

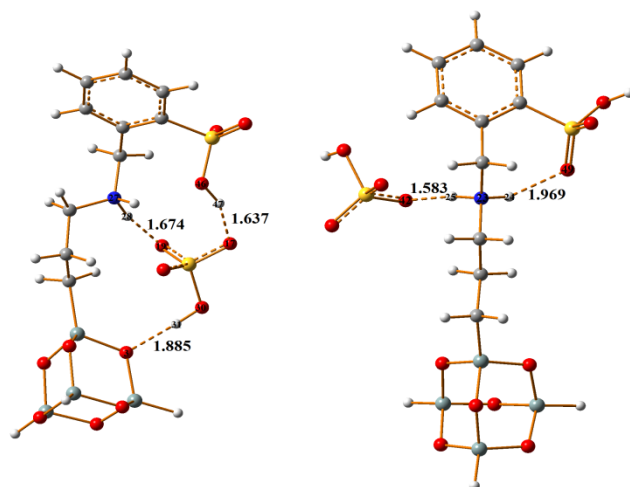
A study on catalytic activity and theoretical modeling of a novel dual acidic mesoporous silica

*Majid Vafaezadeh and Alireza Fattahi**

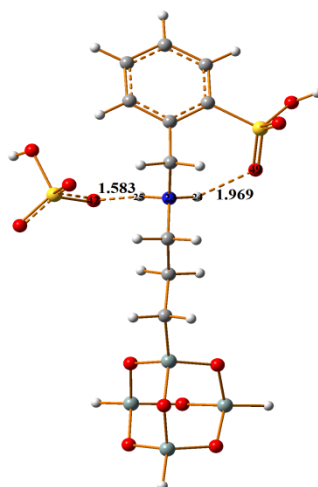
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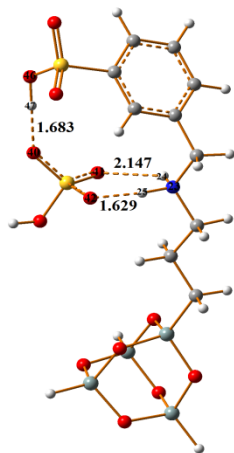
Fig 1S: Optimized structures of O2-3, M2-3 and P2,3.



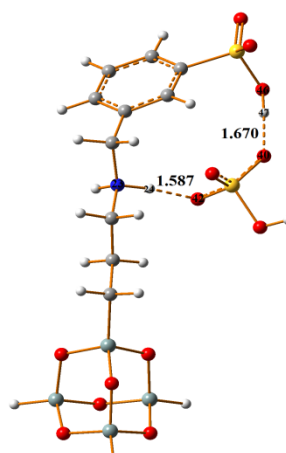
O2



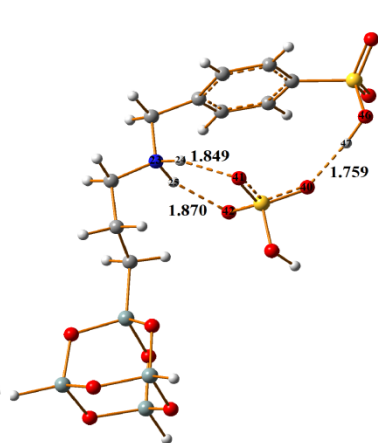
O3



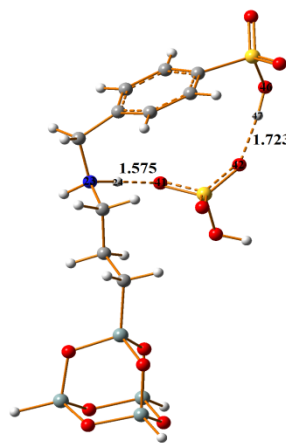
M2



M3



P2



P3

Table 1: Total energy and significant H bonds length of **O2-3**, **M2-3** and **P2,3** (in Å)

Structure	Total energy ^a	(H-bonds)	r _{H...O} ^b
O2	-3380.195640	lp O ₁₇ →σ*H ₄₇ -O ₄₆	1.637
		lp O ₁₉ →σ*H ₂₈ -N ₂₇	1.674
		lp O ₃ →σ*H ₃₁ -O ₃₀	1.885
O3	-3380.188915	lp O ₄₉ →σ*H ₂₄ -N ₂₃	1.969
		lp O ₄₂ →σ*H ₂₅ -N ₂₃	1.583
M2	-3380.198430	lp O ₄₀ →σ*H ₄₇ -O ₄₆	1.683
		lp O ₄₁ →σ*H ₂₄ -N ₂₃	2.147
		lp O ₄₂ →σ*H ₄₅ -N ₂₃	1.629
M3	-3380.196964	lp O ₄₀ →σ*H ₄₇ -O ₄₆	1.670
		lp O ₄₂ →σ*H ₂₄ -N ₂₃	1.587
P2	-3380.192291	lp O ₄₀ →σ*H ₄₇ -O ₄₆	1.759
		lp O ₄₁ →σ*H ₂₄ -N ₂₃	1.849
		lp O ₄₂ →σ*H ₂₅ -N ₂₃	1.870
P3	-3380.186811	lp O ₄₂ →σ*H ₄₇ -O ₄₆	1.723
		lp O ₄₁ →σ*H ₂₄ -N ₂₃	1.575

^a The total energies are reported in atomic unit. ^b r_{H...O} is the length of H bonds that are reported in Å.

