

Table S1. The calculated values of the final 12 descriptors for each complex.

Complexes	No.1	No.2[e]	No.3[e]	No.4[kcal/mol]	No.5	No.6
1	4.15	-0.0276	-21.99	3.18	0.0215	0.0014
2	4.14	-0.0316	-22.09	3.17	0.0219	0.0017
3	4.12	-0.0309	-22.08	3.17	0.0219	0.0009
4	4.13	-0.0289	-23.61	3.16	0.0212	0.0016
5	4.33	-0.0316	-23.25	3.17	0.0215	0.0019
8	4.08	-0.0309	-19.65	3.43	0.0221	0.0018
11	3.68	-0.0285	-20.56	3.20	0.0215	0.0006
12	3.81	-0.0280	-19.11	3.24	0.0215	0.0005
14	3.68	-0.0285	-20.03	3.41	0.0214	0.0020
15	3.81	-0.0280	-19.12	3.45	0.0214	0.0060
16	4.20	-0.0288	-21.12	3.28	0.0210	0.0037
17	4.13	-0.0270	-23.48	3.17	0.0198	0.0012
20	4.09	-0.0289	-25.25	3.05	0.0207	0.0014
21	4.30	-0.0316	-24.20	3.13	0.0196	0.0025
22	4.05	-0.0270	-20.70	3.35	0.0206	0.0028
23	4.07	-0.0316	-19.66	3.37	0.0206	0.0035
24	4.07	-0.0309	-18.58	3.40	0.0211	0.0026
25	4.13	-0.0289	-21.95	3.25	0.0202	0.0024
26	4.33	-0.0316	-21.09	3.29	0.0203	0.0091
27	3.71	-0.0285	-19.89	3.16	0.0215	0.0007
28	3.85	-0.0280	-23.15	3.12	0.0210	0.0004
29	4.25	-0.0288	-22.92	3.13	0.0210	0.0013
30	4.25	-0.0288	-21.51	3.24	0.0210	0.0018
31	4.09	-0.0289	-23.20	3.10	0.0209	0.0013
32	4.09	-0.0289	-21.81	3.22	0.0210	0.0027
33	4.45	-0.0331	-25.15	3.14	0.0159	0.0010
34	4.30	-0.0331	-26.59	3.11	0.0160	0.0021
35	4.25	-0.0331	-22.02	3.21	0.0158	0.0012
36	4.45	-0.0331	-25.74	3.04	0.0160	0.0020
37	4.49	-0.0331	-27.62	2.99	0.0160	0.0020
38	4.45	-0.0331	-26.92	2.95	0.0156	0.0012
39	4.30	-0.0331	-28.15	2.94	0.0156	0.0011
40	4.25	-0.0331	-23.74	2.96	0.0155	0.0007
41	4.45	-0.0331	-27.38	2.92	0.0156	0.0011
42	4.49	-0.0331	-29.33	2.89	0.0157	0.0010
43	4.09	-0.0280	-23.20	3.09	0.0180	0.0012
44	3.88	-0.0316	-22.80	3.12	0.0182	0.0008
45	4.07	-0.0289	-24.29	3.07	0.0178	0.0009
46	4.10	-0.0316	-25.88	3.04	0.0177	0.0008
Complexes	No.7[e]	No.8	No.9[e]	No.10	No.11	No.12
1	-2.61	-52.04	0.0023	0.9948	3.20	0.9251

