Electronic Supplementary File for:

Removal of malachite green using hydrochar from palm leaves

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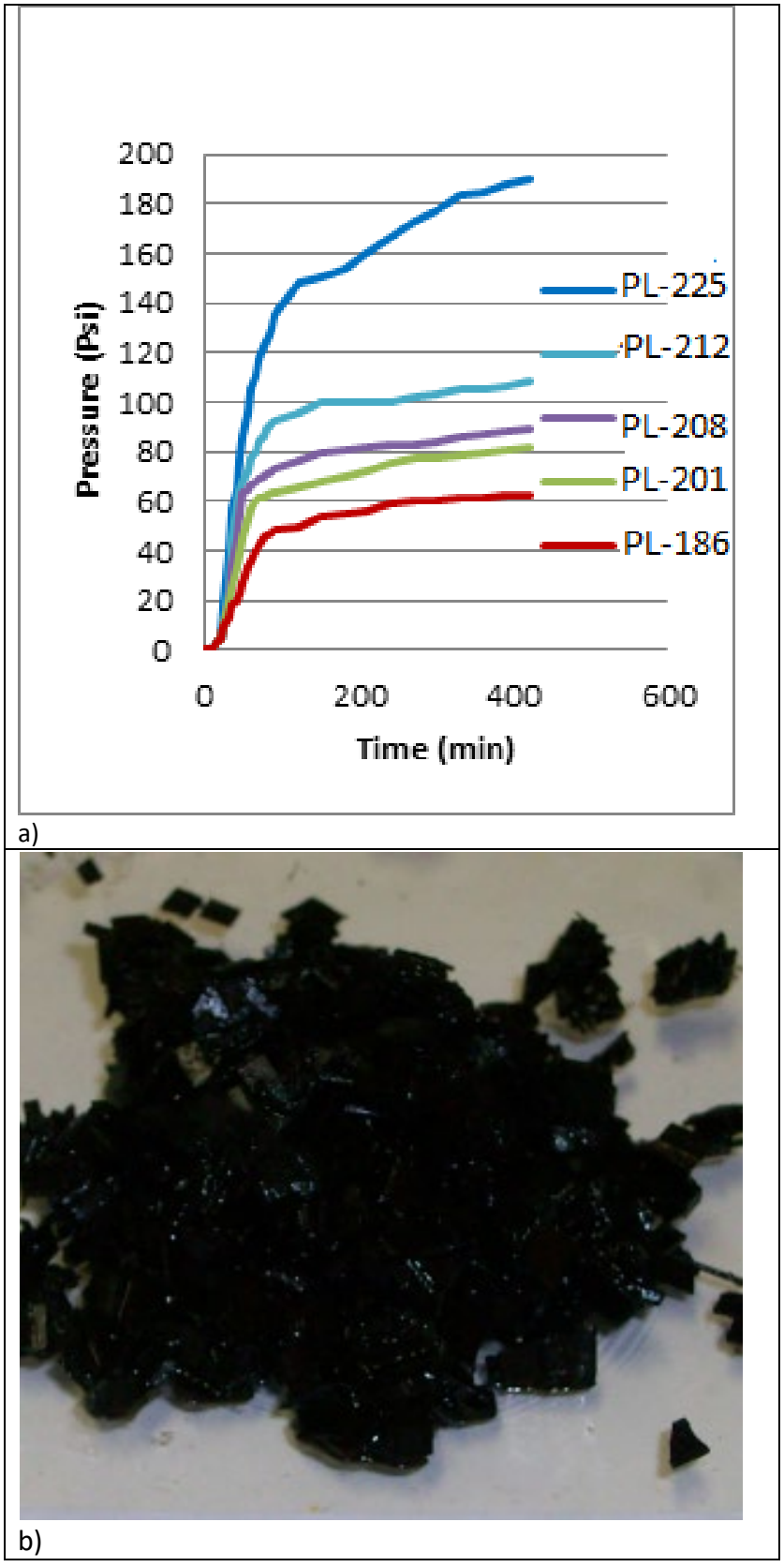


Fig. S1 a) Evolution of reaction pressures psi inside the HTC reactor for hydrothermal carbonization of Palm leaves with temperature Tmax 186°C-225°C. b) Image of wet biocoal HTC PL-208 of Palm leaves.

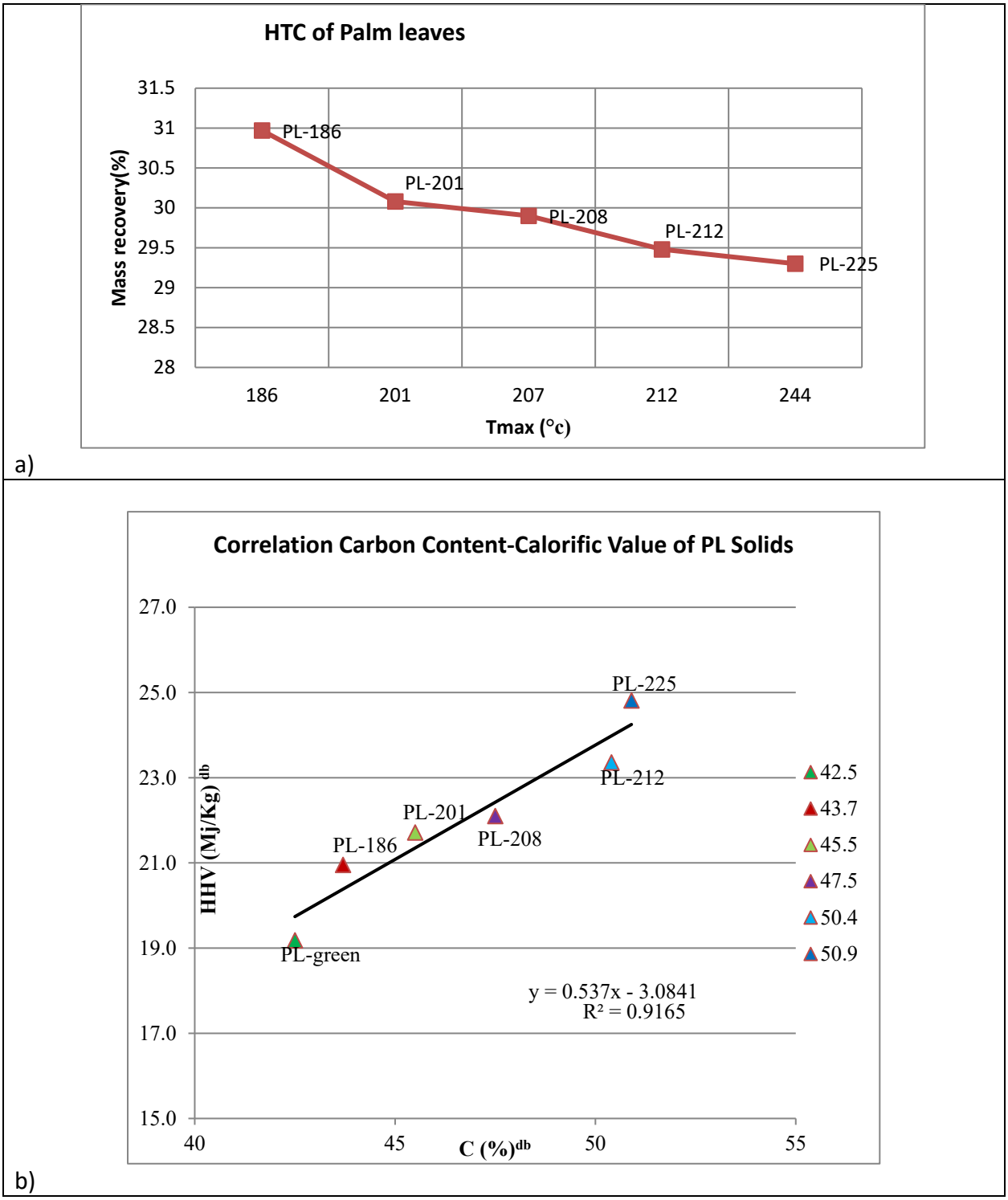


Fig. S2 a) Alteration of mass recovery as coal with the preparation temperature of HTC palm leave biochars. **b)** Relationship between High heating Values HHV and carbon content of the solids.

