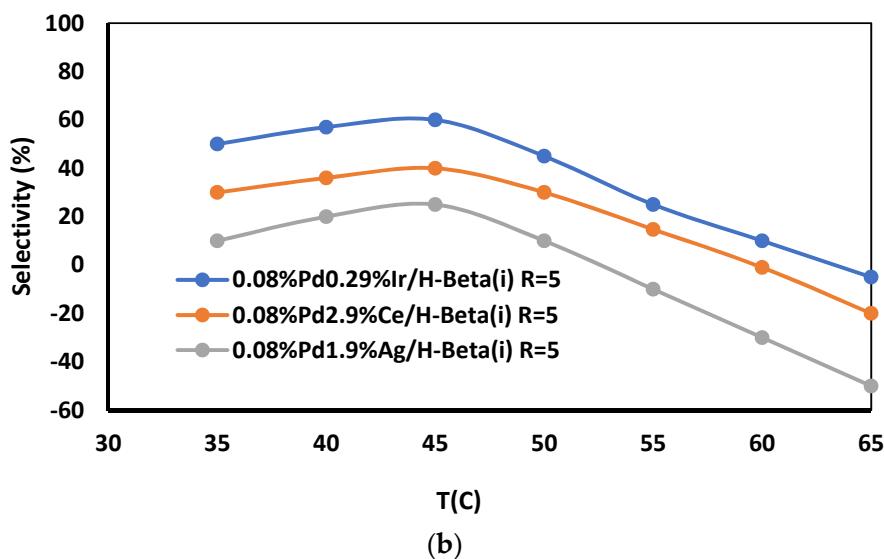
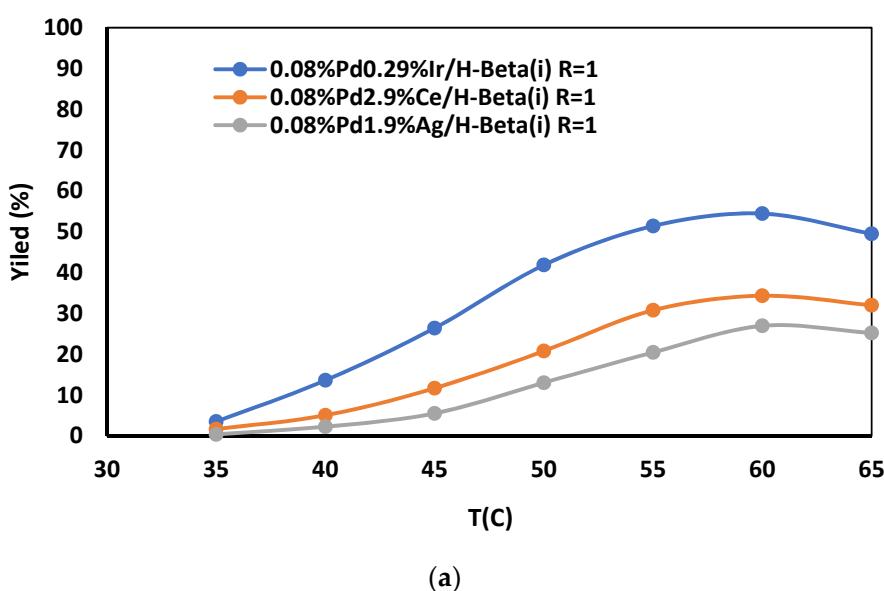
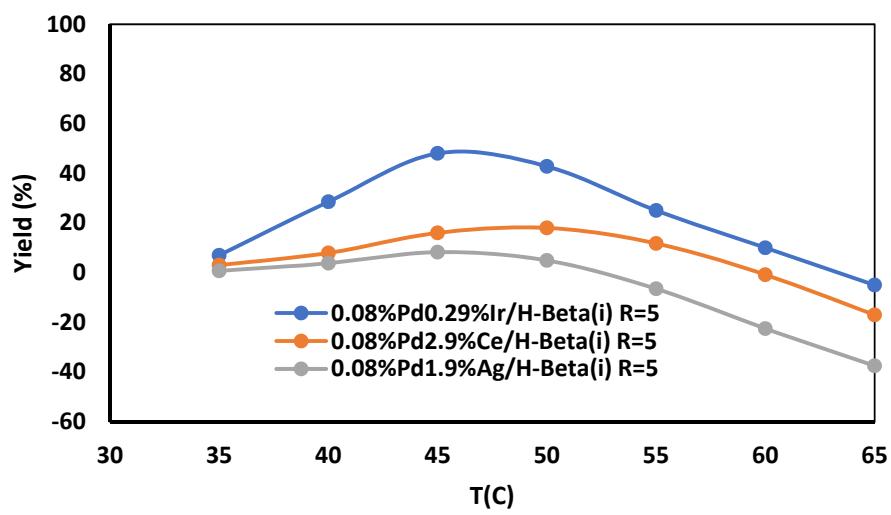


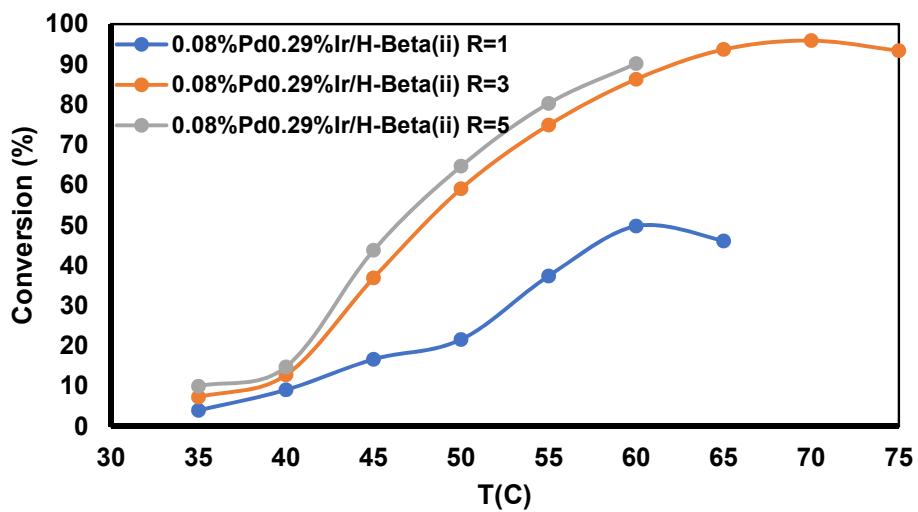
Figure S11. Ethylene selectivity optimum catalysts under  $P=20$  bar and  $GHSV=4030\text{ h}^{-1}$  (a)  $R=1$  and (b)  $R=5$ .





