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Linear and Non-Linear Regression Methods to Study the Adsorption of Cr(VI) from Aqueous Solution using Pomegranate Peel

Supplementary Data

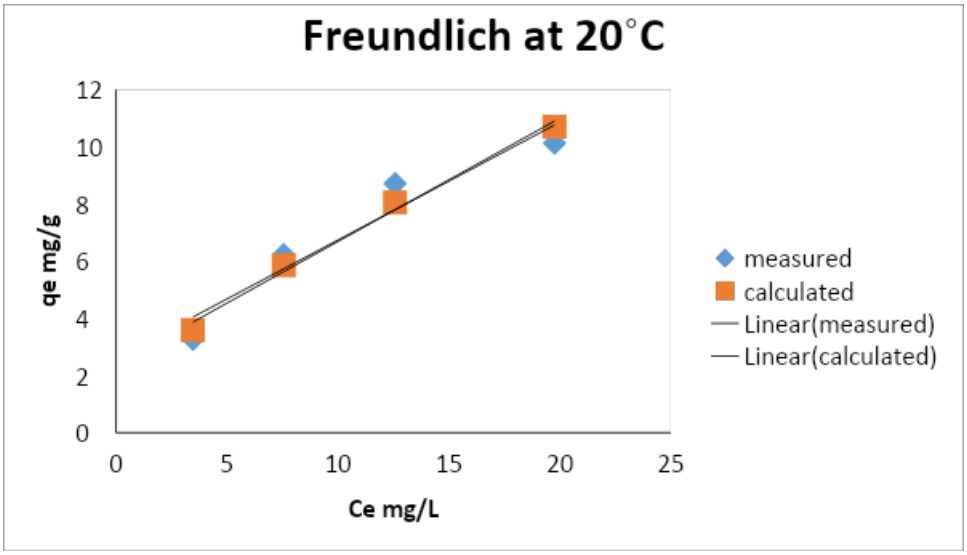

Figure S1. The result of applied nonlinear Freundlich isotherm for adsorption of Cr(VI) onto MPGP at 20 ºC using the data that given a minimum SNE for Error function (HYBRD).

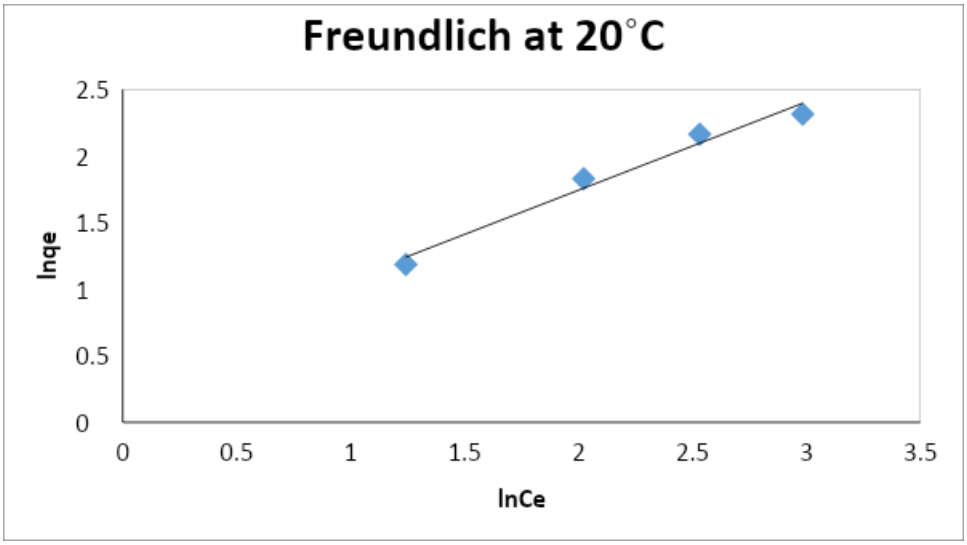

Figure S2. The result of applied linear Freundlich isotherm for adsorption of Cr(VI) onto MPGP at 20 ºC.

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Table S1. The values of Error Functions, SNE, and Langmuir isotherm parameters for linear and non-linear regression for adsorption of Cr(VI) onto MPGP at 20ºC.