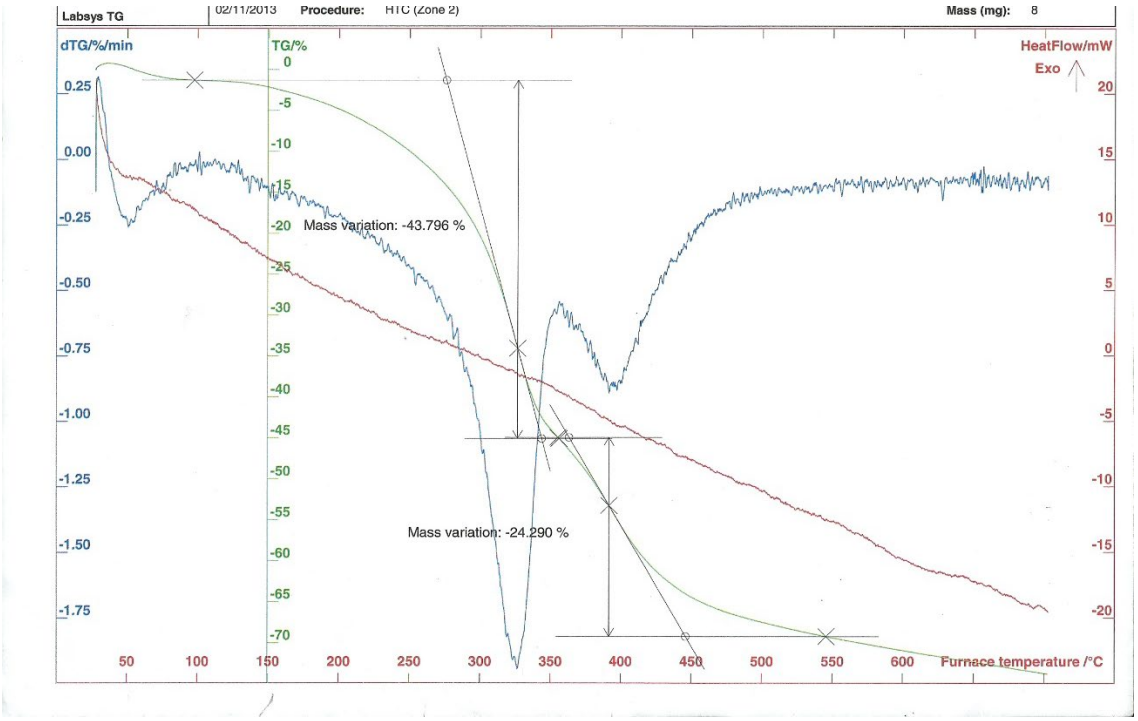
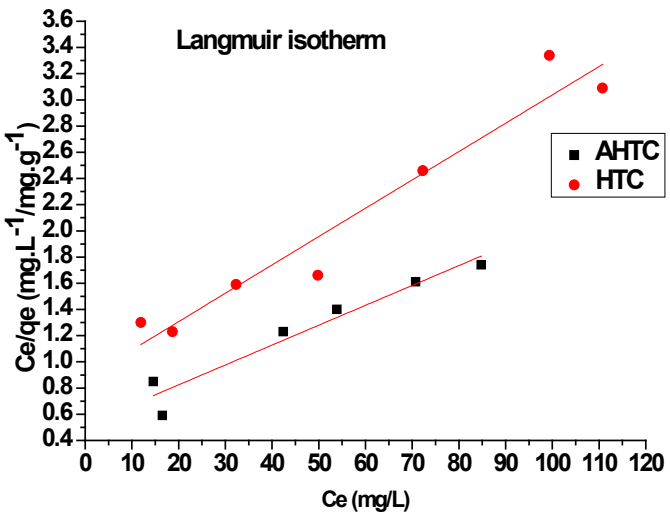
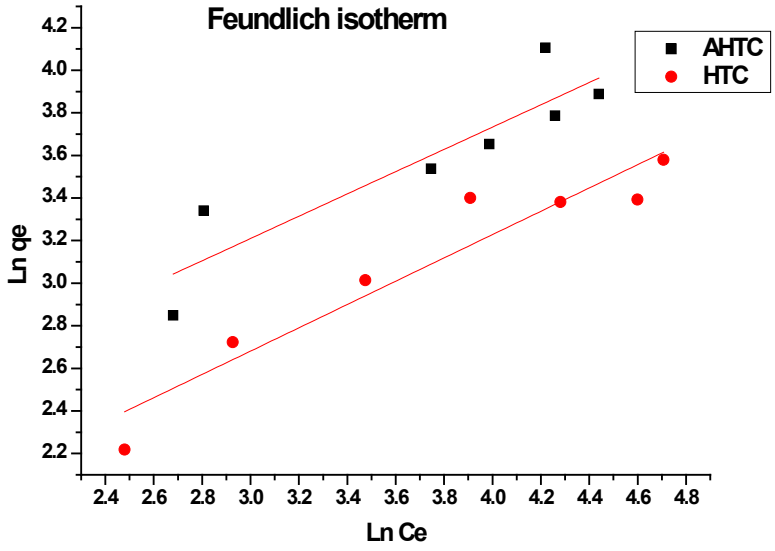


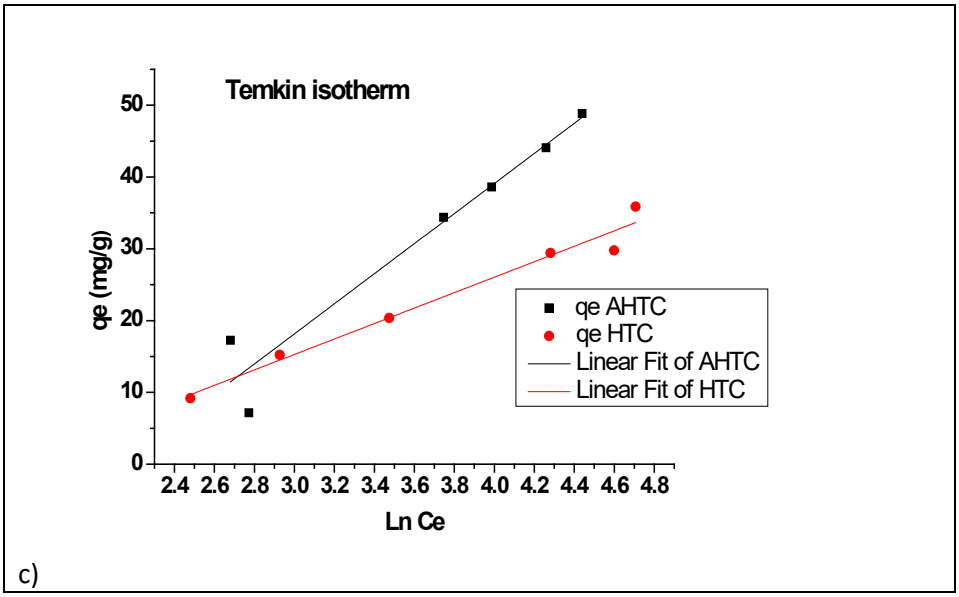
Fig. S3. TG-DTA thermogravimetric analysis curves of AHTC-PL-208.