XYZ coordinates

O1

0 1

H	-6.31183300	1.87497000	-1.00525000
Si	-5.48625700	0.81087300	-0.44552500
O	-3.92731400	0.78404700	-1.04286600
O	-6.08704000	-0.72246600	-0.73886100
O	-5.31687500	0.89795400	1.21455600
Si	-5.22315900	-2.01991300	-0.13956700
H	-5.82689800	-3.31252000	-0.44707900
Si	-2.88395400	-0.38974900	-0.47128400
Si	-4.39331800	-0.27455800	1.96464200
H	-4.30757600	-0.11156500	3.41177800
O	-5.07372500	-1.72950300	1.49877200
O	-3.68043500	-1.84214700	-0.75601900
O	-2.91238100	-0.22479100	1.19550600
C	-1.18819700	-0.33275000	-1.20169400
H	-1.30269900	-0.32120500	-2.29197600
H	-0.75871300	0.63320900	-0.91784900
C	-0.29363400	-1.50874700	-0.76221800
H	-0.14915100	-1.49035500	0.32324600
H	-0.78763900	-2.45858300	-0.98815800
C	1.07263800	-1.55356700	-1.44752500
H	0.97012300	-1.54506000	-2.53576200
H	1.61312300	-2.45772300	-1.15922900
N	1.92782800	-0.38753600	-1.07364000
H	1.53310100	0.53387600	-1.39239700
H	1.97902000	-0.29772000	-0.03751400
C	3.33819600	-0.41252300	-1.61100300
H	3.68315600	0.61996700	-1.57670800
H	3.27112000	-0.70882300	-2.65764700
C	4.29363100	-1.32701700	-0.87620600
C	6.22325900	-3.00653400	0.31365800
C	4.77308300	-1.08378800	0.42740300
C	4.81233100	-2.43310400	-1.55405200
C	5.76403100	-3.26915900	-0.97100100
C	5.72520200	-1.90962500	1.01498000
H	4.47598600	-2.63349800	-2.56579400
H	6.14639000	-4.11732800	-1.52664200
S	1.40516000	3.19103100	-0.62681100
O	0.22338700	2.48616000	0.31329800
H	0.08879300	3.02262300	1.10790100
O	2.61722400	3.21476200	0.25590500
O	0.94466700	4.50728000	-1.01887900
O	1.50611900	2.17071600	-1.70368300

H	6.06921400	-1.68375100	2.01624900
H	6.96810100	-3.64509100	0.77317400
S	4.11971100	0.24440100	1.46665400
O	4.40265900	1.51120600	0.57454300
H	3.61109800	2.20275800	0.48942800
O	2.65714700	0.03179000	1.54845000
O	4.87568300	0.27617000	2.70283800

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2 3 1.0 4 1.0 5 1.0
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38 39 1.0

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45 46 1.0 48 2.0 49 2.0
46 47 1.0
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O2

0 1

H	-4.52946400	-2.92139300	0.38519900
Si	-4.46464400	-1.46603600	0.32109400
O	-3.01170300	-0.91273300	-0.33222100
O	-4.58877000	-0.71393900	1.80217900
O	-5.65097800	-0.77706800	-0.62627300
Si	-4.51211500	0.95340100	1.84469400
H	-4.64050100	1.51165800	3.18600900
Si	-2.79382200	0.76494100	-0.45339200
Si	-5.65321100	0.88747400	-0.77593700
H	-6.73070600	1.39364700	-1.61906300
O	-5.70220400	1.46917000	0.79007400
O	-3.07221200	1.33716300	1.09268600
O	-4.12770000	1.26781800	-1.33547200
C	-1.19180300	1.32958600	-1.19494000
H	-0.75500300	0.45299000	-1.68238900
S	0.40321700	-2.00814100	-0.32246000
O	1.44907000	-2.98670100	0.04367900
O	0.14735600	-0.97300300	0.70395500
O	0.64733000	-1.36786900	-1.66052700
H	-1.44464100	2.04008300	-1.98976200
C	-0.20076400	1.96979400	-0.19680300
H	-0.55443100	2.96633200	0.08172800
H	-0.15290000	1.38545600	0.72303700
C	1.21635900	2.13756900	-0.75254800
H	1.80350500	2.80022000	-0.11406200
H	1.20135100	2.55637200	-1.76200400
N	1.95834600	0.83436300	-0.83595700
H	1.39426400	0.09614800	-1.34409400
H	2.04192900	0.42004800	0.10189000
O	-0.94583600	-2.88479800	-0.47566900
H	-1.69282300	-2.24855500	-0.50603400
C	3.32819000	0.89059700	-1.47562900
H	3.25007600	1.57029600	-2.32429400
H	3.53227700	-0.10904400	-1.85591200
C	4.41050700	1.35250900	-0.52602500
C	6.41160700	2.29275800	1.22101400
C	5.11458200	0.47349600	0.31900300
C	4.75197200	2.70695400	-0.47743300
C	5.73966300	3.17837600	0.38633600
C	6.10088200	0.93456400	1.18428700
H	4.24549400	3.40305300	-1.13779200
H	5.98474800	4.23395600	0.39844900
H	6.61768100	0.22494700	1.81777600
H	7.18145900	2.64989100	1.89453000