Method/error function (parameter set)						
	Linear	Non-linear				
		ERRSQ	HYBRD	MPSD	ARE	EABS
MPGP						
K_L (L/mg^{-1})	0.053855	0.072658	0.066331	0.061383	0.060224	0.073771
q_{max} (mg/g)	20.92	17.51407	18.33524	19.13849	18.93322	17.05961
Coefficient of determination (R^2)	0.98036	0.991613	0.990725	0.988673	0.984675	0.98881
Sum of errors^2(ERRSQ)	0.544672	0.229829	0.254383	0.311321	0.424693	0.307964
Hybrid error function (HYBRD)	0.056818	0.038023	0.033133	0.036120	0.052387	0.043917
Marquardt's PSD (MPSD)	0.006057	0.008065	0.005206	0.004559	0.006627	0.007576
Average relative error (ARE)	0.130087	0.140211	0.134952	0.131791	0.128351	0.138584
Sum of absolute errors (EABS)	1.123206	0.822433	0.912728	0.991120	1.022222	0.821562
Sum of normalized errors (SNE)		4.071529	3.732232	3.897314	4.737041	4.294881

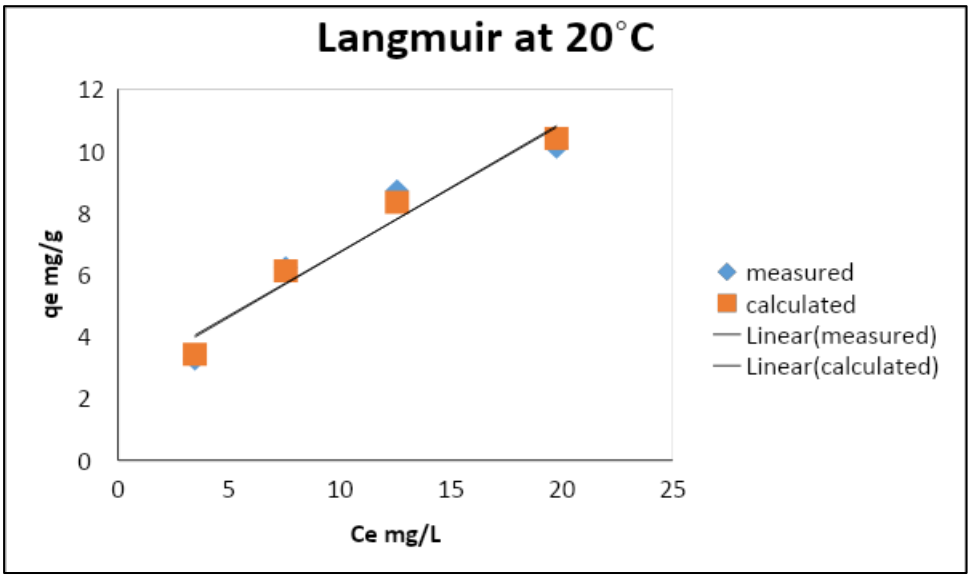

Figure S3. The result of applied nonlinear Langmuir isotherm for adsorption of Cr(VI) onto MPGP at 20ºC using the data that gave minimum SNE for Error function (HYBRD)

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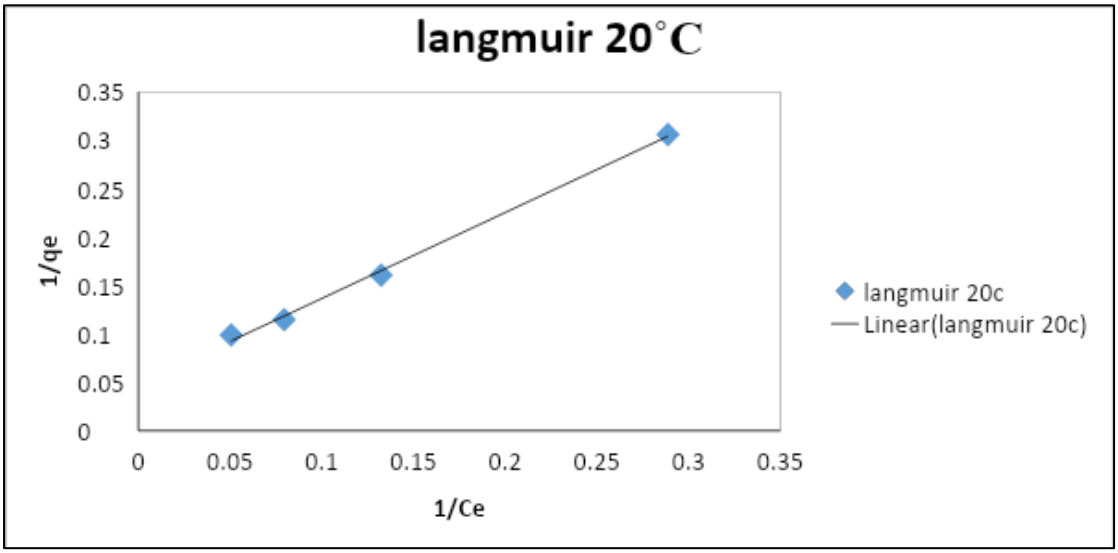

Figure S4. shows the result of applied linear Langmuir isotherm for adsorption of Cr(VI) onto MPGP at 20 ºC

Table S2. The values of Error Functions, SNE, and Dubinin- Radushkevich isotherm parameters for linear and non-linear regression for adsorption of Cr(VI) onto MPGP at 20 ºC.

