Stable Reusability of Nanocellulose Aerogels with Amino Group Modification in Adsorption/Desorption Cycles for CO_2 Capture

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Detailed description of the different isotherm models (BET, Langmuir, Freundlich Temkin) used in this work to fit the experimental data (PDF)

Table SI-1. ADSORPTION ISOTHERM DATA A1

A1 AEROGEL 8-6-2023 - Adsorption

Relative Pressure (P/Po)	Quantity Adsorbed (cm^3/g STP)
0,000892131	1,363326111
0,000999378	1,557560573
0,001121314	1,753216674
0,001200067	1,869039605
0,001279706	1,994748686
0,001355806	2,103279535
0,001457212	2,293225862
0,00154216	2,414713013
0,00159596	2,519743868
0,001638612	2,59883188
0,001722675	2,726011314
0,001782315	2,717131092
0,005589756	3,842707891
0,005628513	3,99316377
0,005657537	4,084730022
0,005692401	4,18963973
0,005734698	4,316316992
0,005791684	4,397152431
0,005844422	4,388776951
0,010124209	5,41958118
0,010150401	5,566146156
0,010185619	5,703120633
0,010205794	5,786309429
0,020522552	6,269745786
0,030289803	6,295215704
0,061291042	6,376559048
0,077721581	6,415643173
0,092839673	6,493226445
0,123678268	6,602686738
0,247758283	6,449986595
0,311253357	6,341751596
0,374389568	6,286836271
0,438305825	6,167968878
0,50133406	6,060999094
0,562461933	5,945867268

0,623436215	5,773803916
0,684868662	5,639115996
0,745803592	5,429047567
0,86824116	5,172033762
0,898975332	5,044400376
0,929475323	4,939681576
0,990886247	4,712587089

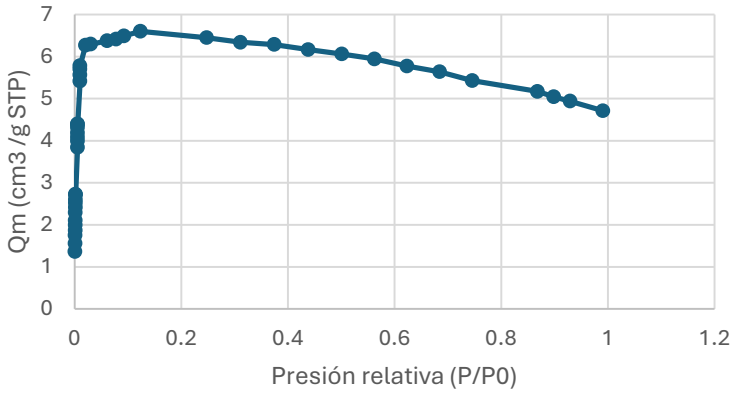


Figure SI-1. ADSORPTION ISOTHERM A1

Table SI-2. BET Report A1

BET Report

BET Surface Area:	21.0253 ± 0.7886 m^2/g
Slope:	0.221671 ± 0.008072 g/cm^3 STP
Y-Intercept:	-0.004431 ± 0.001113 g/cm^3 STP
C:	-49.023099
Qm:	4,6032 cm^3/g STP
Correlation Coefficient:	0.9980169
Molecular Cross-Sectional Area:	0.1700 nm^2

BET Surface Area Plot

A1 AEROGEL 8-6-2023 Not Fitted

Relative Pressure (P/Po)	1/[Q(Po/P - 1)]	Relative Pressure (P/Po)	1/[Q(Po/P - 1)]
0,061291042	0,010239521		
0,077721581	0,013135281		
0,092839673	0,01576119		
0,123678268	0,021375147		
0,247758283	0,051063662		

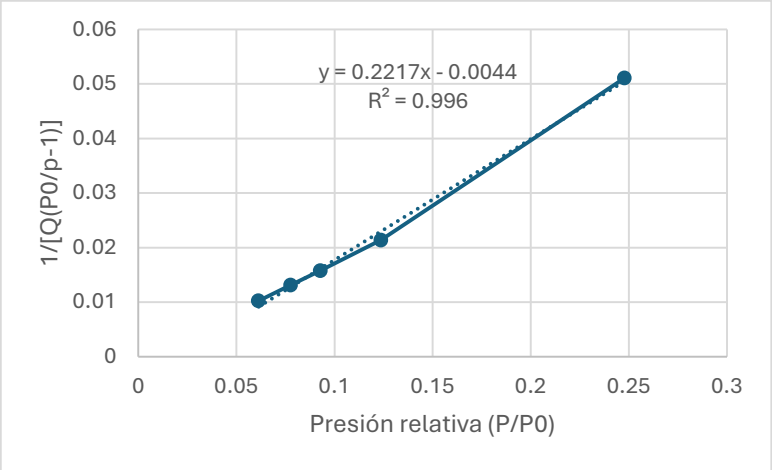


Figure SI-2. ADSORPTION ISOTHERM A1 IN BET COORDINATES

Table SI-3. Langmuir Report A1

Langmuir Report	
Langmuir Surface Area:	26,9316 ± 0,3930 m²/g
Slope:	0,169597 ± 0,002475 g/cm³ STP
Y-Intercept:	-1,255 ± 0,635 mmHg·g/cm³ STP
b:	-0,135137 1/mmHg
Qm:	5,8963 cm³/g STP
Correlation Coefficient:	0.998831
Molecular Cross-Sectional Area:	0.1700 nm²