(b)

Figure S12. Yield over optimum catalysts under  $P=20$  bar and  $GHSV= 4030\text{ h}^{-1}$  (a)  $R=1$  and (b)  $R=5$ .



(a)

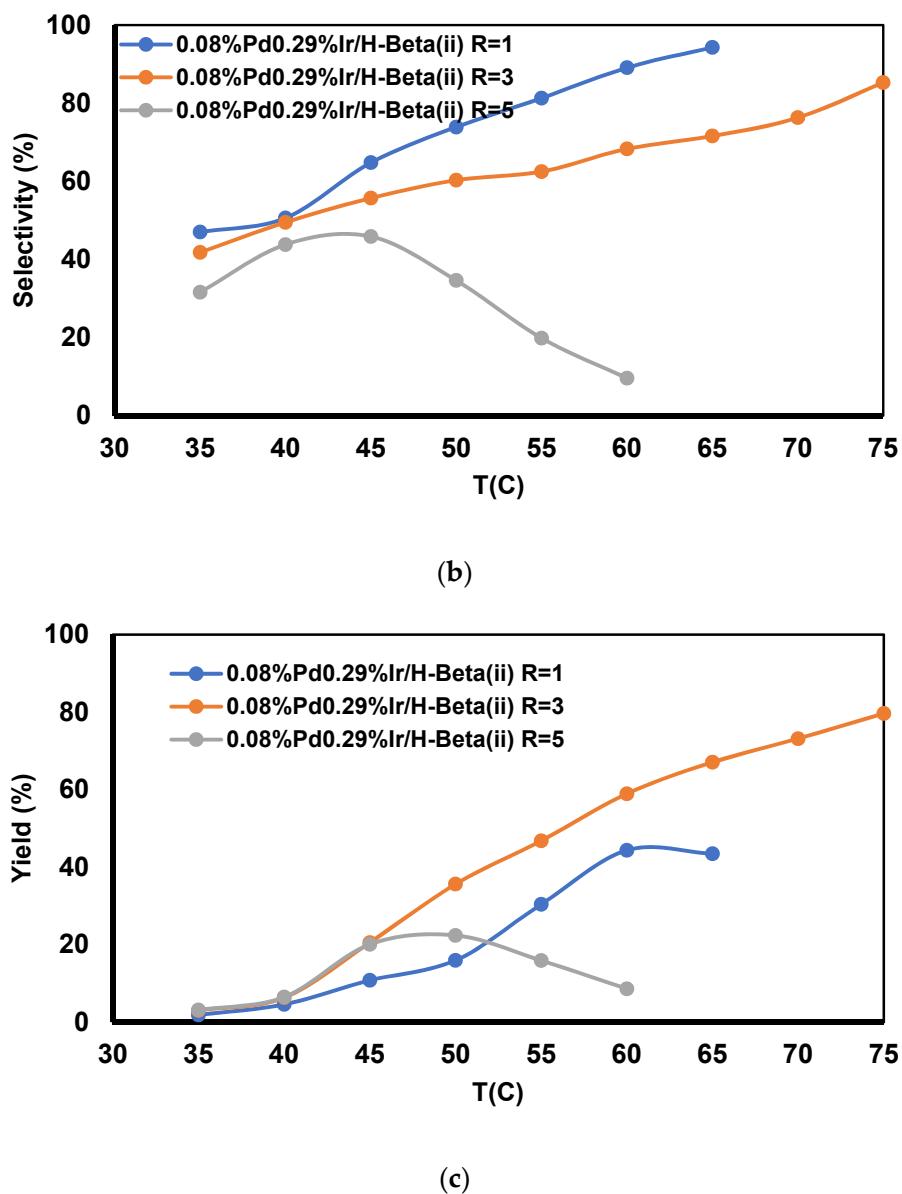
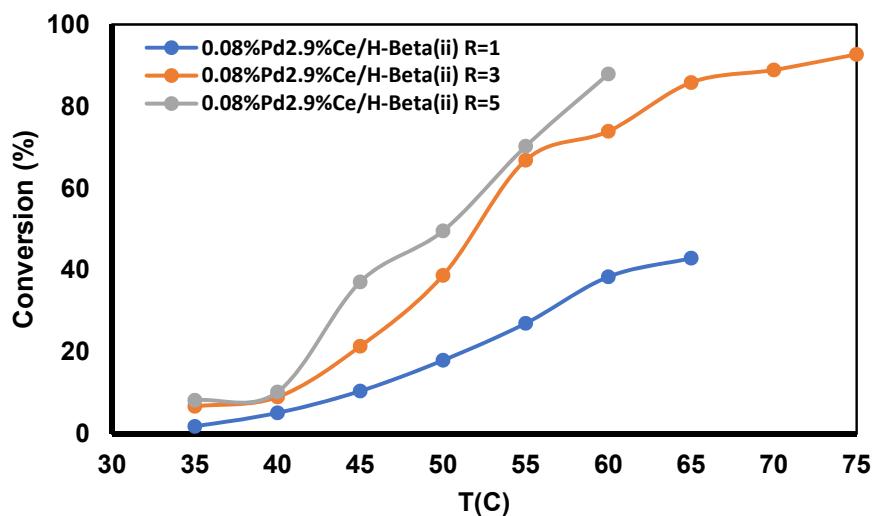
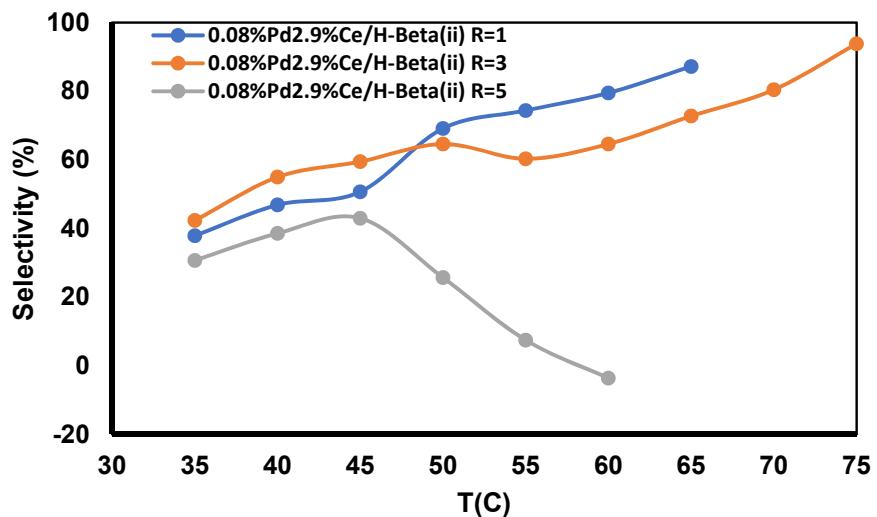