Method/error function (parameter set)						
	Linear	Non-linear				
		ERRSQ	HYBRD	MPSD	ARE	EABS
MPGP						
K_{DR} $(mol/J)^2$	2.87E-06	3.42E-06	2.74E-06	2.74E-06	2.74E-06	2.92E-06
q_{max} (mg/g)	9.46704	9.86190	9.34702	9.34702	9.34702	9.9867
E (J/mol)	4.18E+02	3.82E+02	4.27E+02	4.27E+02	4.27E+02	4.14E+02
Coefficient of determination (R^2)	0.92447	0.93568	0.91784	0.91784	0.91784	0.91977
Sum of errors^2(ERRSQ)	2.220981	1.869366	2.434242	2.434242	2.434242	2.400362
Hybrid error function (HYBRD)	0.291397	0.319393	0.309305	0.309305	0.309305	0.363018
Marquardt's PSD (MPSD)	0.040655	0.064044	0.041586	0.041586	0.041586	0.056028
Average relative error (ARE)	0.319914	0.419249	0.308718	0.308718	0.308718	0.317068
Sum of absolute errors (EABS)	2.336875	2.360621	2.410178	2.410178	2.410178	2.270963
Sum of normalized errors (SNE)		4.627211	4.237733	4.237733	4.237733	4.559429

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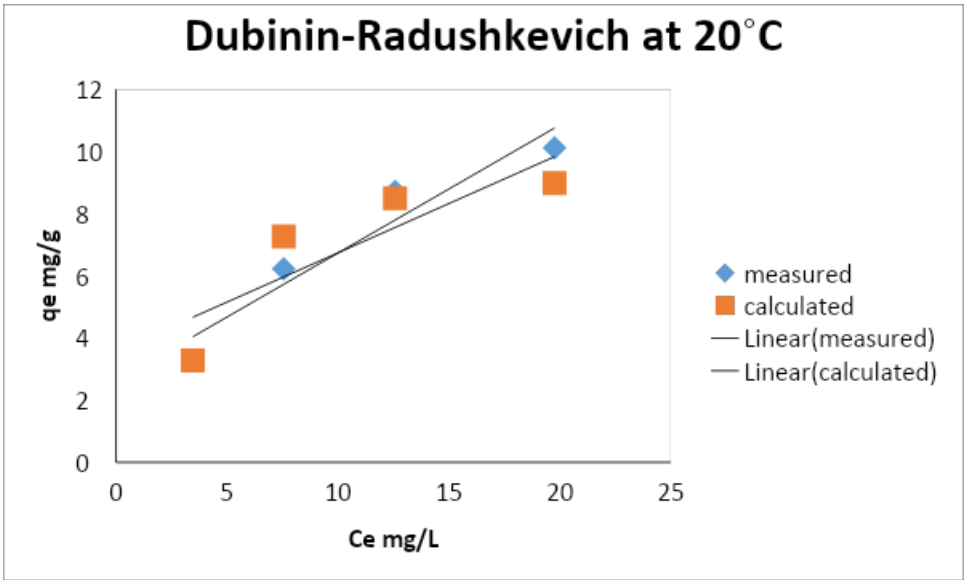

Figure S5. The result of applied nonlinear Dubinin-Radushkvich isotherm for adsorption of Cr(VI) onto MPGP at 20ºC using the data that gave minimum SNE for Error functions (HYBRD,ARE,MPSD).