Langmuir Surface Area Plot

A1 AEROGEL 8-6-2023 Pressure (mmHg)	P/Q (mmHg·g/cm³ STP)	Not Fitted Pressure (mmHg)	P/Q (mmHg·g/cm³ STP)

15,59713936	2,487682897
23,02025032	3,656784994
46,58119202	7,305067147
59,06840134	9,206933699
70,55815125	10,86642393
93,9954834	14,23594472
188,2962952	29,19328473
236,5525513	37,3008226
284,5360718	45,2590237
333,1124268	54,00682677
381,0138855	62,86321439
427,4710693	71,89381297
473,8115234	82,0622817

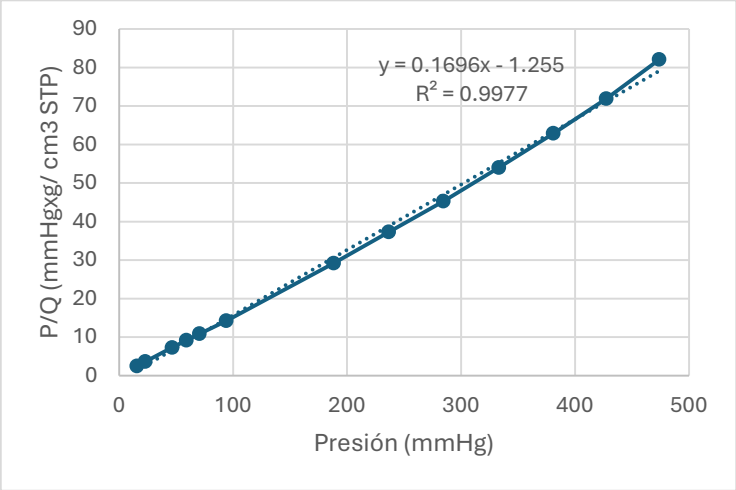


Figure SI-3. ADSORPTION ISOTHERM A1 IN LANGMUIR COORDINATES

Table SI-4. Freundlich Report A1

Freundlich Tabular Report

Qm·C:	2.7227 ± 0.0828 cm³/g STP
m:	6.8946 ± 0.8778
Correlation Coefficient:	0.778878

Freundlich Plot

A1 AEROGEL 8-6-2023

log(P)	log(Q)
-0,1687578	0,13459975
-0,1194567	0,19244495
-0,0694593	0,24383559
-0,03998075	0,2716185
-0,01207612	0,29988819
0,01301099	0,322897
0,04433638	0,36044683
0,06894305	0,38286552
0,08383572	0,4013564
0,0952896	0,41477819
0,11701685	0,43552765
0,1317981	0,43411059
0,62820641	0,58463737
0,63120727	0,60131712
0,63344097	0,61116336
0,63610908	0,62217668
0,63932413	0,63511333
0,64361842	0,64317152
0,64755519	0,64234351
0,8861747	0,73396573
0,8872968	0,74555461
0,88880104	0,75611256
0,88966039	0,76240165
1,19304495	0,79724993
1,36211004	0,79901062
1,6682106	0,80458639
1,77135522	0,8072402
1,84854719	0,81246055
1,97310699	0,81972069
2,27484178	0,80955881
2,37392764	0,80220923
2,45413733	0,79843215
2,52259083	0,79014217
2,5809408	0,78254422
2,63090673	0,77421521
2,67560562	0,76146203
2,71642089	0,75121103
2,75343806	0,73472365

2,81945396	0,71366135
2,83456137	0,70280955
2,84905146	0,69369895
2,87683739	0,67325939

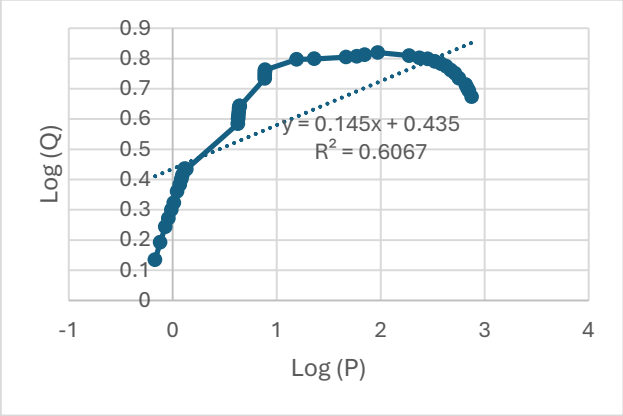


Figure SI-4. ADSORPTION ISOTHERM A1 IN FREUNDLICH COORDINATES

Table SI-5. Temkin Report A1

Temkin Tabular Report	
q·alpha/Qm:	1.202170 ± 0.148123 kJ/mol·(cm³/g STP)
A:	268.6050 ± 223.6366 1/mmHg
Correlation Coefficient:	0.788781

Temkin Plot

A1 AEROGEL 8-6-2023

ln(P)	Quantity Adsorbed (cm³/g STP)
-0,3885792	1,36332611
-0,27505921	1,55756057
-0,15993596	1,75321667
-0,09205908	1,86903961
-0,0278063	1,99474869
0,02995891	2,10327953