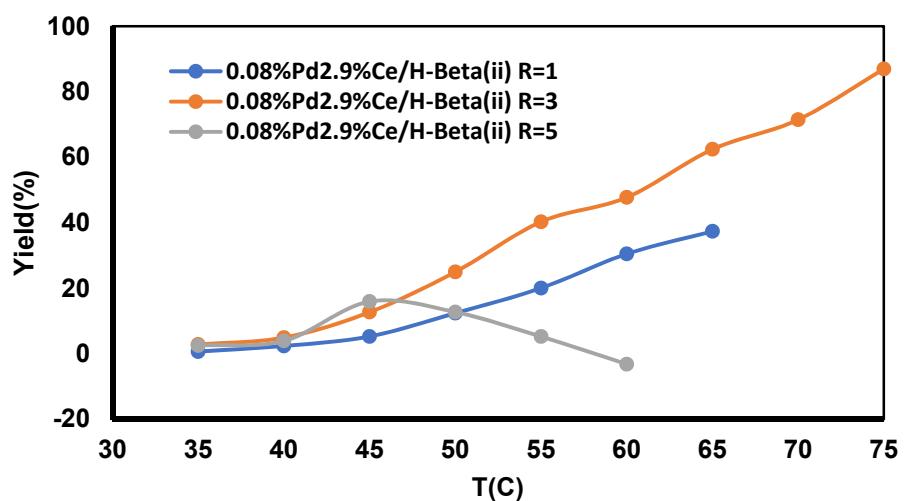
Figure S13. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd0.29%Ir/H-Beta(ii) catalysts under different H<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> ratios, GHSV = 4030 h<sup>-1</sup>, and P = 20 bar.



(a)

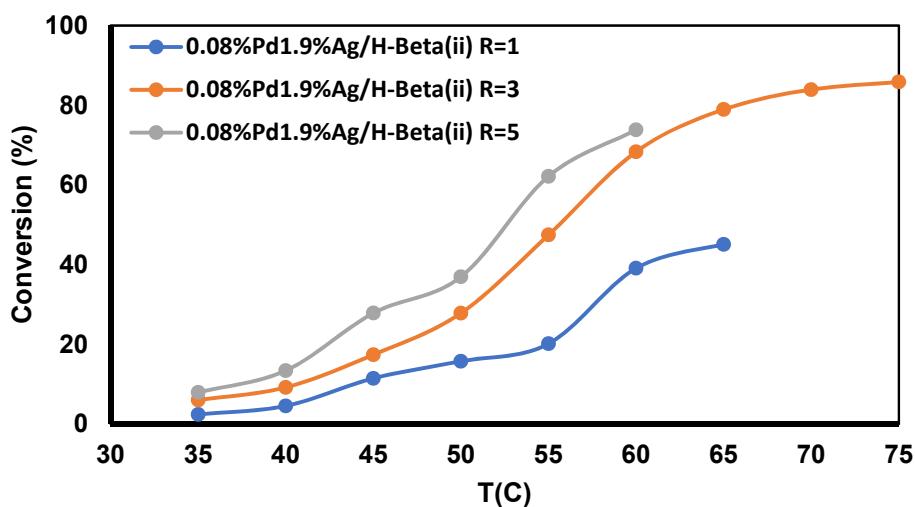


(b)



(c)

Figure S14. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd 2.9%Ce/H-Beta(ii) catalysts under different H<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> ratios GHSV=4030 h<sup>-1</sup>, and P=20 bar.



(a)