Langmuir isotherm
Ce/qe (mg.L-1/mg.g-1)
Ce (mg/L)
AHTC
HTC

a)

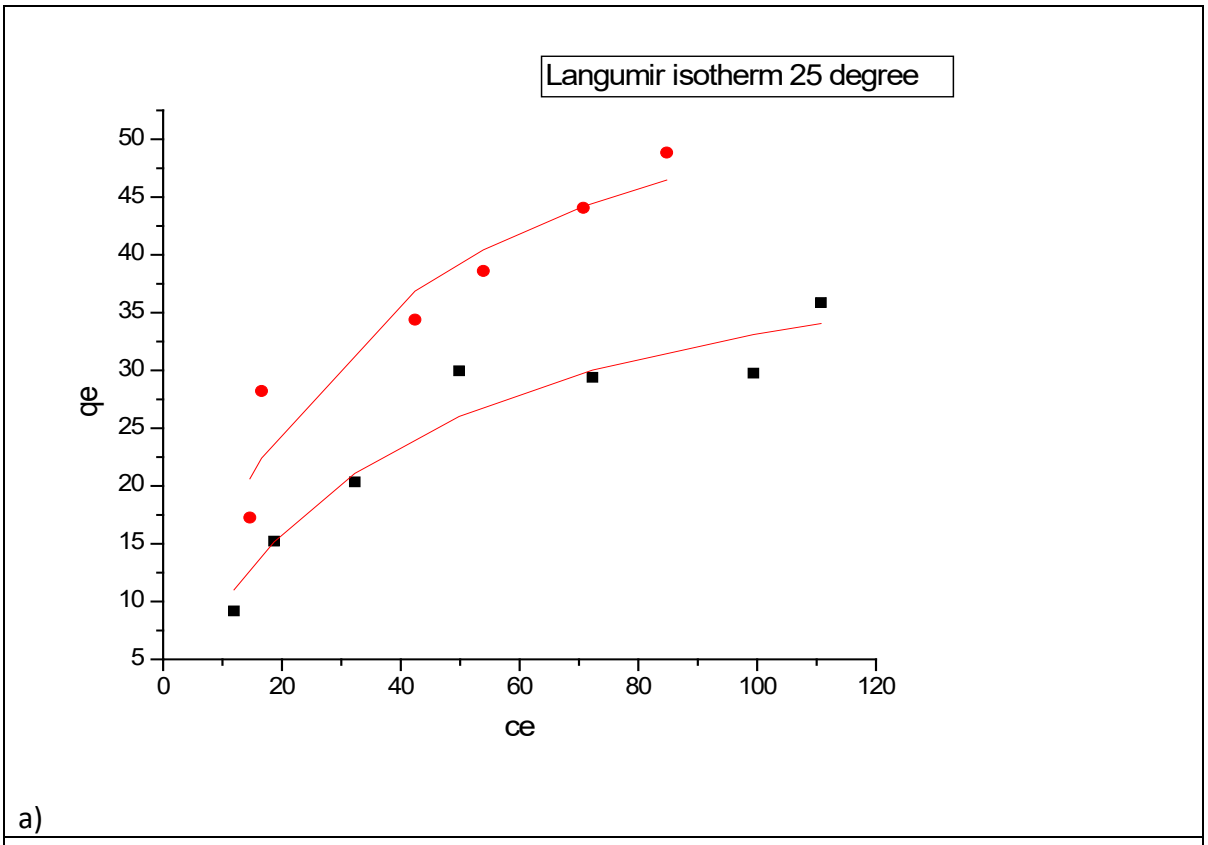

Feundlich isotherm
Ln qe
Ln Ce
AHTC
HTC

b)

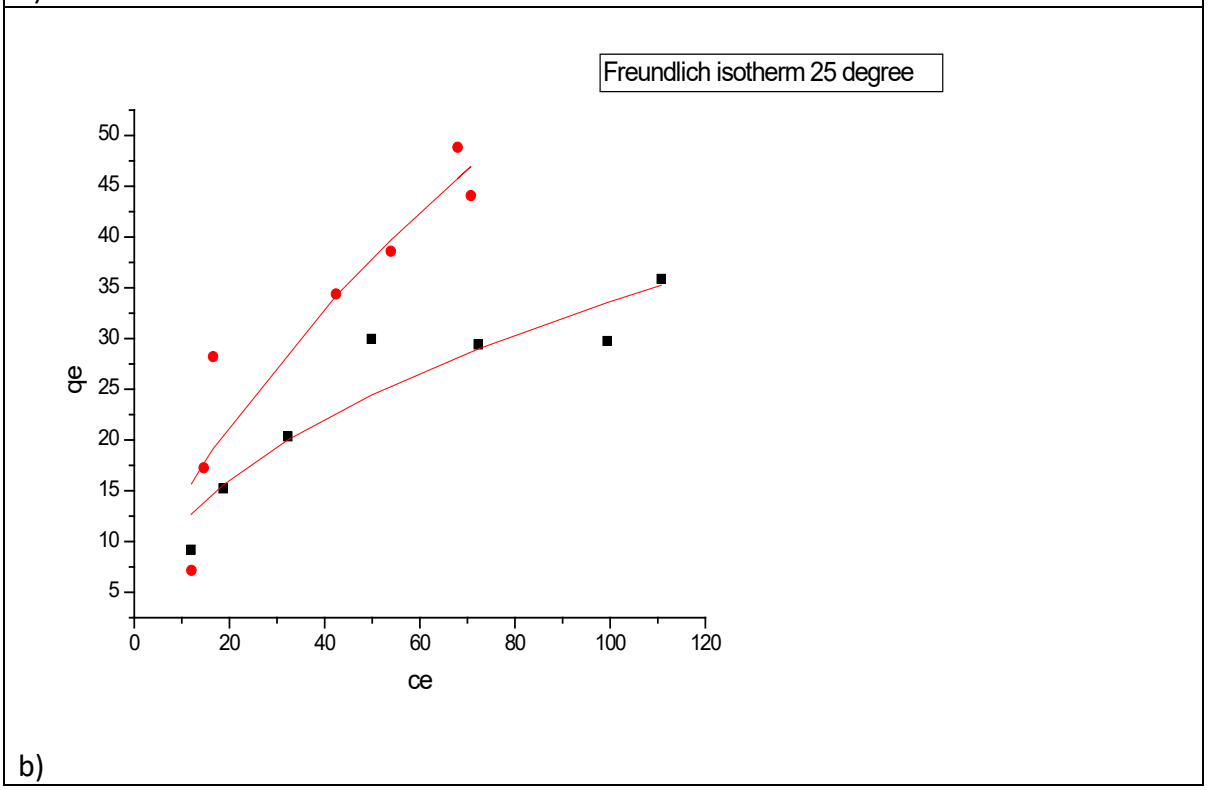


c)

Fig. S4 a) Linear Langmuir, **b)** Linear Freundlich **c)** Linear Temkin plot; for MG adsorption on HTC-PL-208 and AHTC-PL-208. A 0.1 g of biochar was used in 50 ml of MG solution with concentration ranged from 20-200 mg/l, at 25 °C for 24 h (HTC) and 4 h (AHTC).


Langumir isotherm 25 degree
qe
ce
0
20
40
60
80
100
120
5
10
15
20
25
30
35
40
45
50

a)


Freundlich isotherm 25 degree
qe
ce
0
20
40
60
80
100
120
5
10
15
20
25
30
35
40
45
50

b)