0,10208828	2,29322586
0,15874723	2,41471301
0,19303889	2,51974387
0,21941241	2,59883188
0,26944125	2,72601131
0,30347634	2,71713109
1,44649872	3,84270789
1,45340845	3,99316377
1,45855175	4,08473002
1,46469529	4,18963973
1,4720982	4,31631699
1,48198618	4,39715243
1,49105092	4,38877695
2,04049265	5,41958118
2,04307639	5,56614616
2,04654002	5,70312063
2,04851875	5,78630943
2,74708752	6,26974579
3,13637428	6,2952157
3,84119685	6,37655905
4,07869612	6,41564317
4,25643721	6,49322644
4,54324673	6,60268674
5,23801676	6,4499866
5,46617039	6,3417516
5,65086004	6,28683627
5,80848005	6,16796888
5,94283582	6,06099909
6,05788661	5,94586727
6,16080961	5,77380392
6,25479024	5,639116
6,34001953	5,42904757
6,49203266	5,17203376
6,52681875	5,04440038
6,56018341	4,93968158
6,6241629	4,71258709

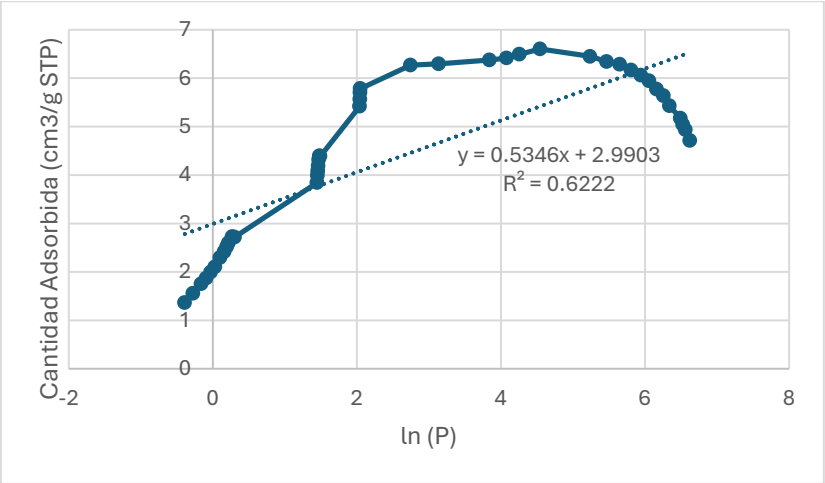


Figure SI-5. ADSORPTION ISOTHERM A1 IN TEMKIN COORDINATES

Table SI-6. ADSORPTION ISOTHERM A2 DATA

A2 AEROGEL 8-6-2023 - Adsorption

Relative Pressure (P/Po)	Quantity Adsorbed (cm^3/g STP)
0,001063974	1,926874279
0,001208031	2,155389105
0,001322003	2,329347941
0,00140819	2,462026619
0,001544461	2,696631802
0,001623038	2,777088611
0,001699668	2,884236435
0,001780192	3,000216155
0,001827975	3,098122303
0,001897526	3,183409375
0,001954158	3,299335875
0,00202601	3,355356357
0,004723994	4,118057707
0,004767353	4,237523233
0,004797792	4,328857891
0,00483655	4,387788041
0,004878493	4,477079504
0,004954415	4,425299546
0,009563552	5,787516397
0,009597177	5,947113747
0,009637528	6,07880611
0,00967133	6,19471901

0,009730439	6,324324422
0,020156391	7,296950413
0,030078659	7,415590463
0,061479523	7,498544991
0,077327282	7,611386202
0,092680389	7,74692606
0,123840031	7,78474978
0,247638281	7,726188217
0,310960468	7,706115012
0,37436937	7,683794808
0,438432553	7,566173398
0,501197253	7,480241792
0,562735186	7,467076734
0,623419551	7,397411046
0,685007437	7,347234342
0,745732438	7,199973814
0,86807781	6,968040788
0,898993884	6,94340972
0,929719543	6,878338163
0,990964468	6,731049251

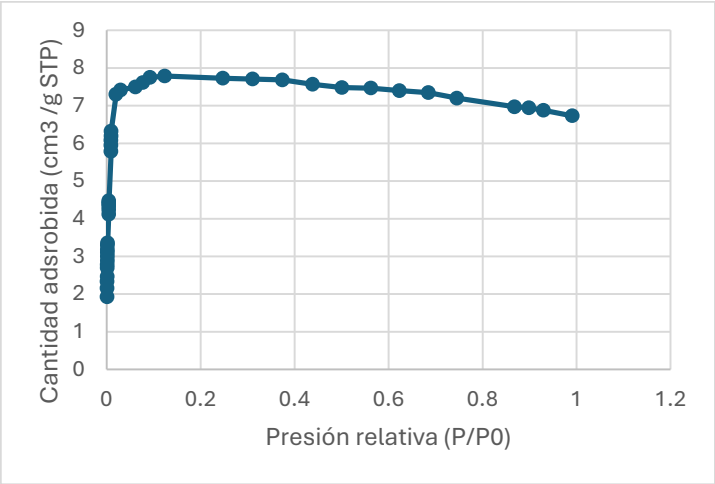


Figure SI-6. ADSORPTION ISOTHERM A2

Table SI-7. BET Report A2

BET Report

BET Surface Area: 25.2545 ± 0.8818 m²/g

Slope:	0.184353 ± 0.006256 g/cm³ STP
Y-Intercept:	-0.003494 ± 0.000862 g/cm³ STP
C:	-51.768397
Qm:	5,5292 cm³/g STP
Correlation Coefficient:	0.9982771
Molecular Cross-Sectional Area:	0.1700 nm²