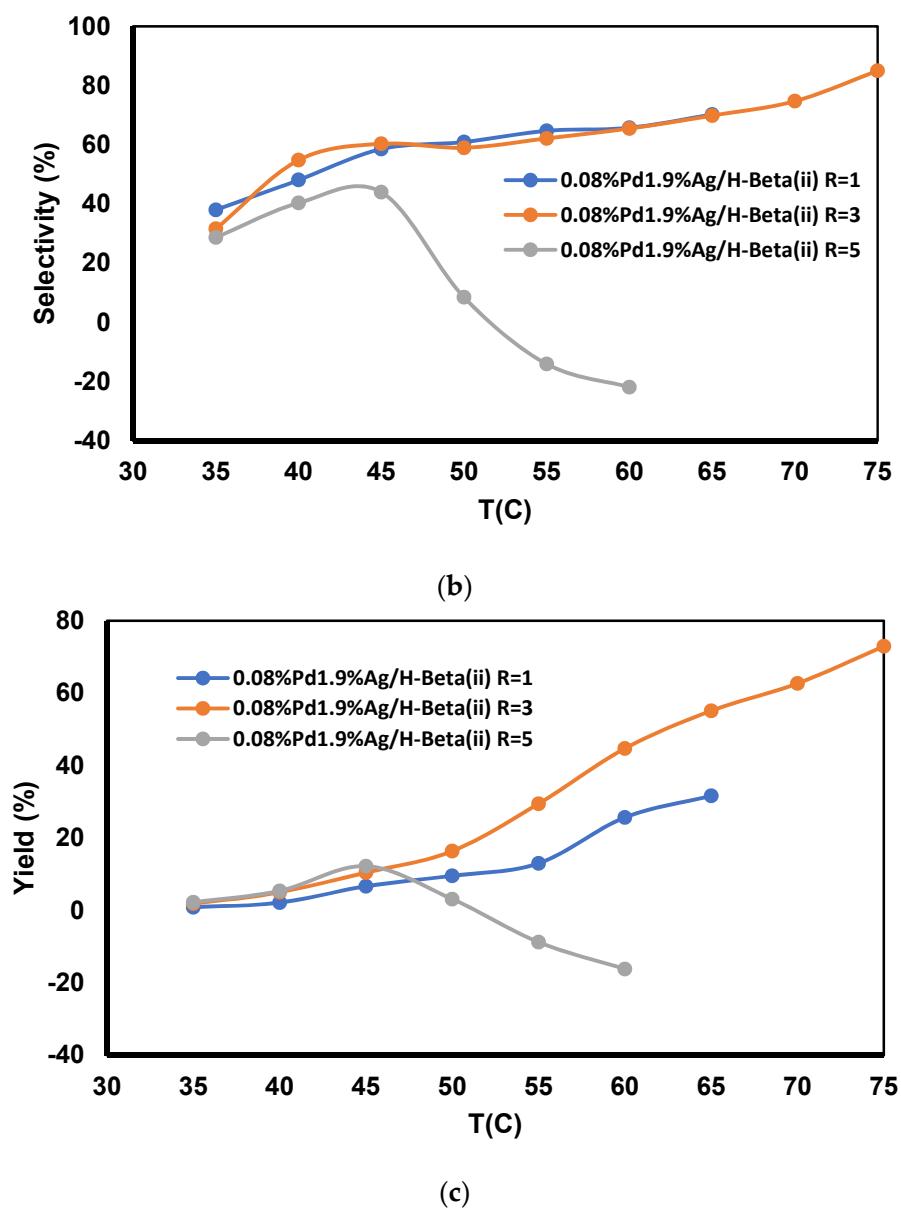
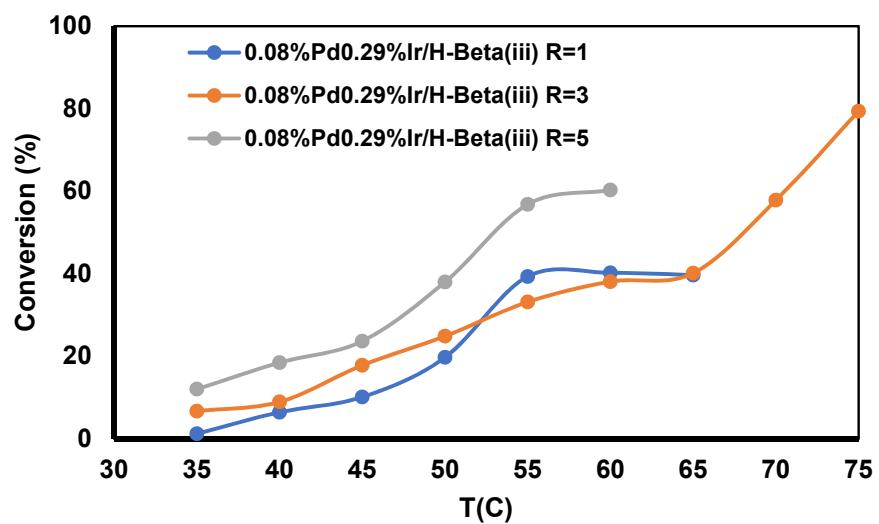
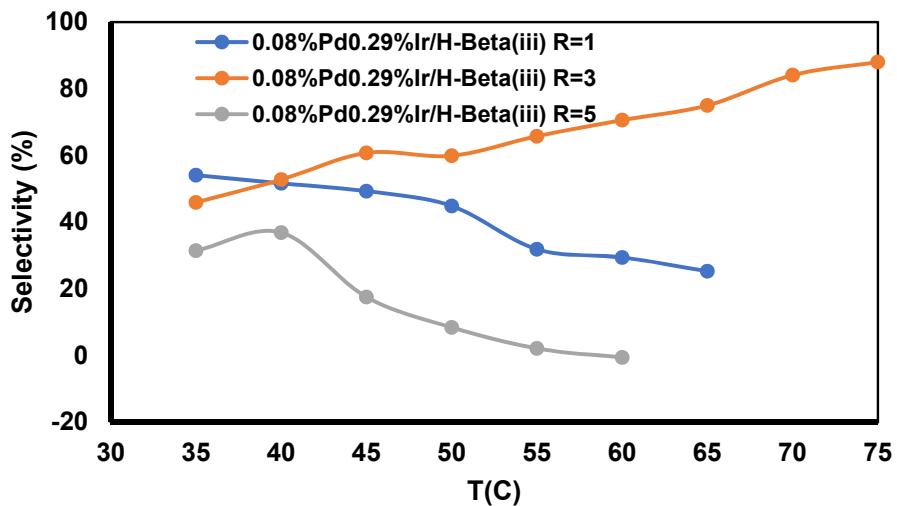


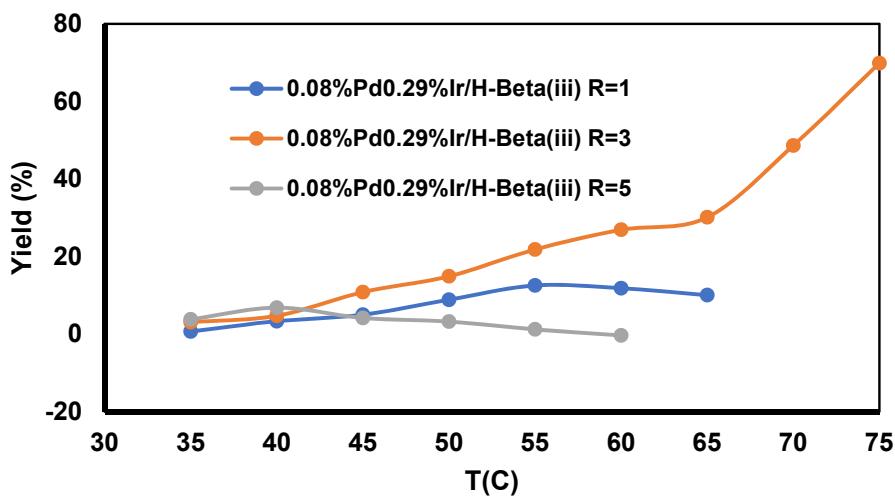
Figure S15. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd1.9%Ag/H-Beta(ii) catalysts under different  $\text{H}_2/\text{C}_2\text{H}_2$  ratios GHSV=4030  $\text{h}^{-1}$ , and P=20 bar.