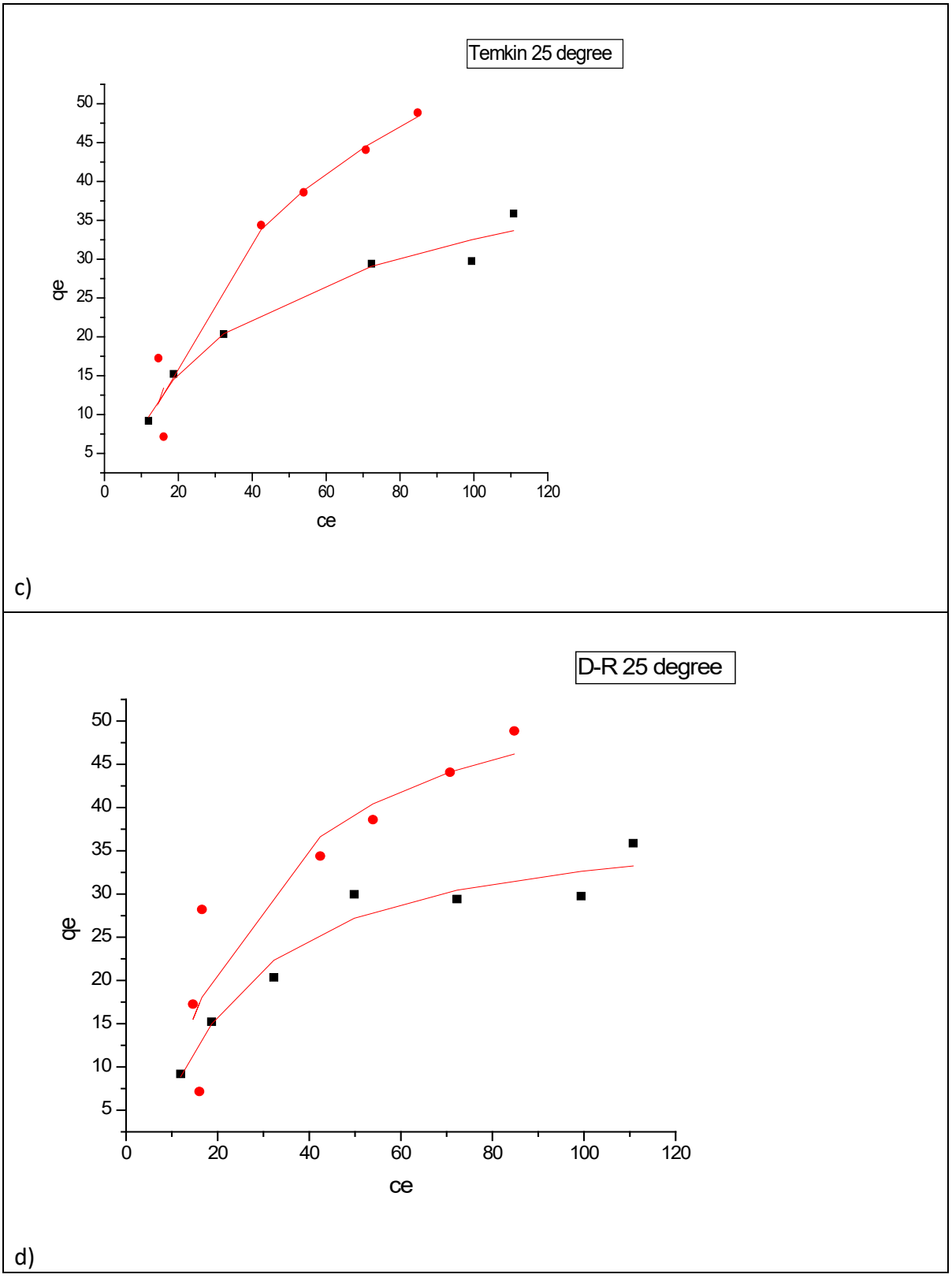


Fig. S5. Non linear MG adsorption isotherm plot qe (mg/l) vs Ce (mg/l) for HTC (black) and AHTC (red) **a)** Langmuir isotherm; **b)** Freundlich isotherm; **c)** Temkin isotherm and **d)** Dubinin-Radushkevich isotherm. Conditions: at 25°C. (0.1 g of biochar was used in 50 ml of MG solution with concentration ranged from 20-200 mg/l, at 25 °C for 24 h (HTC) and 4 h (AHTC).

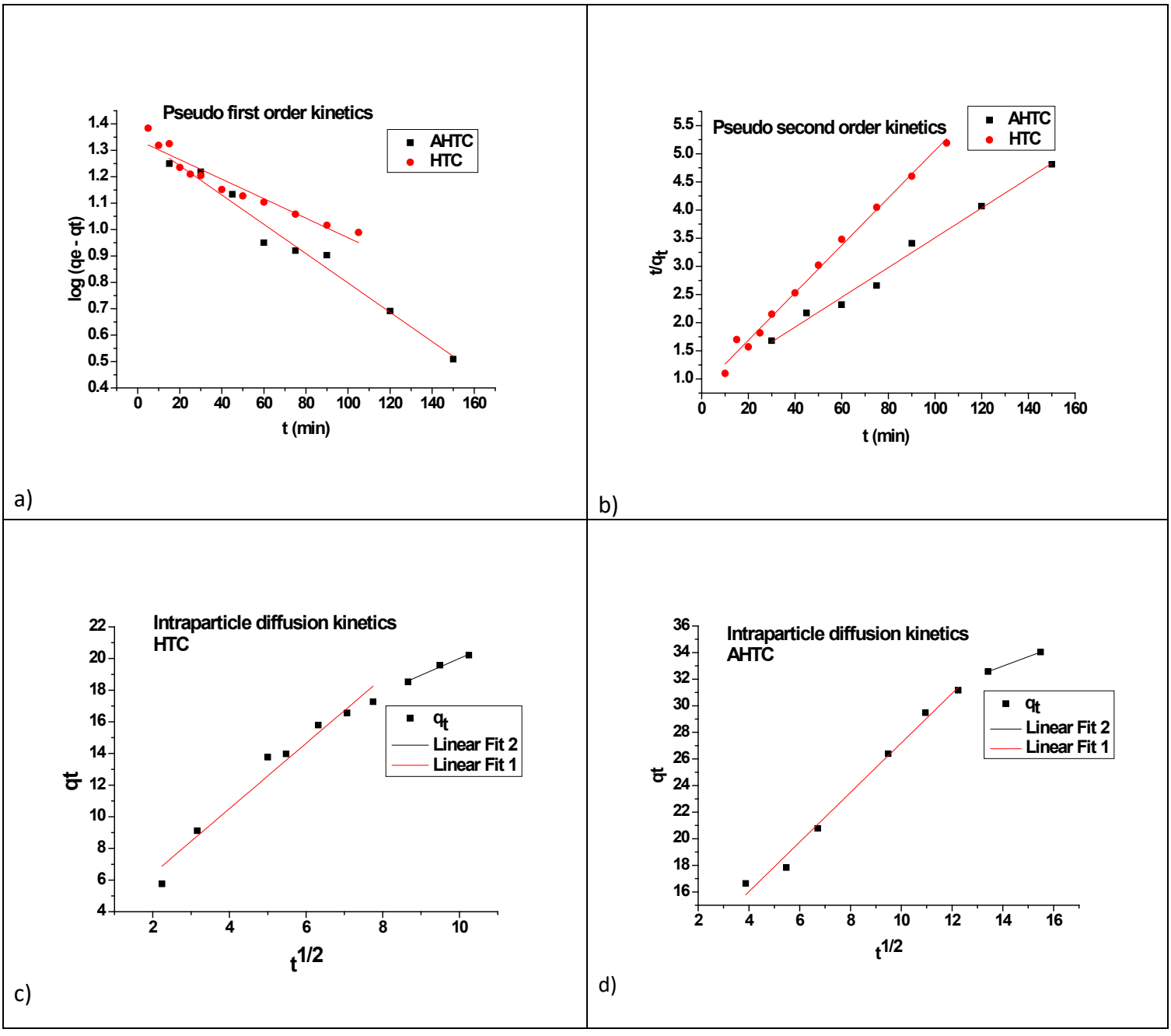
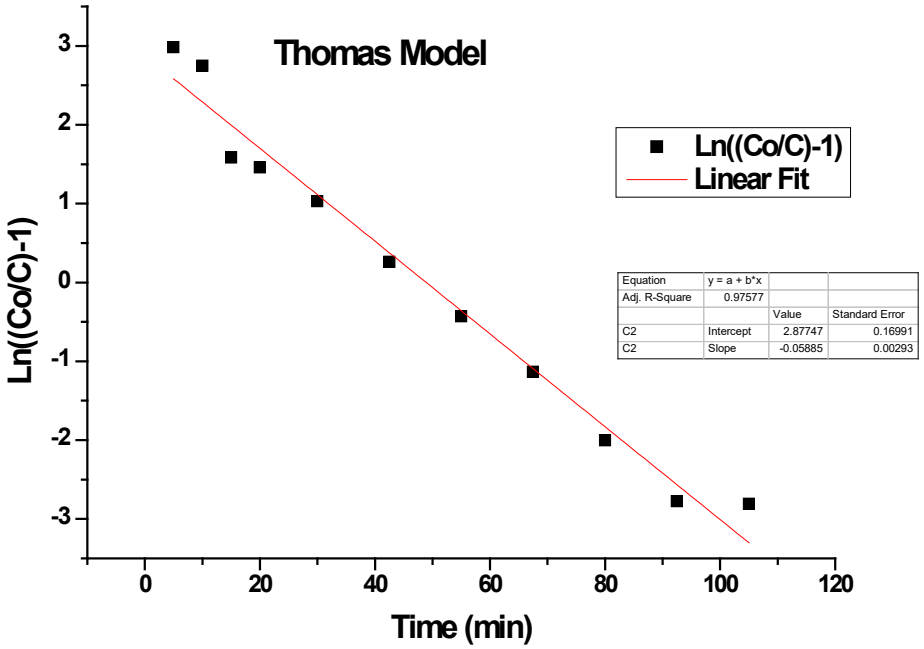
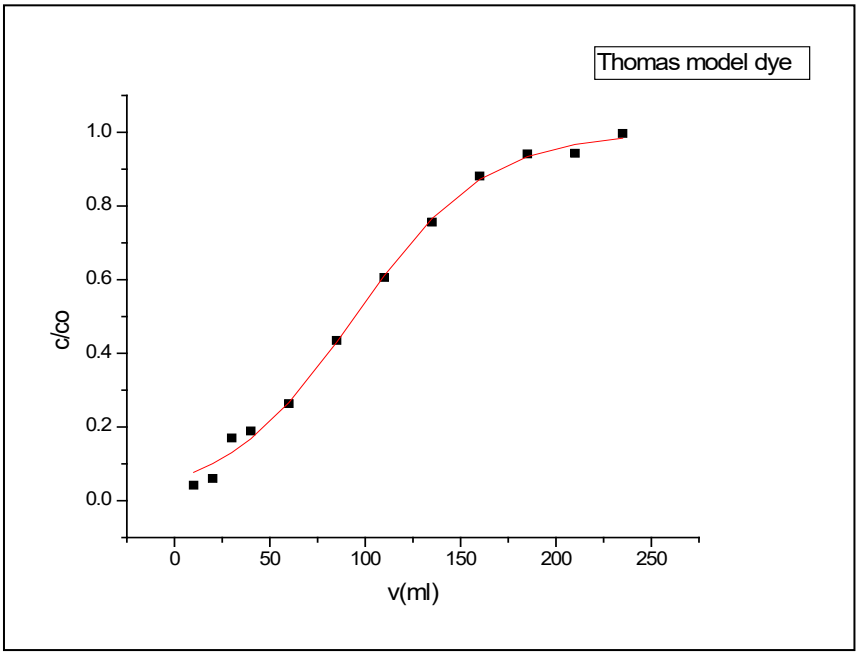