A2 AEROGEL 8-6-2023		Not Fitted	
Relative Pressure (P/Po)	1/[Q(Po/P - 1)]	Relative Pressure (P/Po)	1/[Q(Po/P - 1)]
0,061479523	0,008735942		
0,077327282	0,011010862		
0,092680389	0,013185547		
0,123840031	0,018156536		
0,247638281	0,04260159		

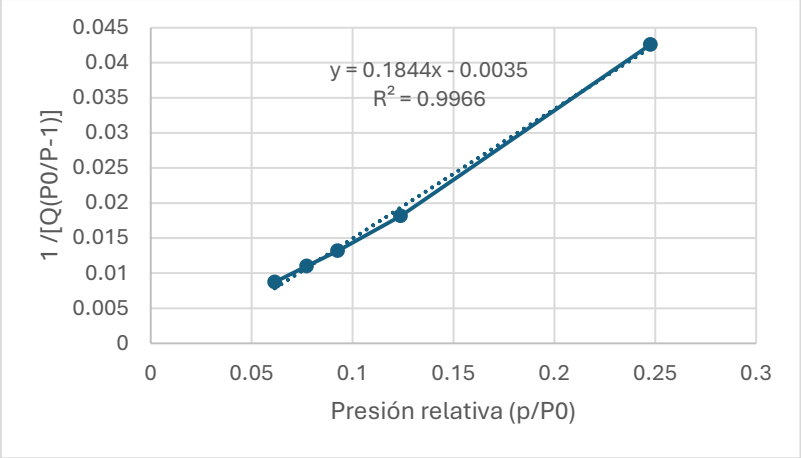


Figure SI-7. ADSORPTION ISOTHERM A2 IN BET COORDINATES

Table SI-8. Langmuir Report A2

Langmuir Report

Langmuir Surface Area:	34,0477 ± 0,2228 m²/g
Slope:	0,134151 ± 0,000878 g/cm³ STP
Y-Intercept:	-0,350 ± 0,225 mmHg·g/cm³ STP
b:	-0,383784 1/mmHg
Qm:	7,4543 cm³/g STP
Correlation Coefficient:	0.999765

Molecular Cross-Sectional Area:	0.1700 nm²

Langmuir Surface Area Plot

A2 AEROGEL 8-6-2023		Not Fitted	
Pressure (mmHg)	P/Q (mmHg·g/cm³ STP)	Pressure (mmHg)	P/Q (mmHg·g/cm³ STP)
15,31885719	2,099350595		
22,8597908	3,082666298		
46,72443771	6,231133876		
58,76873398	7,721160432		
70,43709564	9,092263834		
94,11842346	12,09010259		
188,2050934	24,35937206		
236,3299561	30,66784699		
284,5207214	37,02867249		
333,2087402	44,03926829		
380,9099121	50,92213898		
427,6787415	57,27525733		
473,7988586	64,04928098		

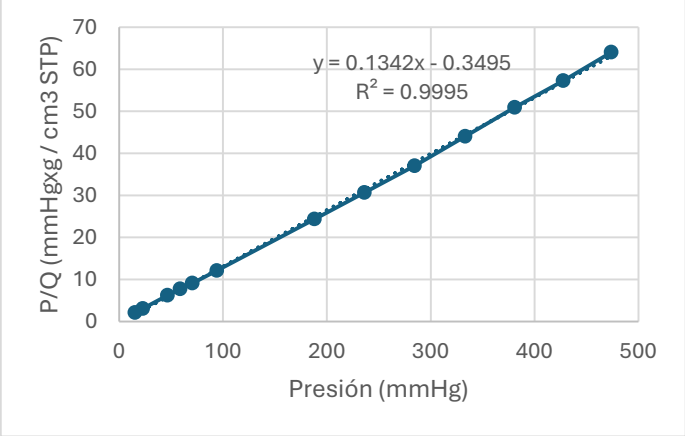


Figure SI-8. ADSORPTION ISOTHERM A2 IN LANGMUIR COORDINATES

Table SI-9. Freundlich Report A2

Freundlich Tabular Report

	3.2204 ± 0.0768 cm³/g
Qm·C:	STP
m:	6.5043 ± 0.6139
Correlation Coefficient:	0.858657

Freundlich Plot

A2 AEROGEL 8-6-2023

log(P)	log(Q)
-0,0922555	0,28485338
-0,03710821	0,33352568
0,00204612	0,36723437
0,02947485	0,39129274
0,06959049	0,43082165
0,09114222	0,44358974
0,11117765	0,46003052
0,13128032	0,47715255
0,14278381	0,49109856
0,15900131	0,50289249
0,17177324	0,51842653
0,18745515	0,52573865
0,5551229	0,61469243
0,55909087	0,62711209
0,56185502	0,63637333
0,56534926	0,64224564
0,56909925	0,65099481
0,575806	0,64594267
0,86143282	0,76249223
0,86295711	0,77430625
0,86477923	0,78381829
0,86629979	0,79202161
0,86894605	0,80101414
1,18522637	0,8631414
1,35907225	0,87014574
1,66954408	0,874977
1,76914634	0,88146376
1,84780144	0,88912941
1,97367464	0,89124466
2,27463137	0,88796528
2,37351877	0,88683549
2,4541139	0,88557576