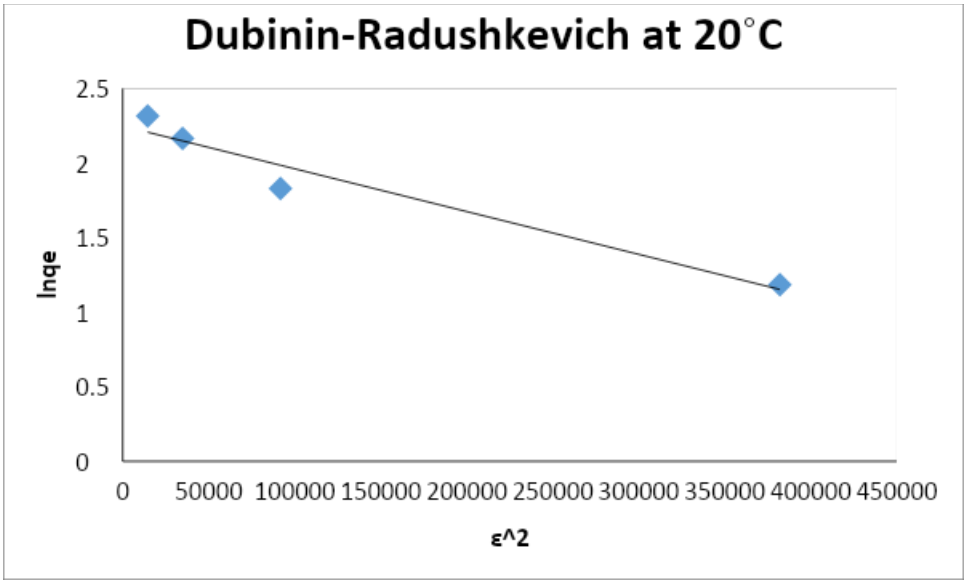

Figure S6. The result of applied linear Dubinin-Radushkevich isotherm for adsorption of Cr(VI) onto MPGP at 20ºC.

Table S3. The values of Error Functions, SNE, and Temkin isotherm parameters for linear and non-linear regression for adsorption of Cr(VI) onto MPGP at 20 Cº.

Method/error function (parameter set)						
	Linear	Non-linear				
		ERRSQ	HYBRD	MPSD	ARE	EABS
MPGP						
b_t (J/mol)	605.7882	605.7862	606.2965	608.3744	619.1753	619.176
A_t (L/mg)	0.647645	0.647641	0.647991	0.650791	0.662474	0.662462
B_t	4.021211	4.021224	4.01784	4.004117	3.934269	3.934264

Coefficient of determination (R^2)	0.9955	0.9955	0.9955	0.9954	0.9944	0.9944
Sum of errors^2(ERRSQ)	0.123354	0.123354	0.123431	0.124301	0.152392	0.152432
Hybrid error function (HYBRD)	0.015203	0.015203	0.015194	0.015255	0.018114	0.018117
Marquardt's PSD (MPSD)	0.001940	0.001940	0.001935	0.001926	0.002179	0.002179
Average relative error (ARE)	0.077524	0.077528	0.077113	0.074066	0.061491	0.061502
Sum of absolute errors (EABS)	0.596271	0.596287	0.592117	0.575206	0.489134	0.489129
Sum of normalized errors (SNE)		4.538635	4.524075	4.461382	4.612826	4.613575

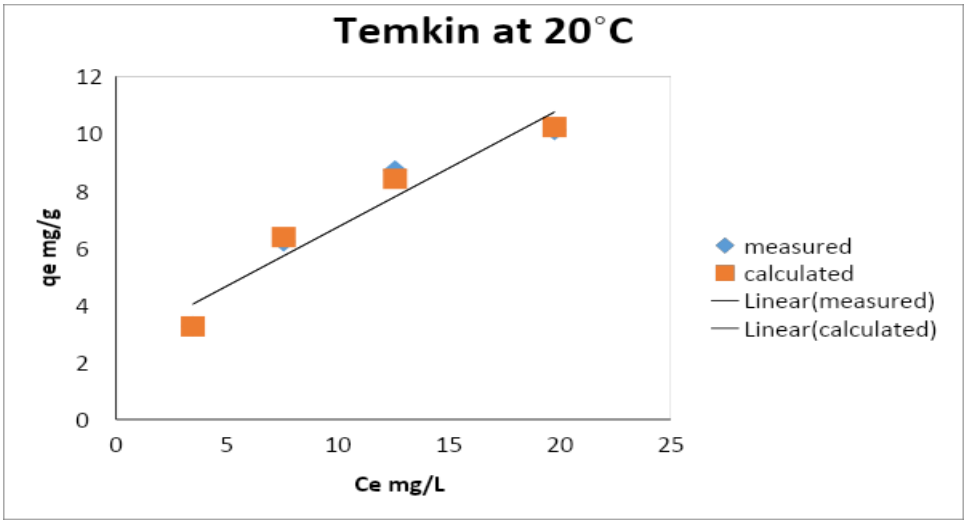

Figure S7. The result of applied nonlinear Temkin isotherm for adsorption of Cr(VI) onto MPGP at 20 ºC using the data that given a minimum SNE for Error function (MPSD).