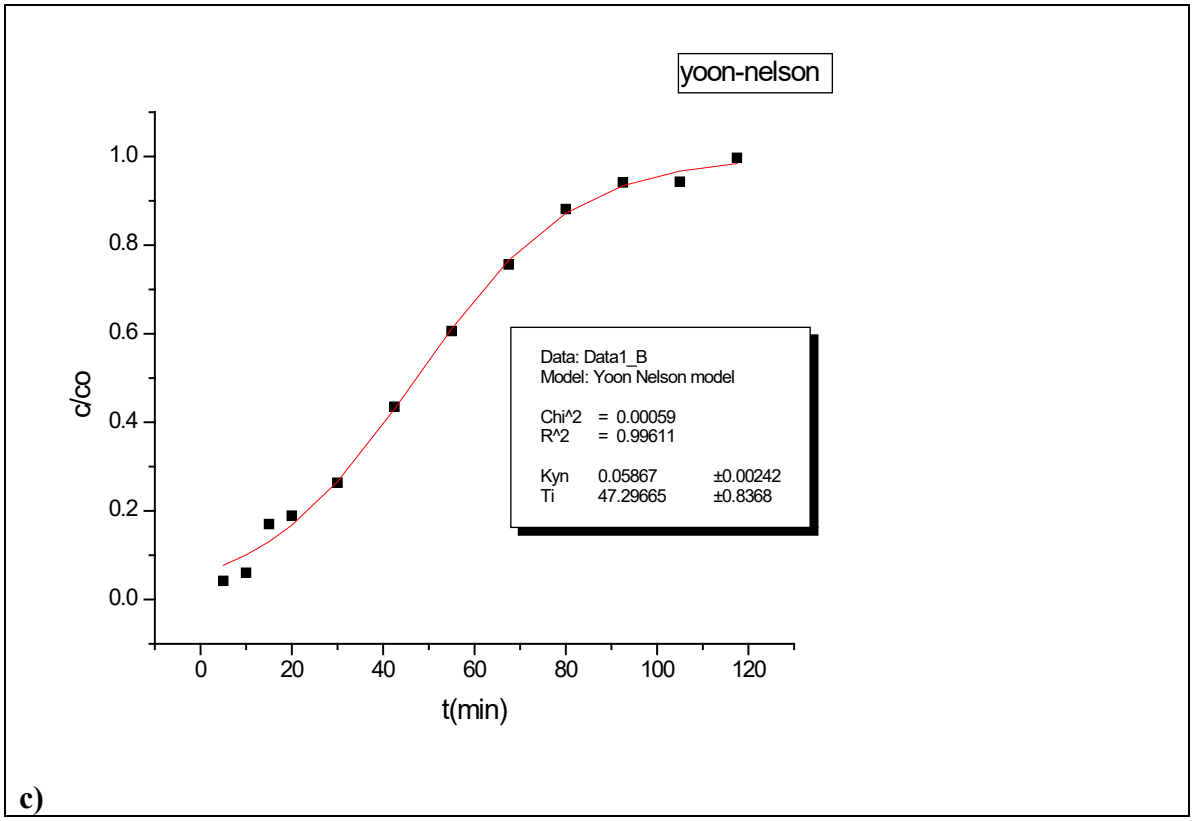
Fig. S6. Kinetics for MG adsorption onto 0.1 gm HTC or AHTC (initial MG solution concentration 100 ppm and volume 50 ml) at 25 °C. **a)** Pseudo-first order kinetic; **b)** Pseudo-second order kinetic; and Intraparticle diffusion kinetics **c)** HTC and **d)** AHTC.


Thomas Model
Ln((Co/C)-1)
Linear Fit
Equation y = a + b*x
Adj. R-Square 0.97577
Value Standard Error
C2 Intercept 2.87747 0.16991
C2 Slope -0.05885 0.00293
Ln((Co/C)-1)
Time (min)

a)


Thomas model dye
c/co
v(ml)

b)



c)

Fig. S7. a) Linear Thomas and **b)** nonlinear Thomas model plot, **c)** nonlinear Yoon-Nelson model plot for MG (100 ppm) adsorption onto AHTC (0.5 gm) packed in a 1 cm diameter column, flow rate is 2 ml/min).

Table S1. Data and results of HTC synthesis of PL-208 sample.

Volume of deionized water (ml)	100
Mass of Palm Leaves m_{bio} (g)	9.96
Mass of citric acid (mg)	10
Final temperature Tf (°C)	208
Final pressure Pf (psi)	90
Mass of Palm Leaves m_{bio}^{db} (g)	4.26
Volume of water collected (ml)	89
Mass of wet coal m_{coal} (g)	19.26
Mass of coal dry basis m_{coal}^{db} (g)	2.98
Mass of water absorbed by coal (g)	16.28
Water content (%)	84.52
Yield coal (%)	69.95
Loss of biomass (%)	70.08

Table S2 Linear parameters, errors, and correlation coefficients: **A)** Langmuir and Freundlich isotherm. **B)** Temkin isotherm for the adsorption of MG by HTC and AHTC.

A) Sample	T °C	Linear Langmuir model						Linear Freundlich model				
		qm (mg/g)	R_L	K_L (L/mg)	SSE	χ^2	R^2	K_F (mg/g) $(L/mg)^{1/n}$	n	SSE	χ^2	R^2
HTC	25°C	46.08	0.570	0.025	3.25E-04	0.00	0.94	2.83	1.8	0.30	0.0885	0.91
	30°C	51.81	0.398	0.041	9.65E-04	0.08	0.97	7.37	2.3	0.75	0.2735	0.91
	35°C	54.53	0.365	0.047	1.69E-03	0.04	1.00	11.75	3.9	0.72	0.2163	0.89
	40°C	59.88	0.294	0.065	1.95E-04	0.00	0.99	15.44	4.0	0.29	0.0891	1.00
AHTC	25°C	65.78	0.530	0.029	8.69E-03	0.18	0.94	5.17	1.9	1.44	0.4603	0.82
	30°C	74.63	0.401	0.049	5.75E-04	0.01	0.96	7.43	1.9	0.29	0.0951	0.83
	35°C	75.19	0.358	0.044	1.75E-04	0.00	0.98	12.36	1.9	0.16	0.0470	0.88
	40°C	85.47	0.279	0.063	9.75E-04	0.03	0.98	16.04	2.5	0.72	0.2023	0.96

B) Sample		Linear Temkin		
		Kt (L/mg)	B (J/mol)	R^2
HTC	25°	0.206	230.23	0.974
	30°	0.622	221.58	0.910
	35°	1.027	244.48	0.909
	40°	1.762	248.45	0.989
AHTC	25°	0.225	82.757	0.944
	30°	0.394	142.65	0.986
	35°	0.376	145.56	0.967
	40°	0.792	146.73	0.958

Table S3: The energies for the hydrothermal carbon (HTC), malachite green (MG) and HTC-MG [values are in Hartree] calculated at the ωB97XD/6-311(d,p).