2,52271638	0,87887629
2,58082227	0,87391564
2,63111766	0,87315061
2,67559401	0,86907975
2,71650888	0,86612389
2,75339663	0,85733092
2,81937225	0,84311068
2,83457033	0,84157279
2,84916555	0,83748352
2,87687167	0,82808277

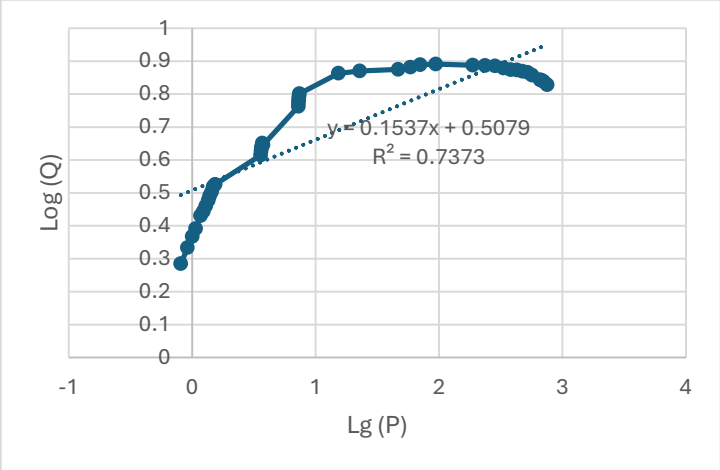


Figure SI-9. ADSORPTION ISOTHERM A2 IN FREUNDLICH COORDINATES

Temkin Tabular Report

q·alpha/Qm:	0.873691 ± 0.072292 kJ/mol·(cm³/g STP)
A:	94.1404 ± 46.0775 1/mmHg
Correlation Coefficient:	0.886013

Table SI-10. Temkin Report A2

Temkin Plot

A3 AEROGEL 7-6-2023

ln(P)	Quantity Adsorbed (cm^3/g STP)
-0,447828534	1,50595474
-0,308002517	1,759583486
-0,138543981	2,089506069
-0,089408121	2,221788543
-0,020091629	2,359220747
0,031002595	2,494223976
0,091343404	2,680652791
0,132234151	2,824663685
0,165153165	2,923678887
0,196028483	3,02977257
0,244371074	3,183328175
0,287965929	3,223978629
1,038672096	4,001742153
1,050596649	4,109359115
1,060193485	4,214491544
1,072510188	4,27986156
1,549050108	5,014004735
1,550048828	5,094652748
1,557019151	5,224362188
1,57611228	5,215743632
2,096261344	5,98015985
2,09806176	6,04308754
2,100320078	6,202773293
2,756844604	6,475458514
3,137699663	6,603161896
3,843818103	6,674072474
4,076920695	6,782663179
4,250447006	6,780156683
4,542983471	7,036342097
5,239036241	6,958253552
5,465966854	6,808896974
5,651048141	6,728156367
5,807785746	6,652385255
5,94285312	6,492604755
6,058089841	6,378341272
6,161220005	6,200712971
6,254796455	6,168285288

6,339969227	6,014719347
6,492287182	5,711260645
6,526630504	5,562970835
6,560115238	5,474287392
6,624318982	5,269364125

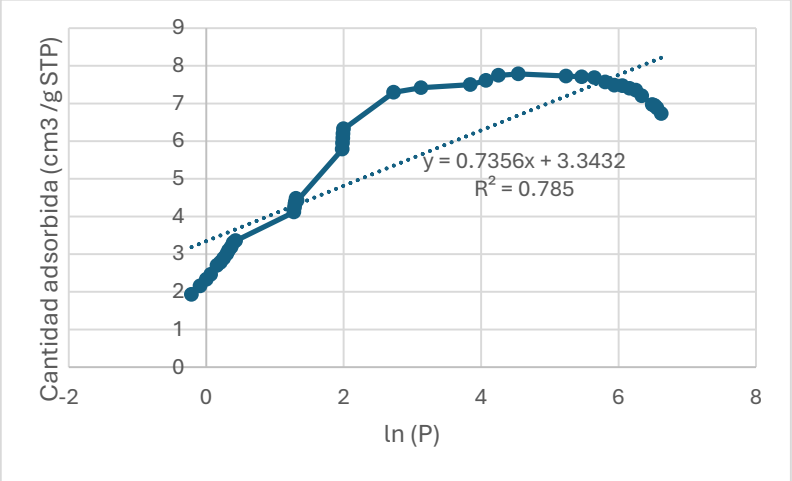


Figure SI-10. ADSORPTION ISOTHERM A2 IN TEMKIN COORDINATES

Table SI-11. ADSORPTION ISOTHERM A3 DATA

A3 AEROGEL 7-6-2023 - Adsorption

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)
0,000840808	1,50595474
0,000966991	1,759583486
0,001145559	2,089506069
0,001203253	2,221788543
0,001289617	2,359220747
0,001357221	2,494223976
0,001441638	2,680652791
0,00150181	2,824663685
0,001552071	2,923678887
0,001600739	3,02977257
0,001680024	3,183328175
0,001754884	3,223978629
0,003717714	4,001742153
0,003762311	4,109359115
0,003798591	4,214491544
0,003845667	4,27986156