S	4.84894300	-1.31867100	0.28296700
O	3.31036600	-1.30568600	0.75819200
H	2.76035500	-2.12325000	0.50706900
O	4.92676200	-1.78624200	-1.09711800
O	5.69230100	-1.92468200	1.29768300

O3

0 1

H	6.60721600	-1.36530600	2.43055200
Si	5.72594600	-1.02145800	1.31966200
O	4.13367200	-0.80008600	1.77571500
O	5.67583900	-2.19019100	0.12507100
O	6.16021200	0.38639900	0.53385100
Si	4.69934600	-1.89815600	-1.19980800
H	4.72537700	-2.97306500	-2.18648400
Si	3.02745200	-0.39821200	0.58341900
Si	5.21852300	0.87783600	-0.75794700
H	5.67993700	2.11496800	-1.37674100
O	5.20735100	-0.42717200	-1.80425700
O	3.18052400	-1.61308700	-0.56493200
O	3.66575700	0.95953800	-0.15441900
C	1.29698500	-0.18669000	1.19663000
H	1.03705100	-1.09280700	1.75665800
H	1.29697200	0.63825200	1.91749200
C	0.27327300	0.07936600	0.07660900
H	0.52435300	1.00483100	-0.44925100
H	0.30784300	-0.73194900	-0.65901200
C	-1.14154800	0.19771700	0.64164000
H	-1.21396100	1.01973900	1.35509200
H	-1.45311600	-0.73205600	1.12180000
N	-2.11129300	0.50920500	-0.45780700
H	-1.79727200	1.44246500	-0.90027100
H	-2.09071600	-0.23507700	-1.16210900
C	-3.54243800	0.72804800	-0.04004800
H	-4.10908800	0.86963000	-0.96177500
H	-3.54504300	1.67064700	0.50575400
C	-4.13240900	-0.36616100	0.82430300
C	-5.26244400	-2.29395800	2.54949100
C	-4.60451200	-1.60238700	0.34250900
C	-4.25774400	-0.12974100	2.19621800
C	-4.81368800	-1.07792300	3.05258900
C	-5.16468700	-2.55895400	1.18562300
H	-3.91637000	0.82083900	2.59072300
H	-4.89604300	-0.86152200	4.11114200
S	-1.56119300	3.91193100	-0.15719100
O	-2.91095900	4.76316200	-0.62453900
H	-2.63717600	5.40004100	-1.29925400
O	-0.47284600	4.87683400	-0.06423900
O	-1.36634500	2.89385000	-1.25592000
O	-2.01976800	3.25947700	1.08415200
H	-5.50956000	-3.50089600	0.78384800
H	-5.69408600	-3.03738800	3.20870700

S	-4.52966000	-1.91418700	-1.42794300
O	-5.59941100	-1.22224100	-2.13243000
O	-3.14777100	-1.73517500	-1.86196400
O	-4.85439100	-3.51571200	-1.49439300
H	-5.60099800	-3.64047300	-2.10160400

M1

0 1

H	-5.78009800	0.18332700	3.22333800
Si	-5.11332700	-0.01832800	1.94230600
O	-3.89120600	1.09165400	1.64953100
O	-6.13179200	0.11303500	0.62480800
O	-4.38776700	-1.51282100	1.78814500
Si	-5.47541500	-0.10766800	-0.89584600
H	-6.44354300	0.02159200	-1.97827400
Si	-3.05903100	0.96118500	0.20998700
Si	-3.59622000	-1.87253500	0.36087100
H	-2.99380000	-3.19770900	0.33237500
O	-4.71976000	-1.59316100	-0.83840700
O	-4.22346800	1.00217400	-0.98393300
O	-2.47602300	-0.62069500	0.20156000
C	-1.68701000	2.18453800	-0.02203200
H	-2.05014000	3.18319100	0.24157000
H	-0.94037800	1.91405200	0.73395400
C	-1.09447500	2.17341400	-1.44911800
H	-0.96717700	1.15291500	-1.81928700
H	-1.79741400	2.65689400	-2.13213300
C	0.24438300	2.90203200	-1.57945500
H	0.19815900	3.91040500	-1.15874800
H	0.53387500	2.97802700	-2.62920700
N	1.34837800	2.16039300	-0.89035100
H	1.10290200	1.98398900	0.08580900
H	1.42902900	1.17057200	-1.33075500
C	2.69893200	2.82892000	-0.94718700
H	2.56334700	3.88225000	-0.69511500
H	3.03169000	2.75934500	-1.98435500
C	3.66338000	2.16303800	0.00219000
C	5.35610500	0.87629600	1.82944800
C	4.14268700	0.87968600	-0.27463800
C	4.05359600	2.80395200	1.18271100
C	4.90451300	2.16862500	2.08541100
C	4.96323200	0.24706400	0.65130600
H	3.69843800	3.80733900	1.39589200
H	5.21119400	2.67817500	2.99117100
S	0.98548200	-1.36756900	-1.20610600
O	0.31702000	-0.58757400	0.11665900
H	-0.63495900	-0.81542400	0.15091800
O	1.55147300	-0.19466600	-1.96460400
O	-0.12287800	-2.03878400	-1.87262400
O	2.04075100	-2.23022500	-0.65794300
H	6.00927100	0.35868400	2.52077900
S	5.49390000	-1.44665900	0.31812000