2	-2.50	-51.85	0.0022	0.9959	3.20	0.9254
3	-2.69	-57.55	0.0017	0.9954	3.19	0.9258
4	-2.58	-56.40	0.0021	0.9948	3.20	0.9250
5	-2.49	-55.92	0.0020	0.9960	3.20	0.9255
8	-2.48	-53.47	0.0012	0.9954	3.20	0.9240
11	-2.36	-48.13	0.0021	0.9934	3.19	0.9234
12	-2.41	-46.77	0.0017	0.9937	3.19	0.9227
14	-2.29	-50.22	0.0020	0.9934	3.20	0.9231
15	-2.41	-51.67	0.0024	0.9937	3.19	0.9224
16	-2.33	-53.37	0.0020	0.9947	3.20	0.9233
17	-2.29	-53.33	0.0024	0.9948	3.20	0.9231
20	-2.28	-56.91	0.0023	0.9948	3.20	0.9225
21	-2.14	-55.14	0.0014	0.9958	3.20	0.9232
22	-2.89	-63.49	0.0023	0.9948	3.19	0.9239
23	-2.83	-60.78	0.0010	0.9960	3.19	0.9242
24	-2.91	-63.48	0.0017	0.9955	3.19	0.9243
25	-2.82	-65.56	0.0021	0.9949	3.19	0.9239
26	-2.74	-64.18	0.0010	0.9960	3.19	0.9242
27	-2.34	-46.47	0.0017	0.9927	3.20	0.9244
28	-2.50	-52.68	0.0010	0.9933	3.20	0.9247
29	-2.40	-54.17	0.0020	0.9951	3.20	0.9239
30	-2.34	-55.25	0.0021	0.9948	3.20	0.9236
31	-2.47	-55.97	0.0021	0.9949	3.20	0.9241
32	-2.39	-55.51	0.0025	0.9949	3.20	0.9238
33	-3.05	-72.25	0.0018	0.9957	3.21	0.9248
34	-3.07	-74.31	0.0000	0.9958	3.20	0.9249
35	-3.07	-69.15	0.0010	0.9957	3.20	0.9259
36	-2.94	-73.00	0.0017	0.9957	3.21	0.9249
37	-2.98	-76.94	0.0005	0.9958	3.20	0.9248
38	-3.12	-71.95	0.0015	0.9957	3.21	0.9259
39	-3.10	-72.73	0.0000	0.9958	3.21	0.9257
40	-3.11	-68.03	0.0007	0.9957	3.20	0.9264
41	-3.01	-74.17	0.0013	0.9957	3.21	0.9258
42	-3.00	-76.30	0.0005	0.9958	3.21	0.9257
43	-2.70	-57.04	0.0023	0.9947	3.21	0.9272
44	-2.58	-54.39	0.0018	0.9958	3.20	0.9264
45	-2.65	-59.42	0.0019	0.9948	3.21	0.9274
46	-2.71	-62.65	0.0006	0.9958	3.21	0.9261

Table S2. The modeling results of the different combinations of training and test sets including R^2 , Q^2 , R_t^2 , $RMSEF$ and $RMSEV$ values for 39 complexes.

Entry	Training	Test	R^2	$RMSEF$	Q^2	$RMSEV$	R_t^2
1	32	7	0.8846	0.3444	0.5391	0.6682	0.8175

2	31	8	0.8961	0.3260	0.7036	0.5356	0.7640
3	30	9	0.8916	0.3299	0.6518	0.5802	0.8137
4	29	10	0.8917	0.3354	0.6974	0.5405	0.8135
5	28	11	0.8984	0.3271	0.7533	0.4878	0.7941
6	27	12	0.8969	0.3266	0.7482	0.4924	0.8064

Table S3. The values of experimental and predicted catalytic activities for the training set of 29 complexes and test set of 10 complexes from 2D-QSAR analysis.