0,006193417	5,014004735
0,006199611	5,094652748
0,00624297	5,224362188
0,006363313	5,215743632
0,010704864	5,98015985
0,010724154	6,04308754
0,0107484	6,202773293
0,020723772	6,475458514
0,030329975	6,603161896
0,061451912	6,674072474
0,077583715	6,782663179
0,092285206	6,780156683
0,123645712	7,036342097
0,248010997	6,958253552
0,311190013	6,808896974
0,374459999	6,728156367
0,438001613	6,652385255
0,501342733	6,492604755
0,562576254	6,378341272
0,623692121	6,200712971
0,684872918	6,168285288
0,745761671	6,014719347
0,868462171	5,711260645
0,89880612	5,562970835
0,929411958	5,474287392
0,991040922	5,269364125

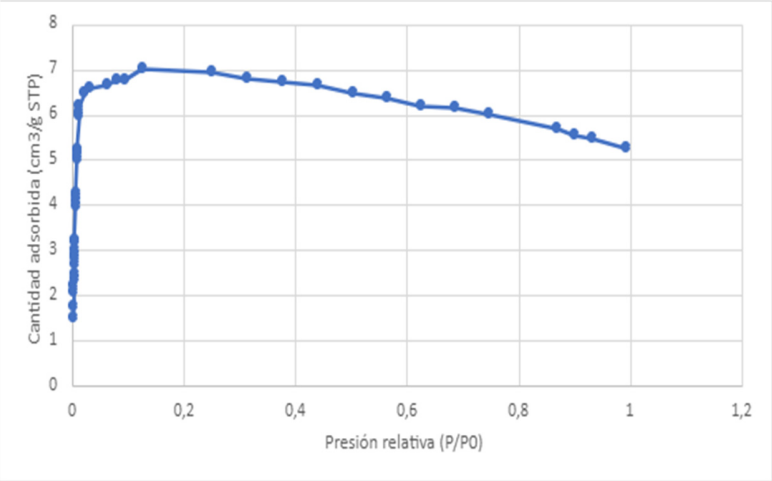


Figure SI-11. ADSORPTION ISOTHERM A3

Table SI-12. BET Report A3

BET Report

BET Surface Area:	22.8268 ± 0.8259 m²/g
Slope:	0.203733 ± 0.007172 g/cm³ STP
Y-Intercept:	-0.003638 ± 0.000989 g/cm³ STP
C:	-54.999087
Qm:	4,9976 cm³/g STP
Correlation Coefficient:	0.9981463
Molecular Cross-Sectional Area:	0.1700 nm²

A3 AEROGEL 7-6-2023		Not Fitted	
Relative Pressure (P/Po)	1/[Q(Po/P - 1)]	Relative Pressure (P/Po)	1/[Q(Po/P - 1)]
0,061451912	0,009810428		
0,077583715	0,012400619		
0,092285206	0,014994878		
0,123645712	0,020051727		
0,248010997	0,047397911		

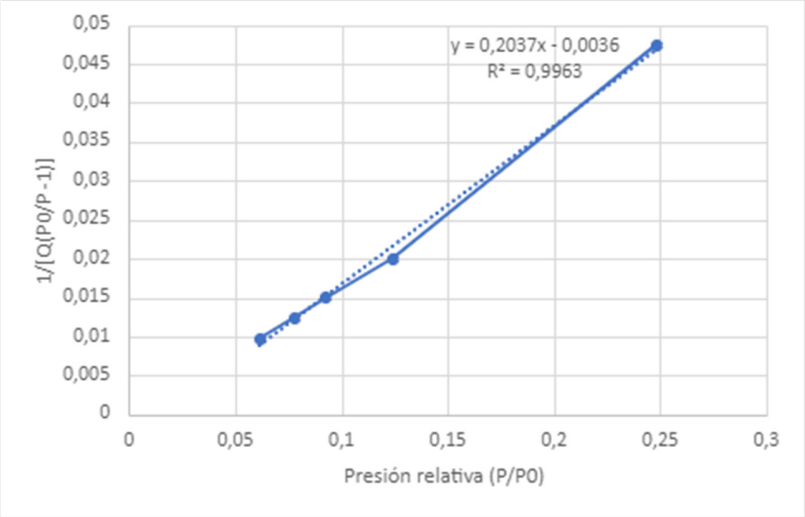


Figure SI-12. ADSORPTION ISOTHERM A3 IN BET COORDINATES

Table SI-13. Langmuir Report A3

Langmuir Report			
Langmuir Surface Area:	28,9786 ± 0,4361 m²/g		
Slope:	0,157617 ± 0,002372 g/cm³ STP		
Y-Intercept:	-1,036 ± 0,609 mmHg·g/cm³ STP		
b:	-0,152151 1/mmHg		
Qm:	6,3445 cm³/g STP		
Correlation Coefficient:	0.998757		
Molecular Cross-Sectional Area:	0.1700 nm²		
A3 AEROGEL 7-6-2023		Not Fitted	
Pressure (mmHg)	P/Q (mmHg·g/cm³ STP)	Pressure (mmHg)	P/Q (mmHg·g/cm³ STP)
15,75003906	2,432270506		
23,05078125	3,490870225		
46,70345306	6,997744368		
58,96362305	8,693284849		
70,1367569	10,34441535		
93,97074127	13,35505579		
188,4883575	27,08845778		
236,5044098	34,73461424		