O	6.58412600	-1.75626100	1.22492600
O	4.23883400	-2.30239200	0.83019700
H	3.45819100	-2.25743200	0.20922100
O	5.63844700	-1.57968700	-1.12364200
H	3.86445300	0.36738100	-1.18858700

M2

0 1

H	-7.91708800	1.29479800	-0.73115400
Si	-6.67271900	0.62717400	-0.36516200
O	-5.30621700	1.52481400	-0.72038200
O	-6.44473500	-0.83464800	-1.13966900
O	-6.55293900	0.28335900	1.26509600
Si	-5.05133900	-1.69173600	-0.79294100
H	-4.94829500	-2.95358100	-1.51666900
Si	-3.81972500	0.85430200	-0.34277200
Si	-5.16860300	-0.48729300	1.79901800
H	-5.16241300	-0.74520600	3.23435600
O	-5.05223300	-1.86799400	0.86770700
O	-3.80387800	-0.62741500	-1.11778200
O	-3.91248200	0.49032500	1.28764000
C	-2.38591700	1.94220000	-0.77414600
H	-2.43526300	2.13583700	-1.85187300
H	-2.55188700	2.90529200	-0.27707700
C	-1.01688700	1.35294200	-0.38711600
H	-0.98480100	1.14315400	0.68610500
H	-0.85602200	0.39821200	-0.89435400
C	0.11280700	2.31556700	-0.75274500
H	-0.00005200	3.27288900	-0.23687800
H	0.13131600	2.50918000	-1.82801000
N	1.45267700	1.75668900	-0.38802100
H	1.47835800	1.49618900	0.60806500
H	1.57096000	0.80209000	-0.84410800
C	2.62015400	2.64548100	-0.73275700
H	2.37851000	3.65224200	-0.38826000
H	2.68389200	2.66124900	-1.82275800
C	3.90002400	2.15674000	-0.10120000
C	6.23680100	1.22015700	1.13547200
C	4.50127200	0.97595700	-0.54710400
C	4.48283200	2.86830600	0.95103900
C	5.65088000	2.40913500	1.55817100
C	5.64660200	0.51458800	0.08942400
H	4.02692000	3.79048200	1.29717200
H	6.09972500	2.97536200	2.36551600
S	1.81827400	-1.47322200	0.23690400
O	0.52793600	-2.48406300	0.31918300
H	0.75529400	-3.30215300	-0.14635100
O	2.99721300	-2.35104000	0.35052500
O	1.58487300	-0.52150900	1.33489200
O	1.72386200	-0.79892000	-1.10095600
H	7.14016400	0.84204600	1.59759800
S	6.34731800	-1.06684400	-0.42458400

O	7.75621900	-1.07286000	-0.07776500
O	5.64833500	-2.09461000	0.59205300
H	4.67032000	-2.18828900	0.42858200
O	5.89673700	-1.31937700	-1.78566500
H	4.08263300	0.40524800	-1.36811700

M3

0 1

H	6.33289100	2.75651500	1.61266200
Si	5.89579900	1.49588100	1.02237900
O	4.50291700	1.63817600	0.10657500
O	5.55504400	0.31265900	2.14957900
O	7.02162900	0.81395400	-0.00575600
Si	5.04504600	-1.17660600	1.58467000
H	4.77723300	-2.14174300	2.64416900
Si	3.90916300	0.25108300	-0.62625700
Si	6.62897100	-0.63626000	-0.73885100
H	7.67701300	-1.15204600	-1.61214700
O	6.23365000	-1.66445200	0.51619400
O	3.71835700	-0.83855500	0.62692400
O	5.18524100	-0.33900900	-1.53017500
C	2.36189000	0.54456600	-1.59743000
H	2.57891200	1.33391400	-2.32652600
H	2.14992300	-0.36357000	-2.17186400
C	1.15013900	0.91904500	-0.72312600
H	0.91167200	0.09559000	-0.04459600
H	1.39274400	1.79101800	-0.10390300
C	-0.07560200	1.22830800	-1.58004200
H	-0.34617600	0.37866900	-2.20896700
H	0.08634600	2.10449600	-2.21334500
N	-1.27787200	1.49143300	-0.71993700
H	-1.48965600	0.58404300	-0.18847000
H	-1.05349900	2.19017300	-0.00945400
C	-2.50301900	1.93949900	-1.48887400
H	-2.63567200	1.20593800	-2.28254200
H	-2.26954900	2.91263900	-1.92617500
C	-3.71041200	1.99003700	-0.58928200
C	-5.86789000	1.96496000	1.20324100
C	-4.57358000	0.89488400	-0.54886900
C	-3.95563300	3.08838800	0.24352700
C	-5.03183000	3.07842800	1.12795400
C	-5.62644600	0.88683700	0.35859300
H	-3.31216200	3.96250900	0.19624600
H	-5.21928300	3.93625200	1.76286200
S	-2.25405300	-1.83737300	-0.40107100
O	-1.15501100	-3.05820800	-0.36243400
H	-1.59183600	-3.86328800	-0.67659000
O	-3.50717500	-2.42946800	0.10412400
O	-2.31665100	-1.33843900	-1.78782400
O	-1.62962500	-0.83335500	0.51205500
H	-6.70176900	1.92989300	1.89315800
S	-6.65939300	-0.58996000	0.45648700