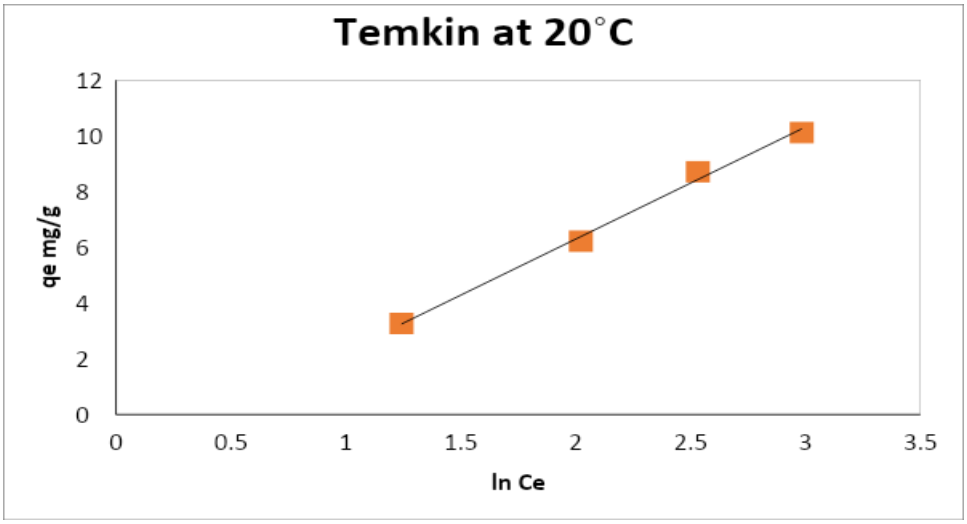

Figure S8. The result of applied linear Temkin isotherm for adsorption of Cr(VI) onto MPGP at 20 ºC

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Table S4. The values of Error Functions, SNE, and Redlich-Peterson isotherm parameters for linear and non-linear regression for adsorption of Cr(VI) onto MPGP at 20ºC.

Method/error function (parameter set)						
	Linear	Non-linear				
		ERRSQ	HYBRD	MPSD	ARE	EABS
MPGP						
a (L/mg)^b	23.417	0.004377	0.005845	0.006761	0.006762	0.004377
K (L/mg)	36.9569	0.964057	0.980673	0.98901	0.988994	0.964044
b	0.35522	1.778428	1.692588	1.64907	1.650755	1.778515
Coefficient of determination (R^2)	0.9584	0.9997	0.9997	0.9996	0.9996	0.9997
Sum of errors^2(ERRSQ)	1.183497	0.007536	0.008121	0.010092	0.010925	0.007542
Hybrid error function (HYBRD)	0.148550	0.001653	0.001247	0.001350	0.001438	0.001654
Marquardt's PSD (MPSD)	0.020032	0.000405	0.000213	0.000191	0.000199	0.000406
Average relative error (ARE)	0.273070	0.029983	0.026256	0.024810	0.023175	0.029900
Sum of absolute errors (EABS)	1.985851	0.142387	0.161807	0.173958	0.156927	0.141469
Sum of normalized errors (SNE)		4.507427	3.828864	4.038508	4.036565	4.500799

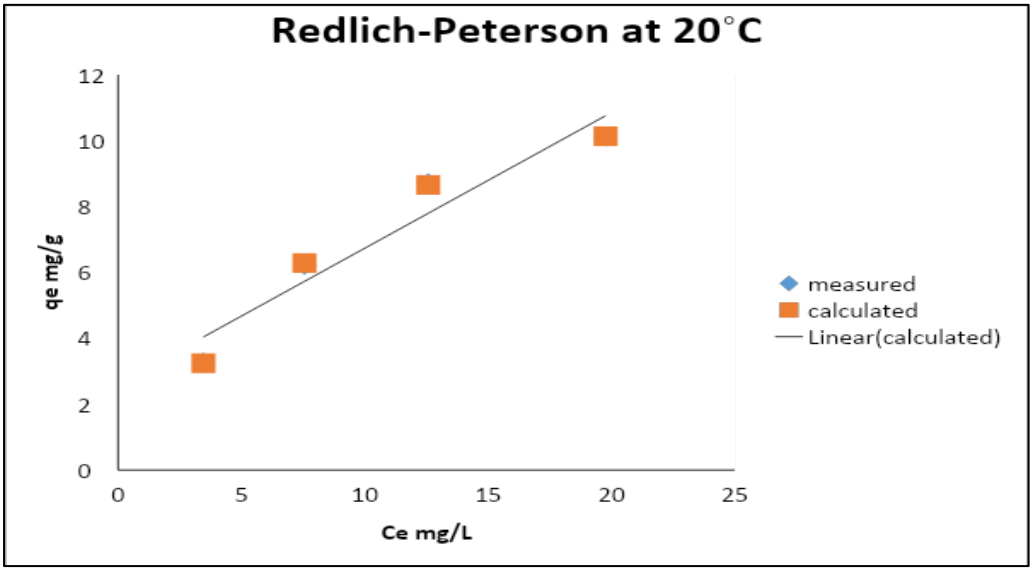

Figure S9. The result of applied nonlinear Redlich-Peterson isotherm for adsorption of Cr(VI) onto MPGP at 20ºC using the data that given a minimum SNE for Error function (HYBRD).