284,5895996	42,29830344
332,8812256	50,03937878
381,0204773	58,685303
427,5579529	67,03278088
474,006012	76,4437919

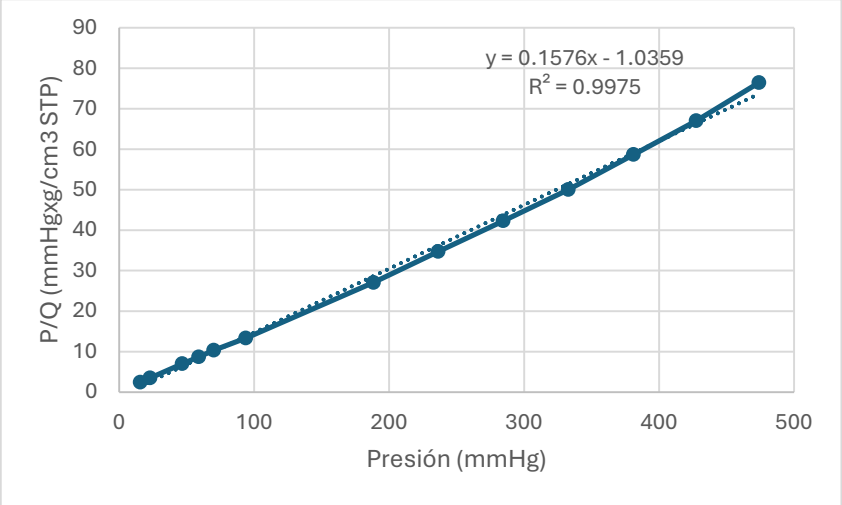


Figure SI-13. ADSORPTION ISOTHERM A3 IN LANGMUIR COORDINATES

Table SI-14. Freundlich Report A3

Freundlich Tabular Report	
Qm·C:	3.1092 ± 0.0854 cm³/g STP
m:	7.4617 ± 0.9322
Correlation Coefficient:	0.784644

Freundlich Plot

A3 AEROGEL 7-6-2023	
log(P)	log(Q)
-0,194489461	0,17781192
-0,133763793	0,245409877

-0,060168886	0,320042725
-0,038829454	0,346702723
-0,008725713	0,372768579
0,013464256	0,39693545
0,039669936	0,428240566
0,057428562	0,450966747
0,071725108	0,465929672
0,085134088	0,481410029
0,106129009	0,502881413
0,125062014	0,508392154
0,45108956	0,602249102
0,456268327	0,613774096
0,46043618	0,624745187
0,465785256	0,631429721
0,672743914	0,70018474
0,673178067	0,707114588
0,676204826	0,718033278
0,684496866	0,717316236
0,910394734	0,776712793
0,911176645	0,781258885
0,91215742	0,792585908
1,197282399	0,811270525
1,362685649	0,819751945
1,669348992	0,824390918
1,770584161	0,831400251
1,84594568	0,83123973
1,972992653	0,847346946
2,27528453	0,84250025
2,373839243	0,833076763
2,454219025	0,827896076
2,522289302	0,822977392
2,580948317	0,812418965
2,630994989	0,804707752
2,67578385	0,792441628
2,716423586	0,790164452
2,753413651	0,779215368
2,819564498	0,756731981
2,834479613	0,745306783
2,849021848	0,738327593

2,87690518 0,72175821

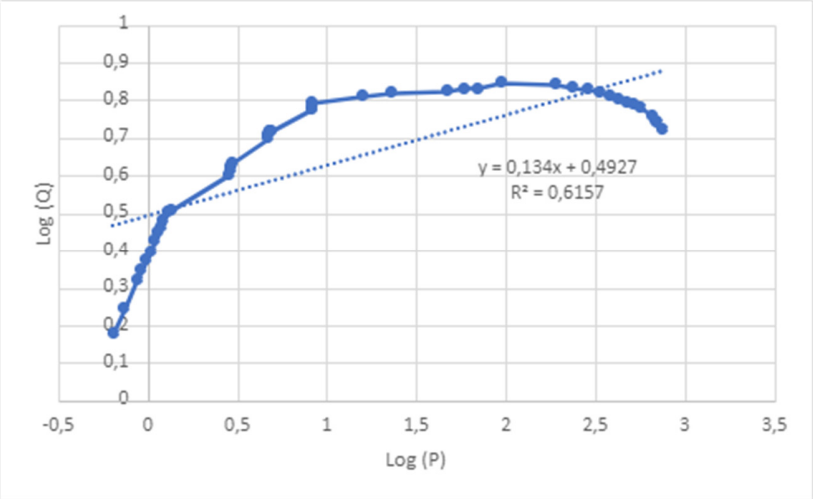


Figure SI-14. ADSORPTION ISOTHERM A3 IN FREUNDLICH COORDINATES

Table SI-15. Temkin Report A3

Temkin Tabular Report	
q·alpha/Qm:	1.165734 ± 0.134397 kJ/mol·(cm³/g STP)
A:	441.9475 ± 365.2043 1/mmHg
Correlation Coefficient:	0.808012