O	-6.80452900	-1.10956200	-0.89498800
O	-5.74931800	-1.58515500	1.33079200
H	-4.95748500	-1.91678100	0.82746900
O	-7.81199600	-0.27931100	1.28138700
H	-4.42106800	0.05180500	-1.21207800

P1

0 1

H	-5.12603600	0.81312500	3.38581400
Si	-5.11602700	0.31631900	2.01524900
O	-4.01446200	1.08897900	1.02429700
O	-6.58343900	0.47366500	1.23143500
O	-4.73170400	-1.30708400	1.89392700
Si	-6.69274900	-0.06416100	-0.34501600
H	-8.01336800	0.11357400	-0.93715400
Si	-3.91710300	0.61340500	-0.57558000
Si	-4.69753600	-1.98447900	0.37051500
H	-4.35042500	-3.40183600	0.36688700
O	-6.19117100	-1.65895700	-0.29682000
O	-5.47618900	0.73780400	-1.16513600
O	-3.61600900	-1.04177400	-0.49834700
C	-2.66878000	1.55967000	-1.56226800
H	-2.85410300	1.37015600	-2.62568300
H	-2.90034900	2.61845900	-1.40515300
C	-1.18621200	1.31167200	-1.21025900
H	-0.56979500	2.08103700	-1.68334800
H	-1.02633700	1.41520800	-0.13292600
C	-0.70413400	-0.06571900	-1.67076100
H	-0.78464500	-0.16639600	-2.75632300
H	-1.28153800	-0.86963000	-1.21113800
N	0.73296800	-0.26929500	-1.31077600
H	1.32206800	0.51611400	-1.67605700
H	0.88209700	-0.12015200	-0.29175100
C	1.32756800	-1.59589600	-1.72590200
H	1.26104000	-1.64972300	-2.81391200
H	0.70121300	-2.37928600	-1.29646200
C	2.74764400	-1.66192700	-1.23092000
C	5.22618900	-1.24857400	-0.08022600
C	3.02038100	-2.16867700	0.04412100
C	3.76396500	-1.04541300	-1.96371100
C	5.00975500	-0.82619500	-1.38672400
C	4.26497300	-1.96629400	0.62707800
H	3.56659600	-0.66710600	-2.96086900
H	5.78523800	-0.28513400	-1.91303000
S	2.67220300	1.97401900	0.14083500
O	2.08508900	3.43089300	0.63564900
H	2.75416200	4.10392300	0.44440700
O	2.41374300	1.90408800	-1.32707800
O	1.83374000	1.01183500	0.88897200
O	4.10526500	1.99757400	0.48602000
H	2.24249500	-2.67209200	0.60868000
H	4.47248300	-2.30812500	1.63334700

S	6.68765800	-0.65590000	0.78689000
O	6.02440700	0.47803400	1.72642800
H	5.40490800	1.07191000	1.23166000
O	7.57209400	-0.04930000	-0.19711400
O	7.17182200	-1.67575000	1.69901100

P2

0 1

H	5.46854400	-2.46772900	2.41991500
Si	5.22781900	-1.50836700	1.34802700
O	3.77102100	-0.70143000	1.48681900
O	5.20165700	-2.19709500	-0.17347600
O	6.38268200	-0.30259100	1.25926700
Si	4.93733300	-1.19179300	-1.48110400
H	4.93500700	-1.88736900	-2.76297400
Si	3.38301700	0.41960300	0.30952000
Si	6.20967400	0.84987800	0.06247700
H	7.26593300	1.85672900	0.06651700
O	6.11578100	-0.01019400	-1.36636200
O	3.50491100	-0.40287800	-1.14163400
O	4.68098200	1.48637000	0.28953900
C	1.76557300	1.27639900	0.57186400
H	1.01870900	0.51621300	0.82240800
H	1.89214600	1.90683500	1.46102100
C	1.32145400	2.12667800	-0.63532400
H	2.13382800	2.78997600	-0.94878300
H	1.10492200	1.48040300	-1.49111200
C	0.12134300	3.03445300	-0.36200300
H	-0.05359500	3.70309600	-1.20788100
H	0.28794800	3.64828400	0.52687000
N	-1.15321500	2.27784600	-0.14360200
H	-1.36965900	1.66002600	-0.95710500
H	-1.04847200	1.54623000	0.59160100
C	-2.34990700	3.15006900	0.17441800
H	-2.41779400	3.89848000	-0.61666000
H	-2.13138200	3.65564700	1.11665000
C	-3.58661000	2.29730300	0.25298300
C	-5.52171300	0.32542300	0.24757900
C	-4.35936600	2.07872600	-0.89263800
C	-3.86908300	1.59328100	1.42527100
C	-4.83359100	0.59184400	1.42542800
C	-5.33609000	1.09140900	-0.90046200
H	-3.28886800	1.77186100	2.32405000
H	-5.01418000	-0.01441600	2.30340600
S	-1.67519100	-0.99340700	-0.29433100
O	-0.48045800	-2.04924700	-0.70041200
H	-0.57061900	-2.83547800	-0.14243800
O	-2.87122300	-1.82401300	-0.07132500
O	-1.71598900	-0.08457500	-1.46273300
O	-1.20096400	-0.28611200	0.93048600
H	-4.16247700	2.64159100	-1.79903200
H	-5.90778700	0.87841600	-1.79502500