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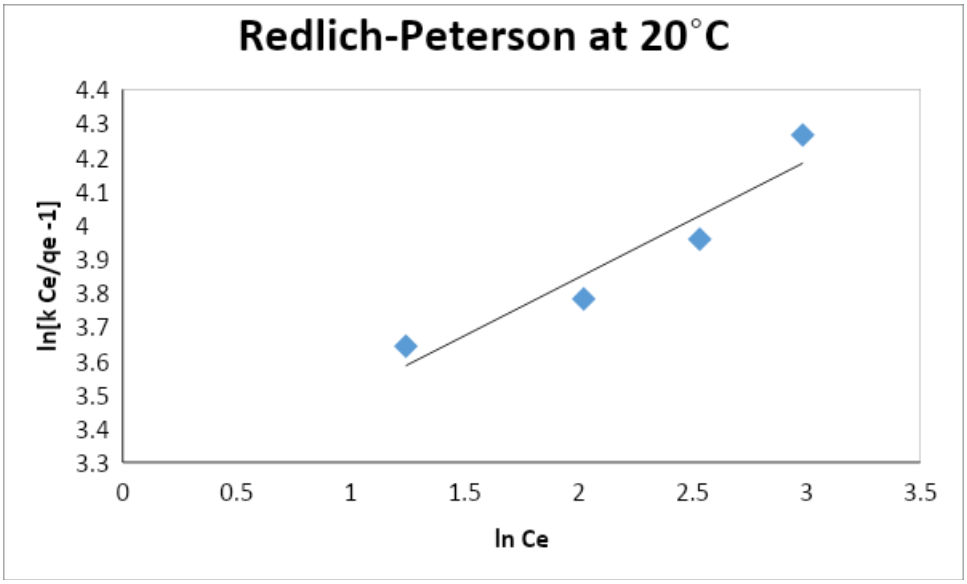

Figure S10: shows the result of applied linear Redlich-Peterson isotherm for adsorption of Cr(VI) onto MPGP at 20ºC.

Table S5. The values of Error Functions, SNE, and Sips isotherm parameters for linear and non-linear regression for adsorption of Cr(VI) onto MPGP at 20ºC.

Method/error function (parameter set)						
	Linear	Non-linear				
		ERRSQ	HYBRD	MPSD	ARE	EABS
MPGP						
n	1.45E+00	0.732723	0.755637	0.773166	0.820599	0.820599
q_m (mg/g))	2.29E+09	13.07917	13.37604	13.64412	14.33362	14.33362
b(L/mg)	4.83E-14	0.126989	0.122128	0.11781	0.10611	0.10611
Coefficient of determination (R^2)	0.9002	0.9982	0.9981	0.9980	0.9965	0.9965
Sum of errors^2(ERRSQ)	3.110649	0.048143	0.050480	0.055558	0.096012	0.096012
Hybrid error function (HYBRD)	0.326890	0.006834	0.006381	0.006607	0.010927	0.010927
Marquardt's PSD (MPSD)	0.038153	0.001074	0.000847	0.000808	0.001245	0.001245
Average relative error (ARE)	0.284999	0.061315	0.053191	0.049468	0.044080	0.044080
Sum of absolute errors (EABS)	2.179122	0.401259	0.391019	0.392842	0.390165	0.390165
Sum of normalized errors (SNE)		3.989222	3.632073	3.617585	4.691265	4.691265