Temkin Plot

A3 AEROGEL 7-6-2023

ln(P)	Quantity Adsorbed (cm³/g STP)
-0,447828534	1,50595474
-0,308002517	1,759583486
-0,138543981	2,089506069
-0,089408121	2,221788543

-0,020091629	2,359220747
0,031002595	2,494223976
0,091343404	2,680652791
0,132234151	2,824663685
0,165153165	2,923678887
0,196028483	3,02977257
0,244371074	3,183328175
0,287965929	3,223978629
1,038672096	4,001742153
1,050596649	4,109359115
1,060193485	4,214491544
1,072510188	4,27986156
1,549050108	5,014004735
1,550048828	5,094652748
1,557019151	5,224362188
1,57611228	5,215743632
2,096261344	5,98015985
2,09806176	6,04308754
2,100320078	6,202773293
2,756844604	6,475458514
3,137699663	6,603161896
3,843818103	6,674072474
4,076920695	6,782663179
4,250447006	6,780156683
4,542983471	7,036342097
5,239036241	6,958253552
5,465966854	6,808896974
5,651048141	6,728156367
5,807785746	6,652385255
5,94285312	6,492604755
6,058089841	6,378341272
6,161220005	6,200712971
6,254796455	6,168285288
6,339969227	6,014719347
6,492287182	5,711260645
6,526630504	5,562970835
6,560115238	5,474287392
6,624318982	5,269364125

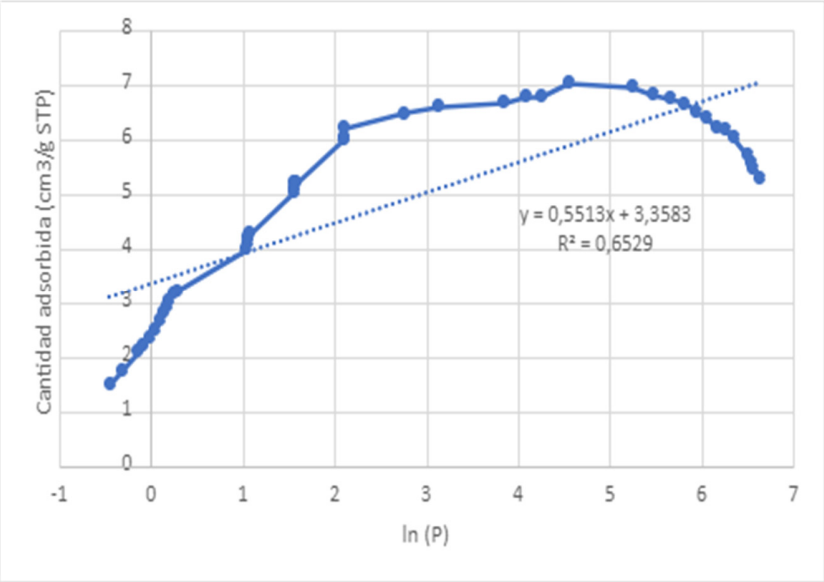


Figure SI-15. ADSORPTION ISOTHERM A3 IN TEMKIN COORDINATES

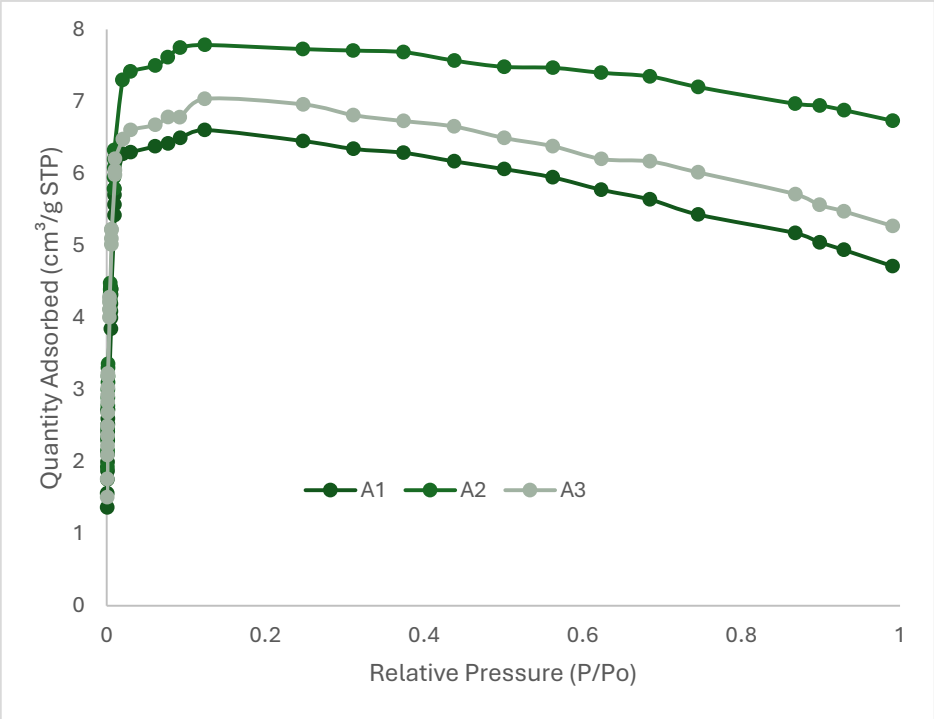


Figure SI-16. ADSORPTION ISOTHERM A1, A2 AND A3