S	-6.50105200	-1.18081000	0.14139800
O	-5.51414600	-2.09892900	-0.74973100
H	-4.57566500	-2.05968200	-0.43681200
O	-7.67119900	-0.95665200	-0.68732500
O	-6.62755500	-1.72397600	1.48562800

P3

0 1

H	-4.96066300	-2.56175000	-2.09684500
Si	-5.05534100	-1.50156300	-1.09996900
O	-3.57470500	-0.91809500	-0.59418600
O	-5.83982500	-1.96731100	0.30051100
O	-5.88834400	-0.15382500	-1.63621900
Si	-6.00907600	-0.83279100	1.51408200
H	-6.70848800	-1.33471100	2.69148900
Si	-3.55650700	0.29531200	0.55651300
Si	-6.06042500	1.12200900	-0.57275100
H	-6.80027700	2.24887200	-1.13159400
O	-6.77057200	0.46817600	0.79035600
O	-4.45758700	-0.29973600	1.83323900
O	-4.50332200	1.51369900	-0.10710700
C	-1.87141100	0.88326000	1.03617800
H	-2.01729400	1.66925200	1.78725700
H	-1.34367100	0.06190500	1.53142700
C	-1.02811600	1.39878700	-0.14427700
H	-0.78792600	0.56278900	-0.80565400
H	-1.59537400	2.13254900	-0.72989800
C	0.26662200	2.03537500	0.35598000
H	0.79997400	1.34172900	1.00488800
H	0.07230900	2.97223800	0.88393100
N	1.19004900	2.34174400	-0.79592500
H	1.53120100	1.39244500	-1.17257800
H	0.64742100	2.78520600	-1.53796900
C	2.39032500	3.22171200	-0.45891800
H	2.08501600	3.88283300	0.35353800
H	2.59083000	3.82908500	-1.34195800
C	3.58623200	2.37940900	-0.10831000
C	5.53449200	0.47305200	0.36196500
C	3.69805400	1.79065200	1.15324500
C	4.52480500	2.07515200	-1.10002100
C	5.51034600	1.12581100	-0.86792300
C	4.66499500	0.81849800	1.38967100
H	4.45656800	2.54494900	-2.07529200
H	6.21676500	0.85582800	-1.64291800
S	1.94268700	-1.23027300	-0.64440400
O	0.91862500	-2.23201100	-1.46043500
H	0.96533100	-3.10705900	-1.04874000
O	1.30166400	-0.90666300	0.64001700
O	1.98893700	-0.06010100	-1.57457500
O	3.20960200	-1.97532200	-0.53720700
H	3.00012900	2.04623200	1.94266700
H	4.72122500	0.29958000	2.33775600

S	6.59567900	-0.96799600	0.56499400
O	5.91514000	-1.98045600	-0.48793400
H	4.92697000	-2.01072900	-0.40485700
O	6.42517600	-1.44948300	1.92798200
O	7.91728200	-0.68923800	0.03325800