Complexes	Exp. Activity ($10^6 \text{ g}\cdot\text{mol}^{-1}\cdot\text{h}^{-1}$)	2D-Pred. ($10^6 \text{ g}\cdot\text{mol}^{-1}\cdot\text{h}^{-1}$)	Sets
1	3.44	3.88	Training
2	1.13	1.96	Training
3	0.60	0.96	Training
4	2.18	2.59	Test
5	1.00	1.47	Training
6	7.18	-	Outlier
7	6.22	-	Outlier
8	4.71	4.06	Training
9	6.85	-	Outlier
10	5.65	-	Outlier
11	3.08	2.61	Training
12	4.97	4.30	Training
13	6.27	-	Outlier
14	3.47	4.02	Training
15	4.76	4.64	Training
16	4.17	4.78	Training
17	3.7	4.08	Training
18	7.1	-	Outlier
19	8.7	-	Outlier
20	2.4	2.34	Training
21	2.5	2.55	Training
22	3.1	3.85	Training
23	3.4	3.11	Test
24	4.1	3.17	Training
25	2.5	2.42	Test
26	4.0	3.62	Training
27	4.85	4.01	Training
28	2.40	3.30	Training
29	4.03	3.47	Test
30	3.39	3.87	Training
31	4.10	2.96	Test
32	2.98	3.33	Test
33	0.3	0.55	Test
34	0.29	0.65	Training

35	0.23	1.07	Training
36	0.34	0.53	Training
37	0.31	-0.05	Training
38	0.48	-0.07	Training
39	0.35	0.63	Test
40	0.32	0.69	Training
41	0.51	-0.15	Test
42	0.37	-0.17	Training
43	3.08	3.13	Training
44	1.01	1.04	Training
45	3.51	2.40	Test
46	1.45	1.93	Training

Table S4. The values of experimental and predicted catalytic activity for the training and test sets from 3D-QSPR analysis.

Complexes	Exp. Activity ($10^6 \text{ g}\cdot\text{mol}^{-1}\cdot\text{h}^{-1}$)	3D-Pred. ($10^6 \text{ g}\cdot\text{mol}^{-1}\cdot\text{h}^{-1}$)	Sets
1	3.44	2.201	Training
2	1.13	1.010	Training
3	0.60	1.006	Training
4	2.18	2.142	Test
5	1.00	0.872	Training
6	7.18	-	Outlier
7	6.22	-	Outlier
8	4.71	3.548	Training
9	6.85	-	Outlier
10	5.65	-	Outlier
11	3.08	3.972	Training
12	4.97	3.870	Training
13	6.27	-	Outlier
14	3.47	3.943	Training
15	4.76	4.058	Training
16	4.17	4.422	Training
17	3.7	3.353	Training
18	7.1	-	Outlier
19	8.7	-	Outlier
20	2.4	3.221	Training
21	2.5	3.048	Training
22	3.1	3.582	Training
23	3.4	3.470	Test
24	4.1	3.179	Training
25	2.5	3.522	Test
26	4.0	3.411	Training
27	4.85	3.860	Training

28	2.40	2.880	Training
29	4.03	4.184	Test
30	3.39	4.057	Training
31	4.10	3.406	Test
32	2.98	3.393	Test
33	0.3	0.603	Test
34	0.29	0.194	Training
35	0.23	0.160	Training
36	0.34	0.550	Training
37	0.31	0.120	Training
38	0.48	0.615	Training
39	0.35	0.253	Test
40	0.32	0.128	Training
41	0.51	0.546	Test
42	0.37	0.157	Training
43	3.08	2.893	Training
44	1.01	2.414	Training
45	3.51	2.823	Test
46	1.45	2.443	Training

Table S5. The values of experimental and predicted molecular weight for the training and test sets from 3D-QSPR analysis.

Complexes	Exp. Molecular weight (g·mol ⁻¹)	3D-Pred. (g·mol ⁻¹)	Sets
1	2700	2735.6	Training
2	4900	4999.7	Training
3	3600	4366.4	Training
4	3800	2992.9	Training
5	5100	5262.7	Training
6	2453	-	Outlier
7	3481	-	Outlier
8	4180	2752.5	Test
9	2825	-	Outlier
10	3830	-	Outlier
11	2360	2681.6	Training
12	3640	3395.1	Training
13	1910	-	Outlier
14	2320	2528.6	Training
15	3210	2809.4	Test
16	1830	2869.2	Training
17	59	382.3	Training
18	60	-	Outlier
19	59	-	Outlier
20	62	721.1	Training