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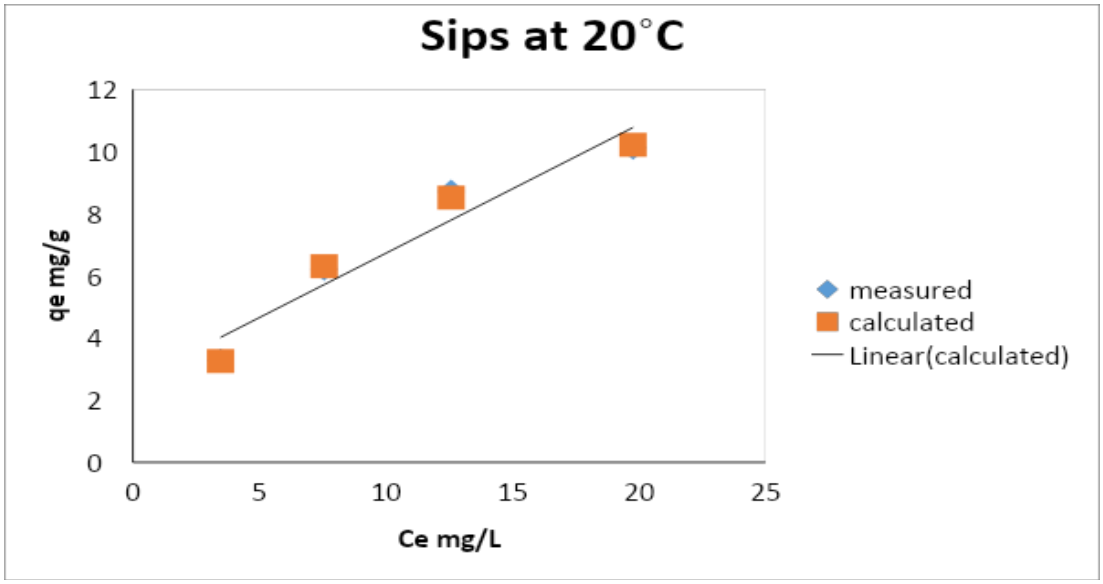

Figure S11. shows the result of applied nonlinear Sips isotherm for adsorption of Cr(VI) onto MPGP at 20ºC using the data that given a minimum SNE for Error function (MPSD).

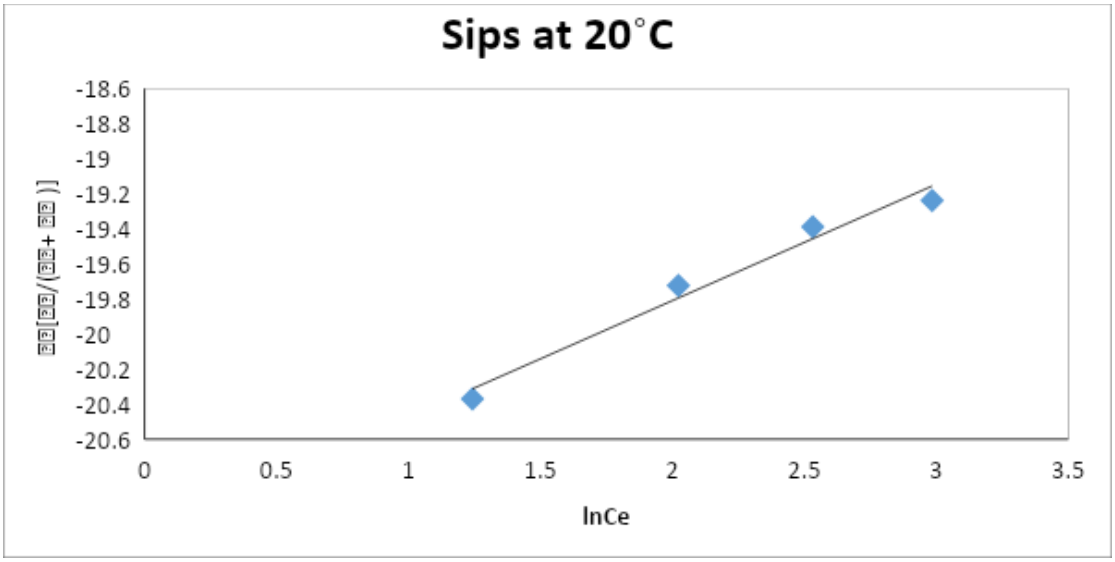

Figure S12. The result of applied linear Sips isotherm for adsorption of Cr(VI) onto MPGP at 20 ºC.

Table S6. The values of Error Functions, SNE, and Toth isotherm parameters for linear and non-linear regression for adsorption of Cr(VI) onto MPGP at 20 ºC.