(a)

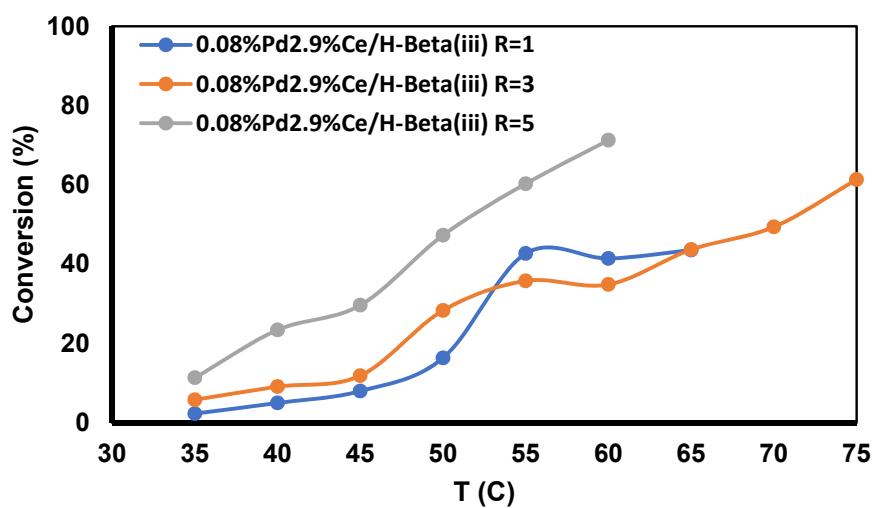


(b)



(c)

Figure S16. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd 0.29%Ir/H-Beta(iii) catalysts under different H<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> ratios, GHSV=4030 h<sup>-1</sup>, and P=20 bar.



(a)

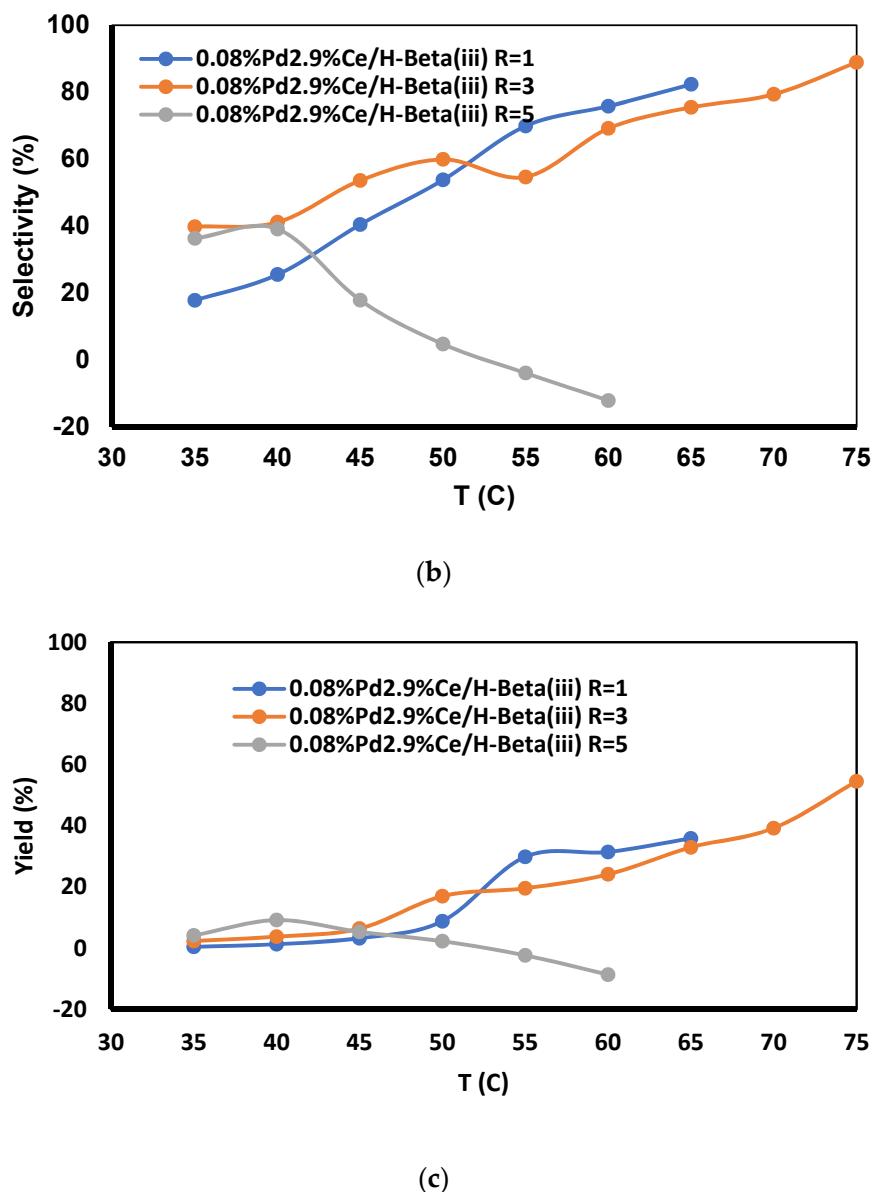
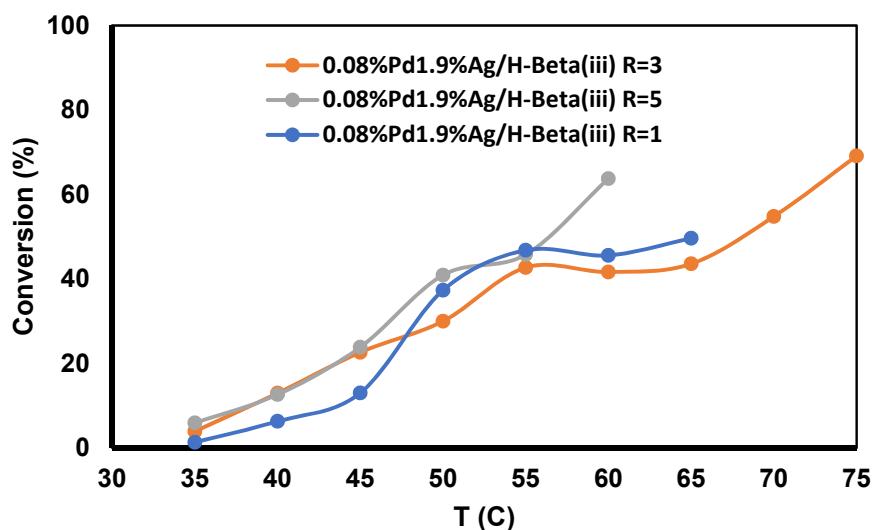
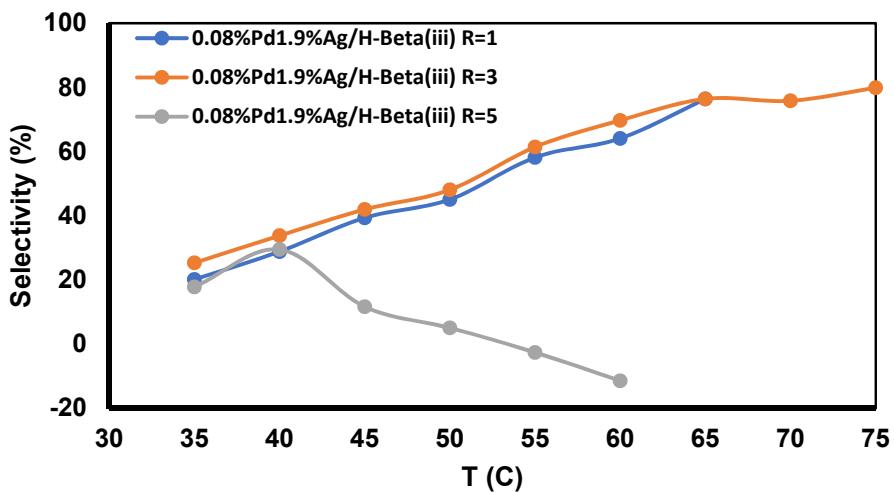