Compound No.	**Total Electronic Energy**	**Sum of Electronic and Zero-point Energies**	**Sum of Electronic and Thermal Enthalpies**	**Gibbs Free Energy**
HTC	-4556.8284966	-4555.465305	-4555.372451	-4555.601793
MG	-1461.0831211	-1460.652637	-1460.626508	-1460.709178
HTC-MG	-6017.9557675	-6016.156607	-6016.038616	-6016.321707

Table S4: The Cartesian coordinates for the hydrothermal carbon (HTC), malachite green (MG) and HTC-MG, computed at the ωB97XD/6-311(d,p).

HTC			
C	-3.74342600	1.08784600	2.20975000
C	-3.73000900	-0.21417200	2.56766100
C	-4.17723700	-1.35227600	1.73606700
C	-3.22415000	-0.59822900	3.94841800
O	-4.47296700	-2.41680200	2.23694900
C	-4.07696800	-1.29228100	0.19710100
O	-4.74726800	-1.99779000	-0.50275700
C	-4.25744600	1.73136700	1.04192600
C	-4.04402000	2.99227000	0.54000100
C	-4.72346700	3.03022500	-0.71394100
C	-5.31331100	1.81654200	-0.88424000
O	-5.05251900	1.03652000	0.18569400
C	-3.22281100	4.06924000	1.08799700
C	-2.32272600	4.87327200	0.30289200
C	-1.74074900	5.74864800	1.14902000
O	-2.23200700	5.56943500	2.40253600
C	-3.12696500	4.54987100	2.36043700
C	-0.69826300	6.78904700	0.98973400
C	-3.81870600	4.27555800	3.66015300
O	-5.03198900	3.58380700	3.51830400
C	-6.14134600	1.19673900	-1.95581200
C	-5.46518100	1.11306800	-3.34365600
C	-6.41279900	0.49095300	-4.31346400
C	-4.11453800	0.34808800	-3.32802500
C	-2.96466700	1.16648500	-2.84838500
C	-2.30219200	2.22933300	-3.36868100
C	-1.33837800	2.63036600	-2.38729800
C	-1.47199000	1.77759700	-1.34110800
O	-2.45605100	0.88180100	-1.61973700
C	-0.78276900	1.63090000	-0.03785200
C	-6.99876700	0.92211400	-5.45557000
C	-7.79844100	-0.16789700	-5.93394700
C	-7.63835500	-1.17939700	-5.04682000
O	-6.79597900	-0.78754900	-4.05481500
C	-8.17710700	-2.55932800	-4.95445500
C	-4.30397100	-1.36455800	4.70454900
C	-1.85602700	-1.30418600	3.91479700
O	-3.84698800	-2.47423600	5.30822500
O	-5.43493200	-0.98312000	4.81469200
C	-0.77077200	-0.41830000	3.39430900
C	0.44316600	-0.60300200	2.79191500
C	1.01622000	0.71546600	2.67727600
C	0.13621500	1.58592600	3.21228500
O	-0.95376600	0.90904200	3.65066300
C	0.10993400	3.06998600	3.41318800
O	0.38788600	3.80745200	2.24315200
C	1.76107100	4.01849700	1.95077300
C	1.99512400	3.84163400	0.49782000
C	1.92498600	4.67915100	-0.56581500
C	2.14068600	3.88027000	-1.72788900

C	2.31910800	2.60481900	-1.27949900
O	2.24351400	2.57510600	0.07228400
C	2.60746900	1.36901100	-1.95973000
C	2.49838600	0.99681600	-3.26567400
C	3.13752500	-0.28166800	-3.34478800
C	3.56459600	-0.59847000	-2.09508100
O	3.24545500	0.40314400	-1.24066800
C	1.87586800	1.77033200	-4.38115200
C	4.22803000	-1.77984100	-1.50150600
C	1.20400700	-1.79755100	2.40795100
C	2.61850200	-1.72130300	2.15785600
C	3.02516800	-2.96832500	1.82445100
O	1.97739800	-3.81460500	1.84642400
C	0.86582100	-3.10941900	2.19918500
C	-0.36443900	-3.94776900	2.15424400
C	-1.32415800	-3.63651000	0.96792800
C	-0.59997100	-3.11076700	-0.22816800
C	-2.17835300	-4.82761200	0.66309000
C	-3.51440300	-5.01283300	0.55483200
C	-3.69579200	-6.39171800	0.21093000
C	-2.45914400	-6.94058900	0.14042200
O	-1.52294500	-5.99704800	0.41667800
O	0.27740600	-3.93008800	-0.86002900
C	0.85892700	-3.21501800	-1.85943000
C	0.36570000	-1.95200400	-1.86909100
C	-0.58607500	-1.88695500	-0.80333000
C	-1.95836900	-8.30470600	-0.16448100
C	1.84027100	-3.94044800	-2.70435000
C	4.29554500	-3.52301400	1.43712100
O	5.36295700	-2.68608000	1.46916200
C	6.43827900	-3.38412000	1.02020900
C	6.07037400	-4.65146500	0.71001900
C	4.66949200	-4.74746000	0.98121100
C	7.72206300	-2.63300400	0.90758900
C	7.68517600	-1.58640600	-0.15882900
O	7.37953500	-0.31901800	0.23559500
C	7.34342500	0.45667500	-0.87792300
C	7.61469200	-0.29683200	-1.97027400
C	7.83546100	-1.63679500	-1.50541100
C	8.12319100	-2.84116600	-2.34105600
C	7.06596700	1.91370300	-0.66726600
C	6.97625700	2.58530700	-2.04957700
C	5.84158500	2.09507000	0.24108700
O	7.95955200	3.08889800	-2.52686200
C	5.66442400	2.50530300	-2.78458100
C	5.54796800	3.53977100	0.53358000
O	5.79738500	4.46658300	-0.18961600
O	4.94218900	3.70948200	1.72551000
H	-3.30936100	1.78490600	2.91431500
H	-3.11692600	0.32595900	4.52125500
H	-3.30406700	-0.62381200	-0.21135900
H	-4.75300300	3.85827100	-1.40409900
H	-2.12287200	4.75425700	-0.74995900
H	-0.42270500	6.87586800	-0.06153600
H	-1.05124300	7.76242700	1.34010600