21	59	499.2	Test
22	60	179.6	Training
23	60	26.9	Training
24	60	480.3	Training
25	62	359.1	Training
26	59	247.2	Training
27	1840	1687.3	Training
28	3210	2949.1	Training
29	1720	1904.1	Test
30	2190	2055.5	Training
31	2240	1431.8	Test
32	1980	1456	Training
33	84	-155.4	Training
34	86	-181.3	Training
35	82	122.6	Test
36	82	102.5	Training
37	83	43.9	Training
38	86	-179.6	Training
39	86	-241.3	Test
40	84	72.4	Training
41	86	92.7	Training
42	86	92.3	Training
43	670	843.1	Test
44	750	728.7	Training
45	870	1053.5	Training
46	730	998.9	Training

Table S6. Experimental values of catalytic activities, molecular weights and melting temperature of products under the optimum reaction conditions.

Complex	Co-catalyst	P ^a	Ratio ^b	T ^c	Activity ^d	M _w ^e
1	Et ₂ AlCl	10	600	20	3.44	2700
2	Et ₂ AlCl	10	600	20	1.13	4900
3	Et ₂ AlCl	10	600	20	0.60	3600
4	Et ₂ AlCl	10	600	20	2.18	3800
5	Et ₂ AlCl	10	600	20	1.00	5100
6	EASC	10	800	20	7.18	2453
7	EASC	10	800	20	6.22	3481
8	EASC	10	800	20	4.71	4180
9	EASC	10	800	20	6.85	2825
10	EASC	10	800	20	5.65	3830
11	Et ₂ AlCl	10	400	30	3.08	2360
12	Et ₂ AlCl	10	400	30	4.97	3640
13	Et ₂ AlCl	10	400	30	6.27	1910

14	Et ₂ AlCl	10	400	30	3.47	2320
15	Et ₂ AlCl	10	400	30	4.76	3210
16	Et ₂ AlCl	10	400	30	4.17	1830
17	EASC	10	400	20	3.7	59
18	EASC	10	400	20	7.1	60
19	EASC	10	400	20	8.7	59
20	EASC	10	400	20	2.4	62
21	EASC	10	400	20	2.5	59
22	EASC	10	400	20	3.1	60
23	EASC	10	400	20	3.4	60
24	EASC	10	400	20	4.1	60
25	EASC	10	400	20	2.5	62
26	EASC	10	400	20	4.0	59
27	Et ₂ AlCl	10	300	30	4.85	1840
28	Et ₂ AlCl	10	300	30	2.40	3210
29	Et ₂ AlCl	10	300	30	4.03	1720
30	Et ₂ AlCl	10	300	30	3.39	2190
31	Et ₂ AlCl	10	300	30	4.10	2240
32	Et ₂ AlCl	10	300	30	2.98	1980
33	DEAC	10	250	30	0.30	84
34	DEAC	10	250	30	0.29	86
35	DEAC	10	250	30	0.23	82
36	DEAC	10	250	30	0.34	82
37	DEAC	10	250	30	0.31	83
38	DEAC	10	250	30	0.48	86
39	DEAC	10	250	30	0.35	86
40	DEAC	10	250	30	0.32	84
41	DEAC	10	250	30	0.51	86
42	DEAC	10	250	30	0.37	86
43	Et ₂ AlCl	10	500	30	3.08	670
44	Et ₂ AlCl	10	500	30	1.01	750
45	Et ₂ AlCl	10	500	30	3.51	870
46	Et ₂ AlCl	10	500	30	1.45	730

^a atm of ethylene; ^b co-catalyst/catalyst; ^c reaction temperature (°C); ^d 10⁶g·mol⁻¹·h⁻¹; ^e Determined by gel permeation chromatography, g·mol⁻¹.