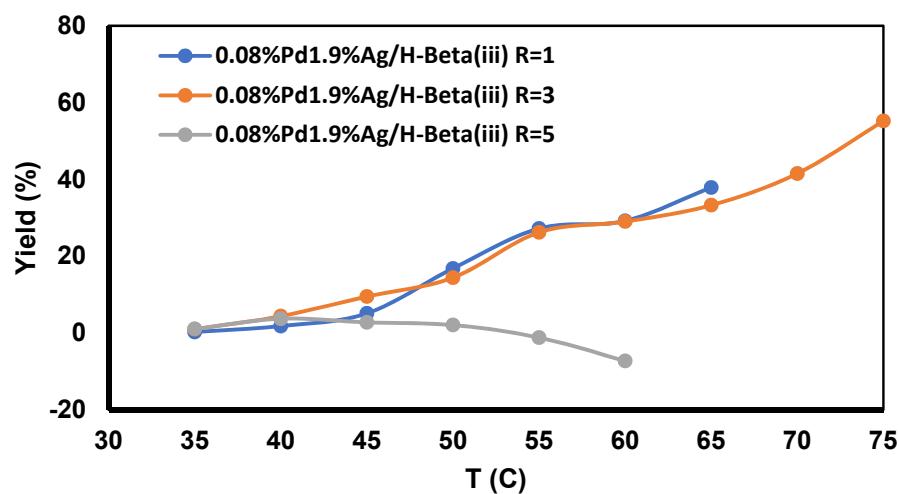
Figure S17. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd2.9%Ce/H-Beta(iii) catalysts under different  $\text{H}_2/\text{C}_2\text{H}_2$  ratios GHSV=4030  $\text{h}^{-1}$ , and P=20 bar.



(a)

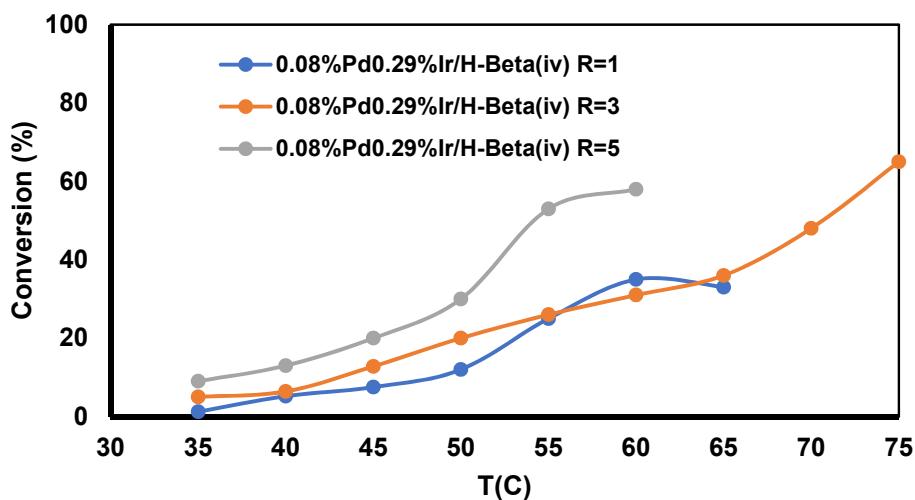


(b)



(c)

Figure S18. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd 1.9%Ag/H-Beta(iii) catalysts under different  $\text{H}_2/\text{C}_2\text{H}_2$  ratios GHSV=4030  $\text{h}^{-1}$ , and P=20 bar.



(a)