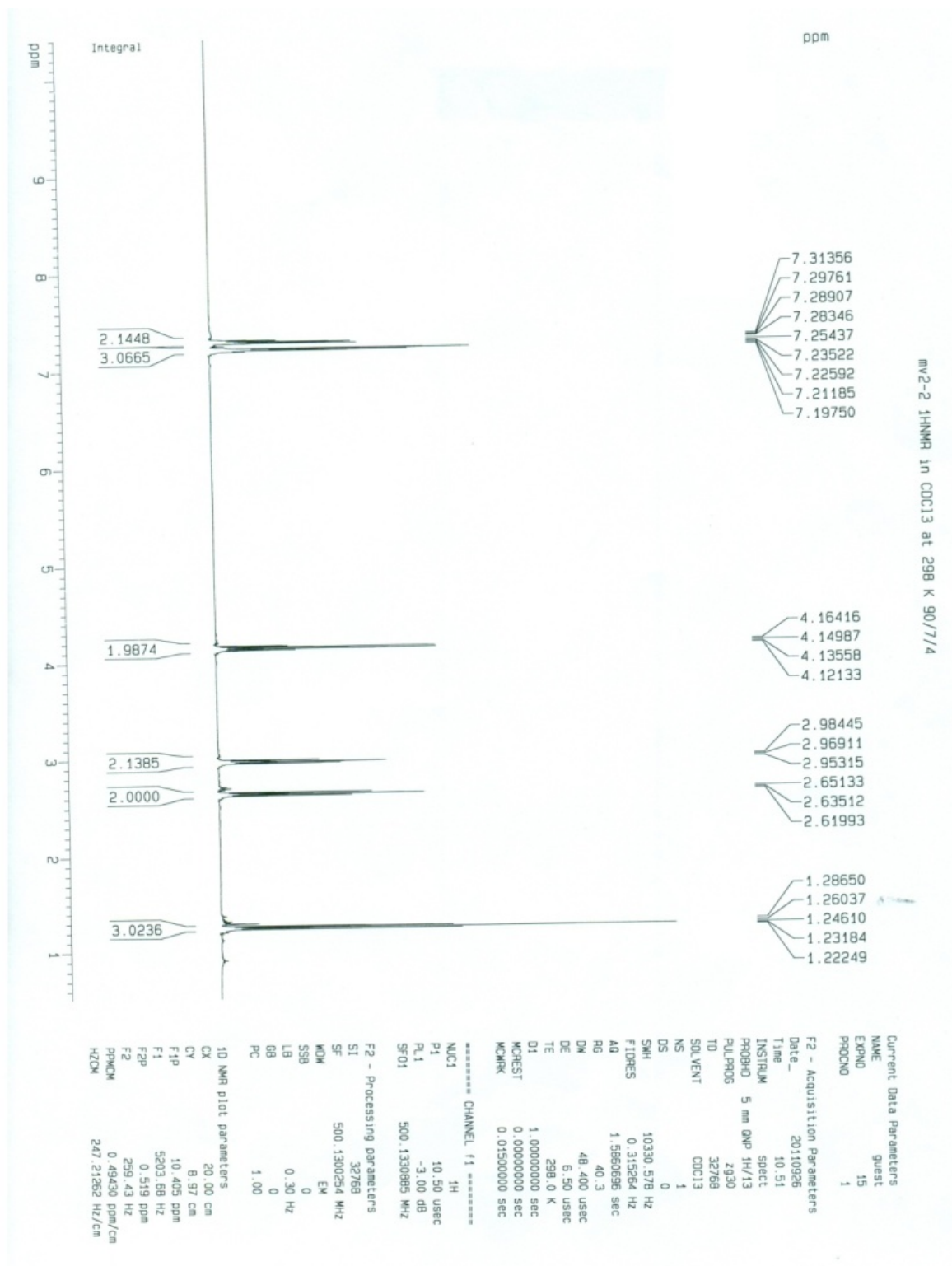


Fig 2S: ¹H NMR of the ethyl-(3-phenylpropionate)