H	0.19100800	6.52080400	1.56661300
H	-3.94534000	5.23594800	4.17834300
H	-3.19328100	3.64984600	4.30838600
H	-5.55812700	4.02770100	2.85077100
H	-6.40330300	0.18658600	-1.63257000
H	-7.07674900	1.75406300	-2.06457500
H	-5.27412200	2.12815300	-3.70605200
H	-4.20683600	-0.55582500	-2.71853900
H	-3.90468500	0.02054000	-4.34941900
H	-2.48641300	2.67906900	-4.33233700
H	-0.62659200	3.43967000	-2.44258300
H	-0.46031800	2.60230500	0.33652600
H	-1.45601800	1.19616900	0.70492000
H	0.09320000	0.98031800	-0.10787500
H	-6.87640700	1.89568600	-5.90387700
H	-8.41139500	-0.19319400	-6.82108000
H	-8.83142300	-2.75803600	-5.80389700
H	-7.36919900	-3.29584800	-4.95643000
H	-8.75050300	-2.69587400	-4.03364000
H	-1.60414100	-1.63473800	4.92675300
H	-1.92960300	-2.20732100	3.31232900
H	-4.60812800	-2.87695000	5.74149300
H	1.95233600	0.96574300	2.20523400
H	-0.89801000	3.35269200	3.72103200
H	0.79600600	3.36309000	4.21923900
H	2.03716400	5.04108900	2.23949100
H	2.40095800	3.32392900	2.50321000
H	1.74929700	5.74198000	-0.52451300
H	2.19362800	4.20722800	-2.75342200
H	3.24642800	-0.89434200	-4.22675800
H	2.58785800	2.47748800	-4.82020200
H	1.54142900	1.10025600	-5.17508600
H	1.00815200	2.33204900	-4.02771400
H	4.61636500	-2.42919300	-2.28613700
H	5.05570700	-1.47737300	-0.85845800
H	3.51529300	-2.34683200	-0.89658400
H	3.25158700	-0.85230400	2.22262500
H	-0.02113900	-4.97713700	2.04824000
H	-0.92684500	-3.90026200	3.08923500
H	-2.00256000	-2.83572900	1.26691200
H	-4.27198500	-4.26014800	0.70446600
H	-4.62927000	-6.90513000	0.04135600
H	0.64368500	-1.16049300	-2.54676600
H	-1.16965900	-1.03474700	-0.50223200
H	-2.79864500	-8.96744300	-0.37471900
H	-1.29788500	-8.29467700	-1.03614300
H	-1.39512400	-8.71685400	0.67777800
H	2.27994100	-3.25011800	-3.42525600
H	2.64233400	-4.36733000	-2.09535600
H	1.36129000	-4.75719300	-3.25173800
H	6.71942700	-5.42528900	0.33125900
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H	7.96512200	-2.15685700	1.86170500
H	8.51681200	-3.34984000	0.69021300
H	7.67247800	0.05526200	-2.98886800

H	8.35461900	-3.70971200	-1.72121100
H	7.25997900	-3.10122100	-2.96119000
H	8.97027300	-2.66569700	-3.00906200
H	7.93914900	2.36735000	-0.18696600
H	4.94629700	1.65844600	-0.21358200
H	5.99311600	1.56154800	1.17983500
H	5.27030100	1.48594400	-2.76522600
H	4.93568000	3.15907500	-2.29898900
H	5.81093800	2.83147100	-3.81331600
H	4.76318300	4.65476900	1.79976200
MG			
C	-3.27049200	-1.55704300	-0.58888400
C	-3.15972100	-0.34494300	-1.34357000
C	-1.98673400	0.32420800	-1.37818700
C	-0.79679100	-0.19813900	-0.77463400
C	-0.86834100	-1.54005000	-0.27992300
C	-2.05193700	-2.19085200	-0.18028600
C	0.29959900	0.61744500	-0.50963800
N	-4.46144000	-2.08763800	-0.30142000
C	-5.66214400	-1.27473300	-0.47760300
C	-4.54768800	-3.13748700	0.70860000
C	1.63784100	0.09022900	-0.30159800
C	0.08243300	2.06353100	-0.35236000
C	2.51167600	0.66448700	0.63621300
C	3.77339100	0.15893100	0.85397800
C	4.25031600	-0.94880700	0.11680400
C	3.38385900	-1.51053500	-0.84797700
C	2.11656800	-1.00513200	-1.03825800
C	0.98234600	2.99452800	-0.88990700
C	0.76248000	4.35122400	-0.72324700
C	-0.33831000	4.79239700	0.00854500
C	-1.21999200	3.87577500	0.56662500
C	-1.02276900	2.51278700	0.38688500
N	5.50286800	-1.45155200	0.32330700
C	5.95672900	-2.60570500	-0.42517000
C	6.37839400	-0.84573600	1.30628500
H	-4.03541700	0.09868400	-1.79145700
H	-1.93819100	1.28558900	-1.87433700
H	0.01443200	-1.98870100	0.15713400
H	-2.08266300	-3.14254600	0.32744200
H	-6.52795900	-1.86336500	-0.18209400
H	-5.58577900	-0.38451300	0.15878000
H	-5.79242300	-0.99308200	-1.52378200
H	-5.58713100	-3.44265300	0.80706600
H	-3.97034100	-4.01494400	0.41377300
H	-4.19095800	-2.74473700	1.66805400
H	2.17156100	1.50550300	1.22908100
H	4.39324500	0.62139500	1.60936600
H	3.71050600	-2.33868100	-1.46152800
H	1.48445900	-1.44220100	-1.80318300
H	1.83921400	2.64411800	-1.45477100
H	1.44822800	5.06798000	-1.16026100
H	-0.50147500	5.85545300	0.14771400
H	-2.06737700	4.21127000	1.15262700
H	-1.70639400	1.79977800	0.85064300

H	5.99419300	-2.40294100	-1.50191500
H	6.96089900	-2.87081300	-0.09971900
H	5.30907600	-3.47430200	-0.26016300
H	7.33029600	-1.37341900	1.31039000
H	6.57813100	0.20648300	1.07455600
H	5.95631000	-0.90251000	2.31630100
Cl	-3.51521900	0.18465900	1.93534800

HTC-MG

C	3.9067795	-0.0703508	0.2117198
C	3.7343965	0.6008892	1.3758108
C	3.8590495	2.0509372	1.5769018
C	3.3769575	-0.1869698	2.6246858
O	4.0360605	2.5193072	2.6853158
C	3.5506255	3.0304582	0.4255138
O	3.9779095	4.1505902	0.4222318
C	4.3299665	0.3684522	-1.0730472
C	4.2419775	-0.2438088	-2.3024632
C	4.7172085	0.7167782	-3.2421712
C	5.0774395	1.8239512	-2.5375102
O	4.8630385	1.6135282	-1.2233722
C	3.6824515	-1.5473438	-2.6412272
C	2.8499935	-1.7790608	-3.7931382
C	2.5039605	-3.0837328	-3.7622352
O	3.0771305	-3.6840828	-2.6937752
C	3.7943545	-2.7578458	-2.0154042
C	1.6426635	-3.9383108	-4.6124042
C	4.5668785	-3.2898038	-0.8459992
O	5.7023465	-2.5065998	-0.5450872
C	5.6334805	3.1571082	-2.8994602
C	4.7249335	4.0260872	-3.7996942
C	5.3960025	5.3318632	-4.0626202
C	3.3044035	4.2435062	-3.2121512
C	2.3708415	3.1096852	-3.4689662
C	1.8024995	2.6237022	-4.6002802
C	1.0573925	1.4616722	-4.2171642
C	1.2152615	1.3252242	-2.8772472
O	2.0077885	2.3299832	-2.4151792
C	0.7077475	0.3565242	-1.8786612
C	5.8509465	5.9381882	-5.1847142
C	6.3861315	7.2024752	-4.7703712
C	6.2159425	7.2695812	-3.4278862
O	5.6142135	6.1336462	-2.9864482
C	6.5401455	8.2913082	-2.4013212
C	4.4196755	0.0089782	3.7131448
C	1.9301765	0.0342622	3.0946648
O	3.9009065	0.3061702	4.9205958
O	5.5963765	-0.1599098	3.5489528
C	0.9426755	-0.4523728	2.0875068
C	-0.3705245	-0.2045338	1.8058868
C	-0.7329155	-1.1531748	0.7824338
C	0.3622075	-1.8984498	0.5255898