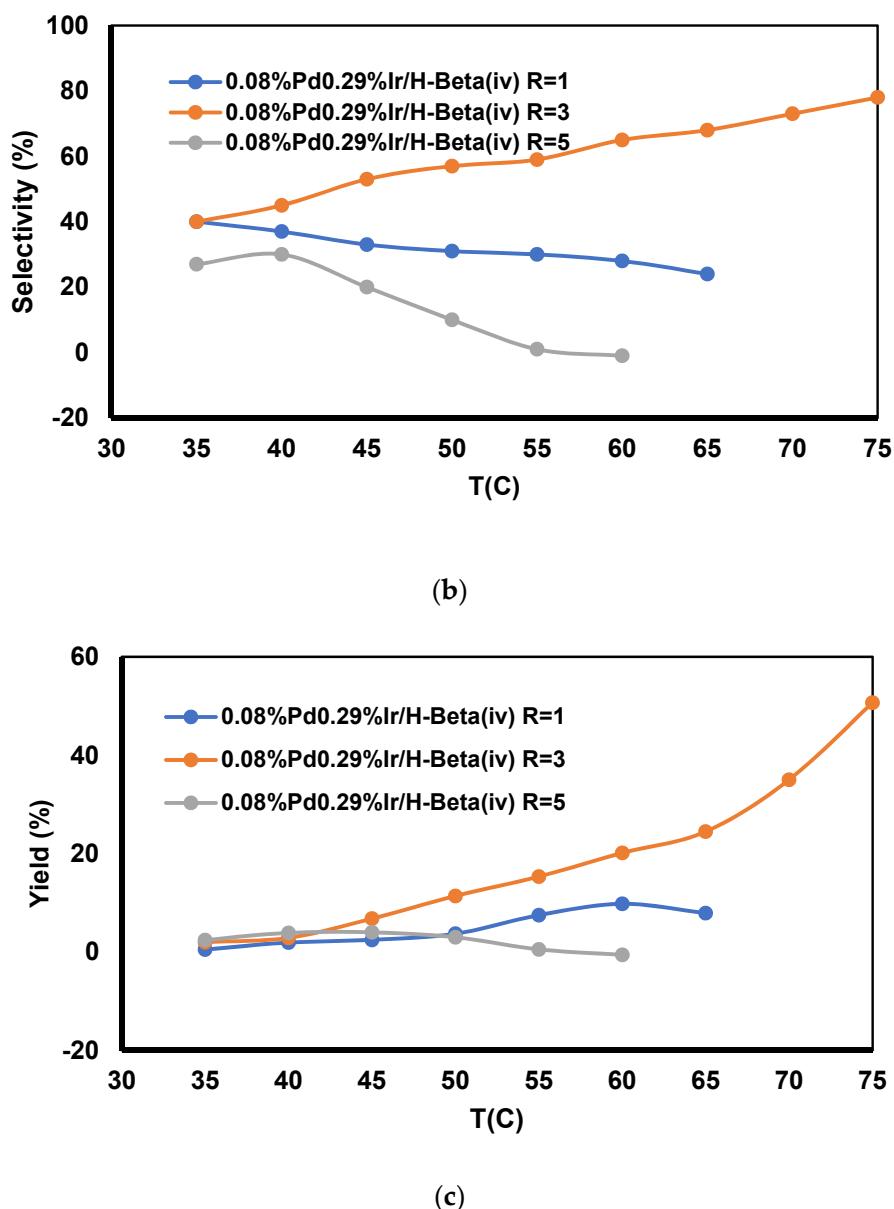
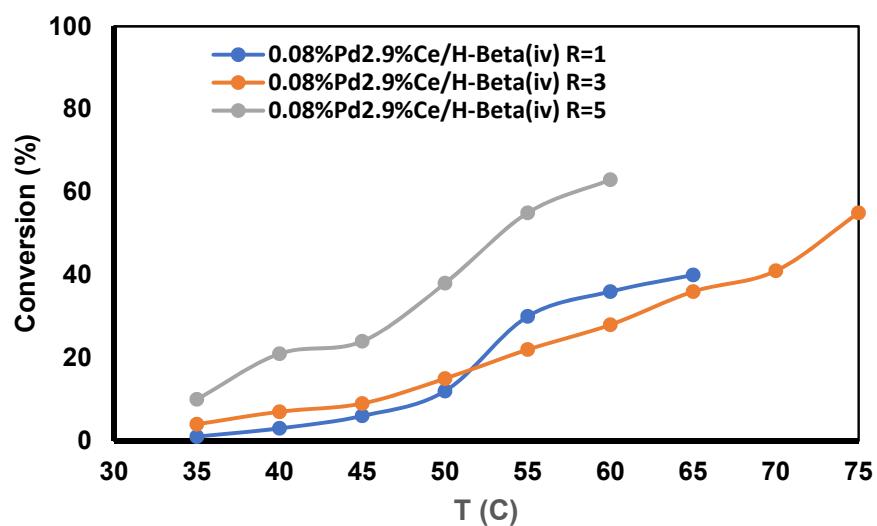
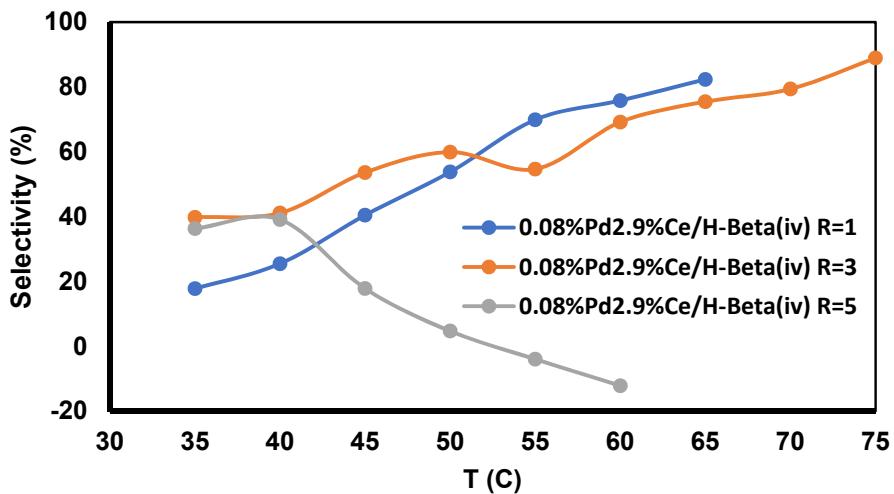


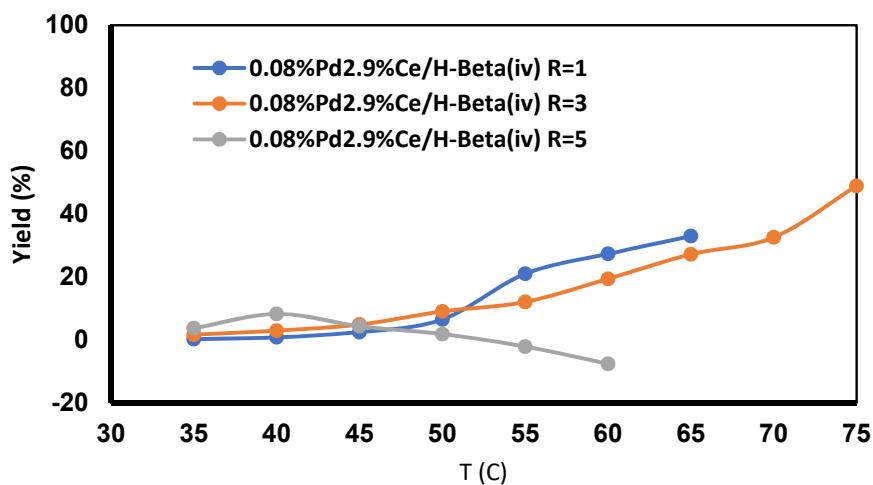
Figure S19. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd0.29%Ir/H-Beta(iv) catalysts under different  $\text{H}_2/\text{C}_2\text{H}_2$  ratios GHSV=4030  $\text{h}^{-1}$ , and P=20 bar.