Method/error function (parameter set)						
	Linear	Non-linear				
		ERRSQ	HYBRD	MPSD	ARE	EABS
MPGP						
n	2.52	2.32656	2.16655	2.05368	2.04117	2.04117
q_m (mg/g))	11.38635	11.41824	11.64747	11.85903	11.7766	11.77655
K_t(L/mg)	0.058	0.08282	0.08261	0.08206	0.08314	0.08314
Coefficient of determination (R^2)	0.9968	0.9994	0.9993	0.9991	0.9990	0.9990
Sum of errors^2(ERRSQ)	0.088577	0.017302	0.019270	0.023297	0.027258	0.027258

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Hybrid error function (HYBRD)	0.018259	0.003185	0.002750	0.002947	0.003439	0.003439
Marquardt's PSD (MPSD)	0.004520	0.000681	0.000433	0.000391	0.000445	0.000445
Average relative error (ARE)	0.102599	0.044488	0.038677	0.035840	0.029710	0.029710
Sum of absolute errors (EABS)	0.527327	0.244463	0.252665	0.264435	0.225594	0.225594
Sum of normalized errors (SNE)		4.48534	3.966717	4.0909	4.173979	4.173979

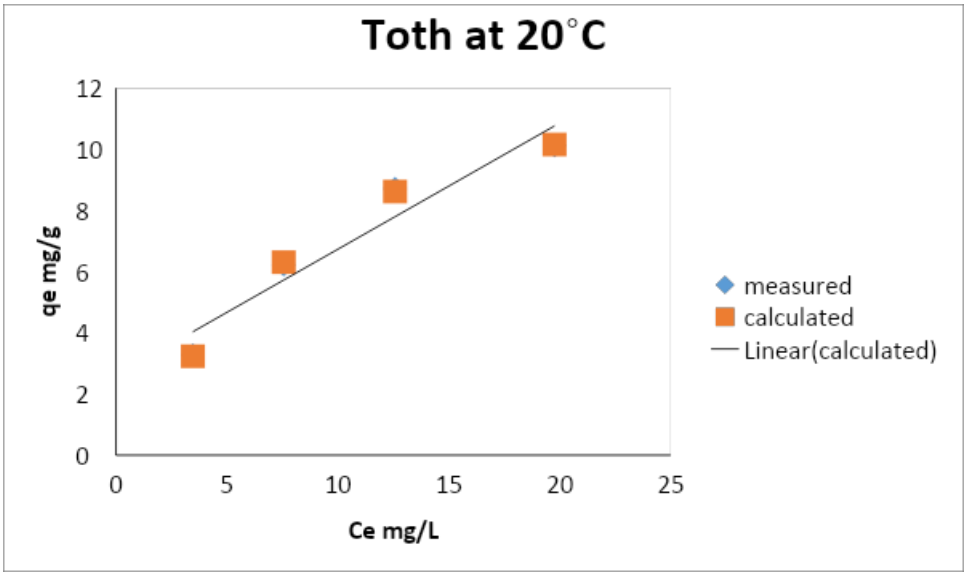

Figure S13. The result of applied nonlinear Toth isotherm for adsorption of Cr(VI) onto MPGP at 20 º C using the data that given a minimum SNE for Error function (HYBRD).

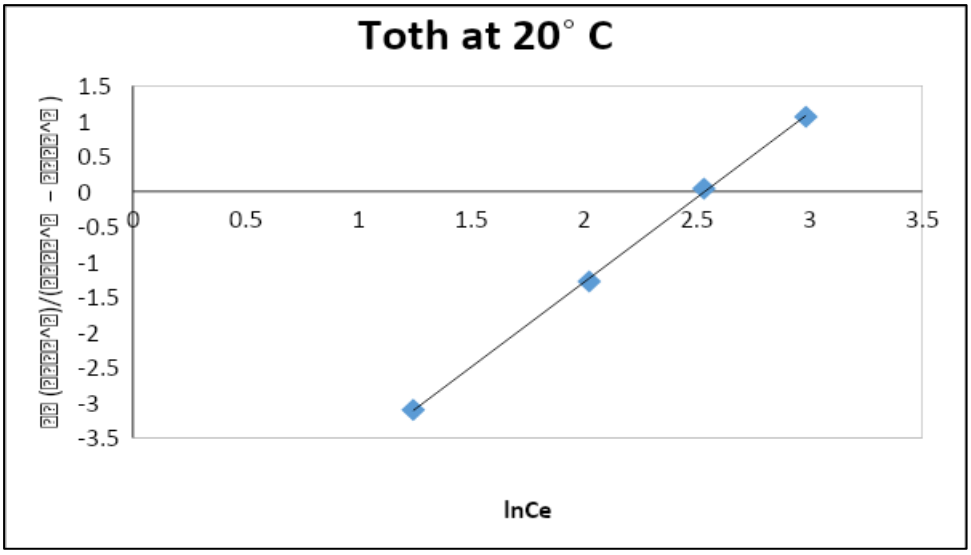

Figure S14. The result of applied linear Toth isotherm for adsorption of Cr(VI) onto MPGP at 20 º C.