O	1.3843465	-1.4772608	1.3098568
C	0.6689635	-3.0736588	-0.3476562
O	0.2887435	-2.9144248	-1.6913712
C	-1.0382645	-3.2890958	-2.0113412
C	-1.6130335	-2.2547178	-2.9027882
C	-1.5703155	-2.0421598	-4.2404462
C	-2.1250785	-0.7466368	-4.4643972
C	-2.4586215	-0.2624298	-3.2337662
O	-2.1598465	-1.1757748	-2.2807902
C	-3.0929365	0.9551702	-2.8035042
C	-3.3584245	2.1239542	-3.4502182
C	-4.1883885	2.8674652	-2.5517822
C	-4.3462195	2.1170432	-1.4307202
O	-3.6812725	0.9446742	-1.5749302
C	-2.8994265	2.5247792	-4.8140062
C	-5.0149635	2.3330842	-0.1282102
C	-1.3708995	0.6525522	2.4435638
C	-2.7719155	0.3533782	2.3299198
C	-3.4322285	1.3024122	3.0345358
O	-2.5537815	2.1654732	3.5813848
C	-1.2948225	1.7776272	3.2219558
C	-0.2455935	2.7139652	3.7129148
C	0.5350055	3.4772402	2.6037428
C	-0.2933995	3.6982292	1.3813418
C	1.1156155	4.7388072	3.1637638
C	2.3696045	5.2441662	3.2176078
C	2.2556825	6.5141472	3.8709478
C	0.9449225	6.6826232	4.1686948
O	0.2367135	5.6039742	3.7457458
O	-1.4154645	4.4512812	1.5014528
C	-2.0375235	4.4554812	0.2923898
C	-1.3301795	3.7085582	-0.5912452
C	-0.1908615	3.2161052	0.1221668
C	0.1762815	7.7659552	4.8323038
C	-3.2733955	5.2720242	0.1984688
C	-4.8319725	1.5666972	3.2374518
O	-5.6949035	0.6765852	2.6856548
C	-6.9522015	1.1307482	2.9223228
C	-6.9004545	2.2899662	3.6239188
C	-5.5151605	2.5792142	3.8324338
C	-8.0662195	0.3345822	2.3309968
C	-8.0540095	0.3550382	0.8361058
O	-7.4752905	-0.7082658	0.2104838
C	-7.5261215	-0.4705728	-1.1257752
C	-8.1194175	0.7249772	-1.3559972
C	-8.4633355	1.2719532	-0.0746232
C	-9.1020605	2.5957292	0.1920798
C	-6.9829295	-1.5439068	-2.0184312
C	-7.1016065	-1.0583558	-3.4755772
C	-5.5727235	-1.9528278	-1.5672092

O	-8.0630625	-1.3751078	-4.1257582
C	-6.0346945	-0.1320778	-3.9959482
C	-4.9968105	-3.0601418	-2.4048322
O	-5.2256735	-3.2505688	-3.5684062
O	-4.1484865	-3.8482018	-1.7110562
H	3.7034305	-1.1327558	0.2376858
H	3.4832745	-1.2370968	2.3549128
H	2.8533535	2.6640862	-0.3443982
H	4.7805495	0.5908052	-4.3112912
H	2.5323455	-1.0381008	-4.5100142
H	1.3407885	-3.3932378	-5.5077762
H	2.1726075	-4.8460508	-4.9120932
H	0.7429095	-4.2309068	-4.0623242
H	4.8134155	-4.3433918	-1.0494332
H	3.9519015	-3.2797868	0.0639828
H	6.3537585	-2.6741038	-1.2275292
H	5.8270165	3.6989052	-1.9706842
H	6.5946395	3.0273942	-3.4057092
H	4.6162585	3.5334752	-4.7709022
H	3.3714355	4.4398812	-2.1381302
H	2.8870255	5.1441072	-3.6698492
H	1.9124755	3.0395232	-5.5901442
H	0.4748295	0.8054432	-4.8455072
H	0.5683405	-0.6234048	-2.3347892
H	1.4275415	0.2402752	-1.0643862
H	-0.2420465	0.6764442	-1.4404862
H	5.8095685	5.5346922	-6.1843952
H	6.8372995	7.9601132	-5.3916372
H	7.0004255	9.1586302	-2.8758532
H	5.6383565	8.6184122	-1.8769362
H	7.2343085	7.8937802	-1.6558992
H	1.7765845	-0.5020758	4.0365978
H	1.7722055	1.0884762	3.3129558
H	4.6565475	0.4252142	5.5076638
H	-1.6821385	-1.2209408	0.2752068
H	1.7468035	-3.2318358	-0.3427332
H	0.2058785	-3.9759508	0.0652808
H	-1.0297625	-4.2636888	-2.5189032
H	-1.6568695	-3.3785728	-1.1126492
H	-1.1799235	-2.7250998	-4.9777772
H	-2.2822915	-0.2522818	-5.4088202
H	-4.6027905	3.8494632	-2.7218792
H	-3.4944665	2.0375302	-5.5939762
H	-2.9926155	3.6030812	-4.9516912
H	-1.8511725	2.2538242	-4.9669602
H	-5.6715015	3.2018252	-0.1796632
H	-5.6109915	1.4633332	0.1538388
H	-4.2685275	2.5023712	0.6529378
H	-3.2267135	-0.4573388	1.7852148
H	-0.7663535	3.4509962	4.3249088

H	0.4727105	2.2118172	4.3673048
H	1.3776825	2.8664862	2.2757888
H	3.2612145	4.7697322	2.8389508
H	3.0504715	7.2103862	4.0884598
H	-1.5824855	3.5272272	-1.6242932
H	0.5910705	2.5789422	-0.2546872
H	0.8520445	8.5704682	5.1246338
H	-0.5825335	8.1766862	4.1602718
H	-0.3324275	7.3987332	5.7283598
H	-3.7253365	5.1393152	-0.7844832
H	-3.9988985	4.9734592	0.9603408
H	-3.0544485	6.3339842	0.3412888
H	-7.7477595	2.8730652	3.9487858
H	-5.0793375	3.4243562	4.3395598
H	-8.0089465	-0.7039808	2.6691808
H	-9.0093625	0.7444992	2.6985678
H	-8.3089595	1.1676212	-2.3218922
H	-9.2880225	2.7410592	1.2580398
H	-8.4563295	3.4129922	-0.1426192
H	-10.0549305	2.6894732	-0.3351862
H	-7.6455615	-2.4133368	-1.9555262
H	-4.8806475	-1.1058858	-1.6233492
H	-5.5922725	-2.2611088	-0.5214262
H	-5.8145135	0.6552202	-3.2705932
H	-5.1163275	-0.6987838	-4.1697482
H	-6.3684065	0.3052152	-4.9359022
H	-3.7894965	-4.4730048	-2.3532332
C	2.2923295	-5.0190978	2.5478748
C	1.5792615	-5.7202358	1.5341098
C	2.1560515	-5.9410848	0.2549068
C	0.2336125	-6.1427918	1.7035628
C	1.4330855	-6.4316318	-0.7954312
H	3.1916985	-5.7039118	0.0349808
C	-0.5042925	-6.6287008	0.6584338
H	-0.2134985	-6.1121758	2.6900498
C	0.0603095	-6.7307908	-0.6468142
H	1.9661985	-6.5552468	-1.7294352
H	-1.5154895	-6.9644388	0.8437128
C	1.6094305	-4.2472888	3.5556668
C	2.2306575	-3.9409258	4.7885388
C	0.3609355	-3.6306288	3.3141908
C	1.6911335	-3.0435958	5.6731138
H	3.1602995	-4.4340308	5.0454428
C	-0.1974925	-2.7340558	4.1886148
H	-0.1404055	-3.7868068	2.3695278
C	0.4766035	-2.3709048	5.3793288
H	2.2102135	-2.8498428	6.6012178
H	-1.1141105	-2.2365498	3.9040638
C	3.7517645	-4.9518218	2.4862618
C	4.4034175	-3.7394218	2.7879778

C	4.5225515	-6.0199438	2.0035458
C	5.7559505	-3.5794758	2.5667958
H	3.8182575	-2.9063248	3.1482438
C	5.8825085	-5.8632658	1.7909408
H	4.0577265	-6.9669678	1.7609128
C	6.4945055	-4.6459188	2.0586648
H	6.2162275	-2.6155628	2.7478998
H	6.4411185	-6.6817858	1.3567468
H	7.5494935	-4.5156948	1.8488758
C	-2.1095425	-7.3674148	-1.5591412
H	-2.6101215	-6.5336578	-1.0561612
H	-2.5571015	-7.4867908	-2.5446592
H	-2.3038215	-8.2817718	-0.9863632
C	-0.0536315	-7.3446308	-2.9981032
H	0.4103125	-6.4326408	-3.3848632
H	0.7202535	-8.1133918	-2.9233122
H	-0.8060465	-7.6792208	-3.7097492
N	-0.6911215	-7.1044618	-1.7100582
N	0.0006285	-1.3939478	6.1883838
C	0.8294485	-0.8720648	7.2615008
H	0.9737895	-1.6084688	8.0595828
H	1.8086615	-0.5632188	6.8810228
H	0.3442595	0.0012622	7.6924418
C	-1.2781135	-0.7613998	5.9040708
H	-1.2538875	-0.1908148	4.9694258
H	-2.0747635	-1.5074458	5.8366588
H	-1.5262755	-0.0806988	6.7159738
Cl	4.8617435	-6.7963878	-1.4461152