Table S7. The calculated bond lengths and bond angles by DFT compared with experimental crystal structures for complex **8** along with the values of standard deviation (δ).

Complex 8		
Bonds	Bond lengths (Å)	
	Exp.	MM
Ni(1)-N(1)	2.044	2.021
Ni(1)-N(2)	2.012	2.011

Ni(1)-Cl(1)	2.202	2.240
Ni(1)-Cl(2)	2.234	2.234
Ni(2)-C(9)	1.293	1.291
N(2)-C(10)	1.451	1.445
N(1)-C(1)	1.367	1.357
N(1)-C(5)	1.362	1.346
δ		0.63
Bond Angles (deg.)		
Angles	Exp.	MM
N(2)-Ni(1)-N(1)	81.6	82.389
N(2)-Ni(1)-Cl(1)	106.7	104.352
N(1)-Ni(1)-Cl(1)	137.8	124.026
N(2)-Ni(1)-Cl(2)	110.2	111.536
N(1)-Ni(1)-Cl(2)	96.68	97.478
Cl(1)-Ni(1)-Cl(2)	117.2	128.010
δ		4.32

Table S8. The values of different self-defined descriptors for each Ni complex.

Complexes	Q [e]	θ [°]	β [°]	ΔE [kcal·mol ⁻¹]	$\Delta \varepsilon_1$ [kcal·mol ⁻¹]	$\Delta \varepsilon_2$ [kcal·mol ⁻¹]
1	0.347	252.199	80.700	15.81	89.23	117.7
2	0.341	245.356	80.708	14.87	89.23	117.3
3	0.340	227.970	80.543	14.06	85.53	117.4
4	0.352	252.153	80.779	15.75	89.98	116.4
5	0.342	245.152	80.743	15.62	89.92	116.7
6	0.399	254.171	81.251	15.37	87.73	123.7
7	0.379	249.817	81.225	15.31	88.16	124.3
8	0.396	236.082	81.350	14.50	88.04	124.7
9	0.404	253.775	81.330	15.50	87.54	120.9
10	0.406	251.373	81.333	15.12	88.73	119.7
11	0.314	226.177	79.440	20.64	96.26	113.1
12	0.317	224.470	80.652	15.88	89.98	118.2
13	0.343	229.684	80.062	12.74	89.92	116.5
14	0.393	229.123	81.243	13.81	87.73	124.5
15	0.377	232.829	80.932	13.18	88.04	125.0
16	0.397	228.396	81.183	14.43	88.10	121.1
17	0.493	245.621	81.854	39.41	82.14	124.6
18	0.482	245.458	81.895	38.15	82.58	124.9
19	0.430	231.371	82.003	41.16	82.71	125.4
20	0.505	247.806	78.889	32.19	82.01	121.9
21	0.488	245.719	81.934	38.03	83.27	122.5
22	0.372	206.864	82.349	40.29	89.04	121.7
23	0.385	207.196	82.519	39.41	89.29	121.9
24	0.366	191.872	82.389	47.30	89.48	122.5

25	0.376	207.048	82.364	39.66	89.73	118.8
26	0.391	201.000	82.551	39.22	90.05	119.3
27	0.355	233.511	81.999	36.65	87.91	118.5
28	0.327	244.494	81.014	5.271	88.60	117.0
29	0.359	235.620	81.965	36.90	88.35	117.3
30	0.414	234.458	82.109	14.93	86.60	121.7
31	0.363	256.267	81.905	37.27	88.29	116.8
32	0.406	257.418	82.058	15.44	86.47	121.4
33	0.414	232.276	82.064	40.47	83.02	122.9
34	0.411	231.405	82.071	40.54	85.47	121.7
35	0.412	217.947	82.205	40.16	83.46	123.9
36	0.419	232.053	82.103	40.66	83.71	119.9
37	0.415	231.281	82.118	40.73	83.83	118.7
38	0.365	232.532	82.041	37.34	84.52	117.1
39	0.361	233.168	82.087	37.40	84.71	116.7
40	0.361	217.888	82.136	37.02	84.90	117.1
41	0.366	232.429	82.070	37.59	84.09	115.8
42	0.364	233.065	82.094	37.59	85.34	114.9
43	0.361	259.254	83.710	16.50	87.03	117.7
44	0.343	244.290	83.881	15.12	87.73	117.8
45	0.366	258.982	83.762	16.44	87.79	116.5
46	0.363	259.339	83.771	14.37	87.91	115.6