(a)

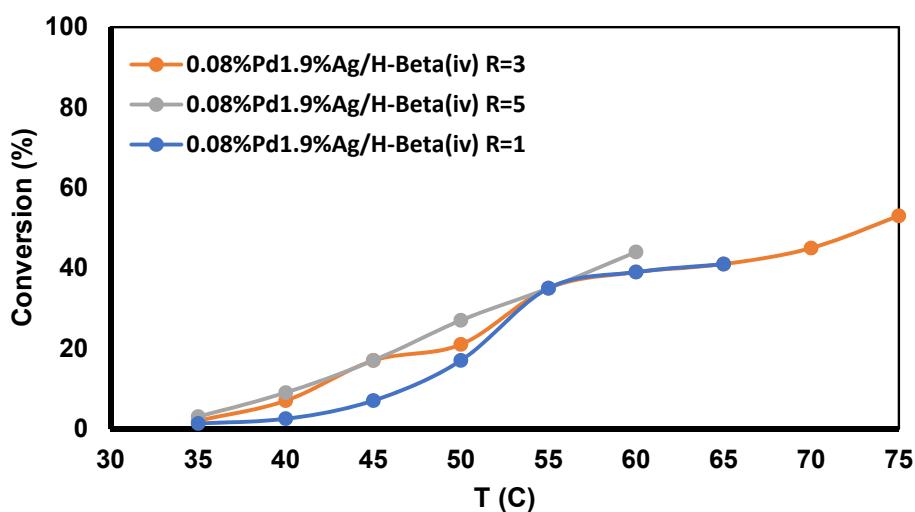


(b)



(c)

Figure S20. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd2.9%Ce/H-Beta(iv) catalysts under different  $\text{H}_2/\text{C}_2\text{H}_2$  ratios GHSV=4030  $\text{h}^{-1}$ , and P=20 bar.



(a)

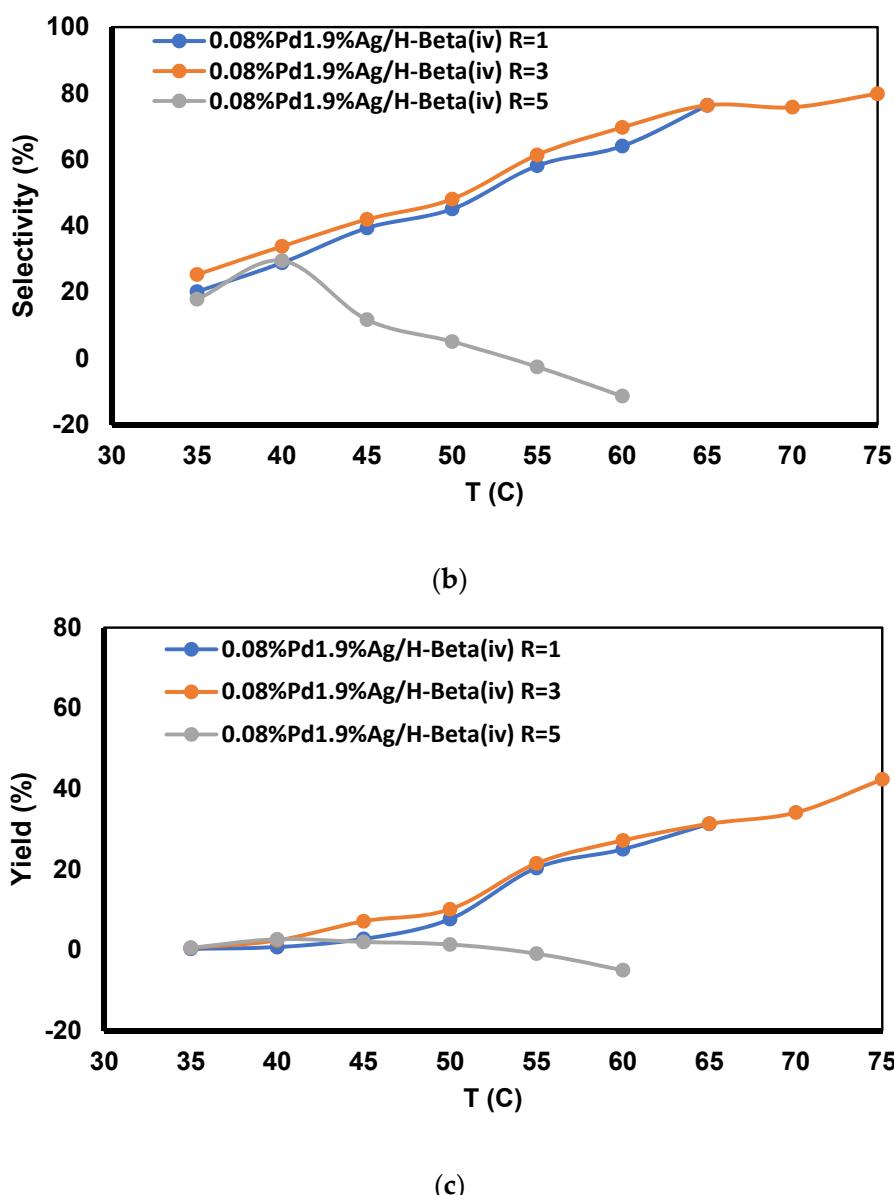


Figure S21. (a) Acetylene conversion, (b) Ethylene selectivity and (c) Yield percentage over 0.08%Pd1.9%Ag/H-Beta(iv) catalysts under different  $\text{H}_2/\text{C}_2\text{H}_2$  ratios GHSV=4030  $\text{h}^{-1}$ , and P=20 bar.

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