Explanation of descriptors

Regarding the remaining descriptors, there are one topological descriptor (No.1) [1,2], and eight quantum-chemical descriptors (Nos.4, 5, 6, 7, 8, 10, 11 and 12) [2-5]. The topological descriptor (No.1) average Information content (order 2) is defined on the basis of the Shannon information theory and is calculated by the equation (S1):

$${}^k\overline{IC} = -\sum_i \frac{n_i}{n} \log_2 \frac{n_i}{n} \quad (S1)$$

where n_i is a number of atoms in the i^{th} class and n is a total number of atoms in the molecule.

As to the quantum-chemical descriptors, No.4 descriptor is the energy gap between the complex's LUMO and HOMO orbitals. No.5 and No. 6 descriptors are max electrophilic reactivity index for a C atom (E_A) and max 1-electronic reactivity index for C atom, respectively. The former is a charge distribution related descriptor calculated by equation (S2):

$$E_A = \sum_{j \in A} C_{jLUMO}^2 / (\epsilon_{LUMO} + 10) \quad (S2)$$

where C_{jLUMO} is the j^{th} AO coefficients on the lowest unoccupied molecular orbital. And ϵ_{LUMO} is the energy of the orbitals. Max 1-electronic reactivity index for C atom depends on the calculated charge distribution in the molecules, referring to the reactivity at the site of C atoms in the molecule. This descriptor is calculated by equation (S3):

$$R_A = \sum_{i \in A} \sum_{j \in A} C_{iHOMO} \cdot C_{jLUMO} / (\epsilon_{LUMO} - \epsilon_{HOMO}) \quad (S3)$$

where the C_{iHOMO} and C_{jLUMO} are the molecular frontier orbital coefficients, the ϵ_{LUMO} and ϵ_{HOMO} are the molecular orbital energy. These two descriptors express the relative reactivity of the atom which is also relevant with the energy of activation of the corresponding chemical reaction.

The quantum-chemical descriptors No.7 and No.8 are FNSA-2 Fractional PNSA(PNSA-2/TMSA) and WNSA-3 Weighted PNSA (PNSA3*TMSA/1000) [Quantum-Chemical PC], respectively. Both the descriptors are classified as the CPSA (Charged Partial Surface Areas) descriptors. The descriptor FNSA-2 Fractional PNSA (PNSA-2/TMSA) is calculated by the equations (S6):

$$FNSA-2 = PNSA-2/TMSA = \frac{Q^- \sum_a^- SA_a^-}{TMSA} \quad (S4)$$

where SA_a^- is the surface area contributions of the a^{th} negative atoms, Q^- the total sum of partial negative charges in the molecule, and the sum is restricted to negatively charged atoms a^- . And TMSA is the total molecular solvent-accessible surface area. The descriptor WNSA-3 Weighted PNSA (PNSA3*TMSA/1000) [Quantum-Chemical PC] is calculated by the equations (1) in the main text. Both descriptors roughly reflect the charge distribution of these negatively charged atoms.

The quantum-chemical descriptor max SIGMA-SIGMA bond order (No. 10) for a given pair of atomic species in the molecule relates to the strength of intra-molecular

bonding interactions and characterizes the stability of the molecules. The descriptors avg valency of a N atom (No. 11) and min valency of a H atom (No.12) are both quantum chemical descriptor describing the interaction of nitrogen atom's bonding and hydrogen-bonding, respectively.

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