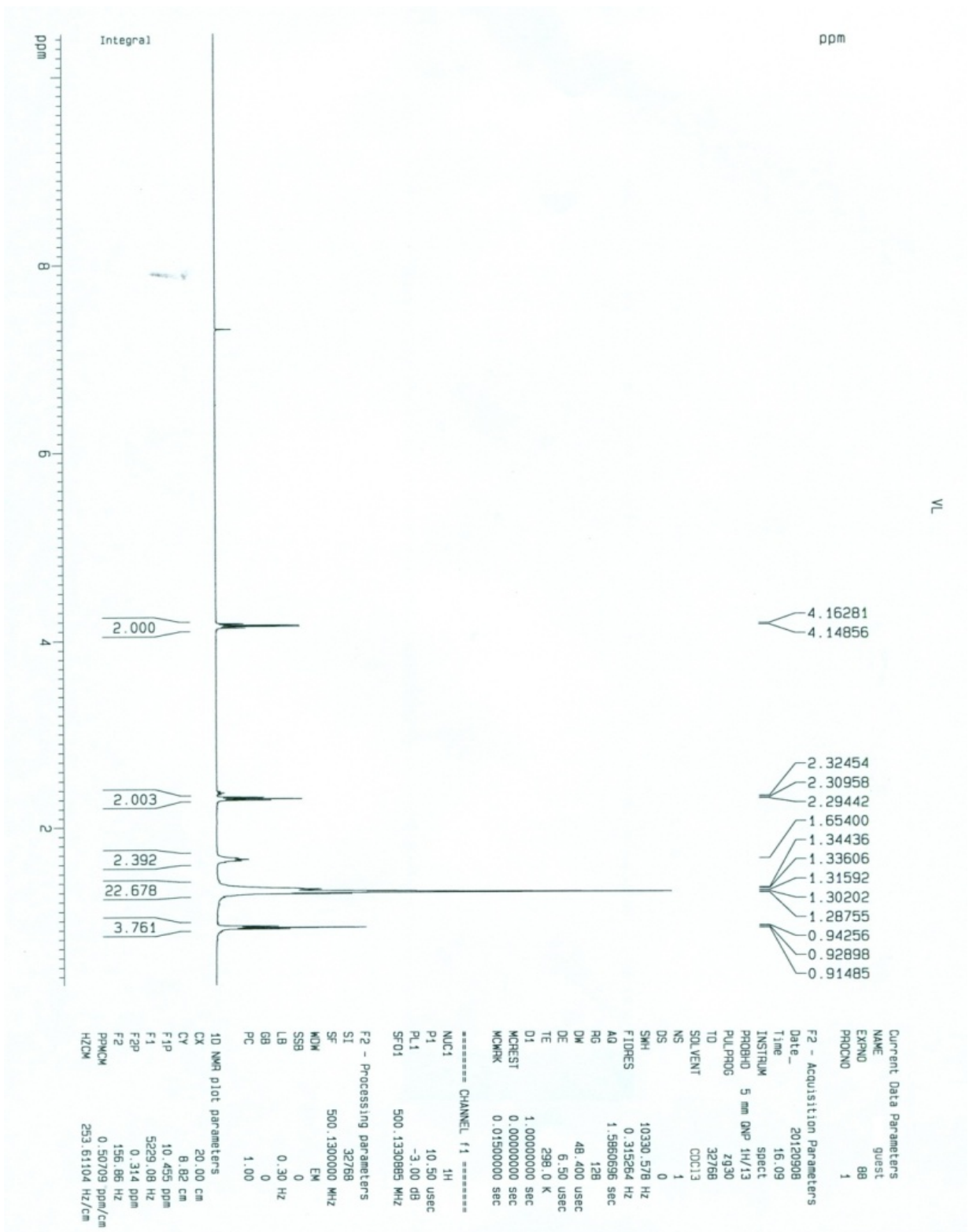


Fig 3S ¹H NMR of the ethyl laurate

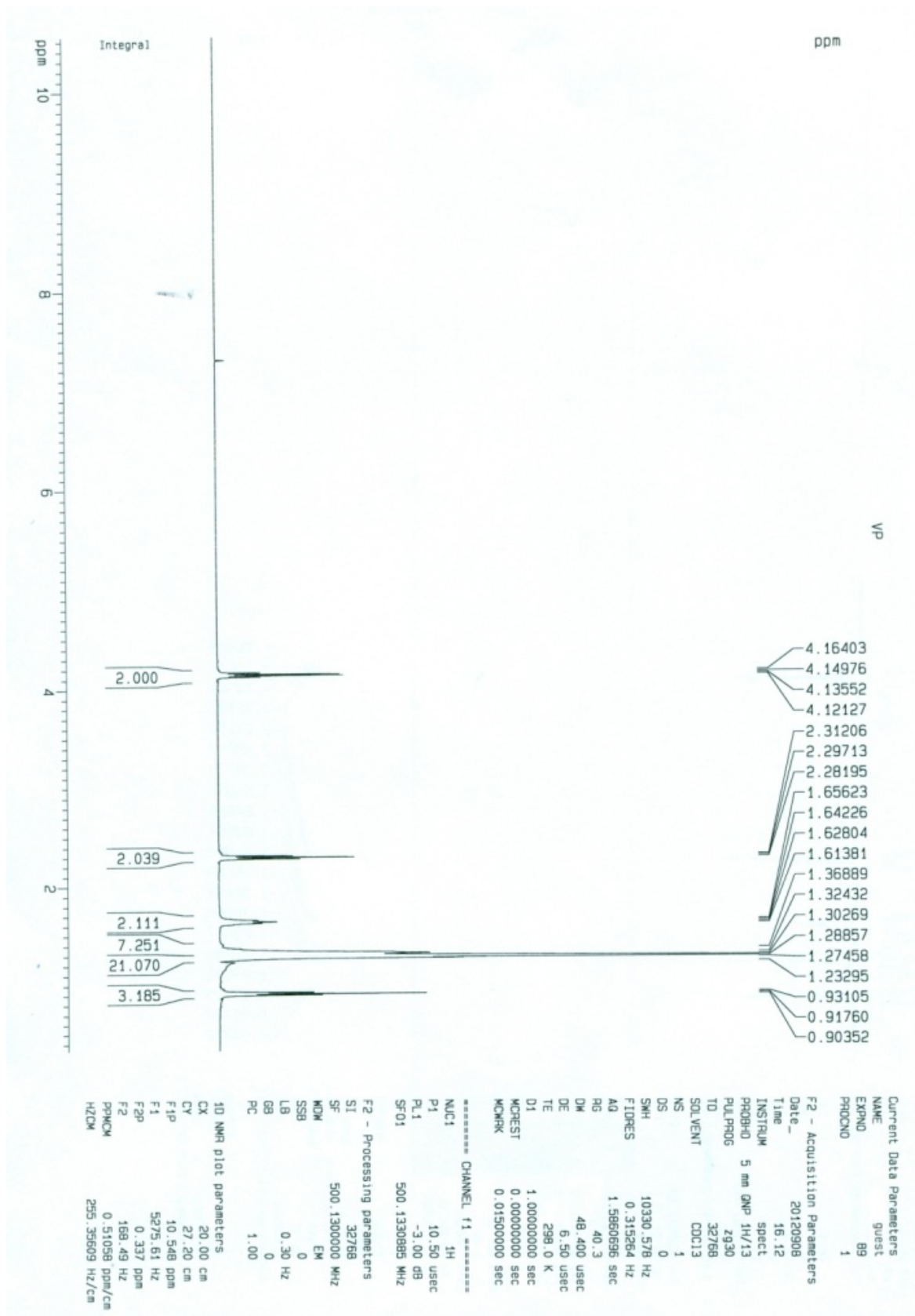


Fig 4S: ¹H NMR of the ethyl palmitate

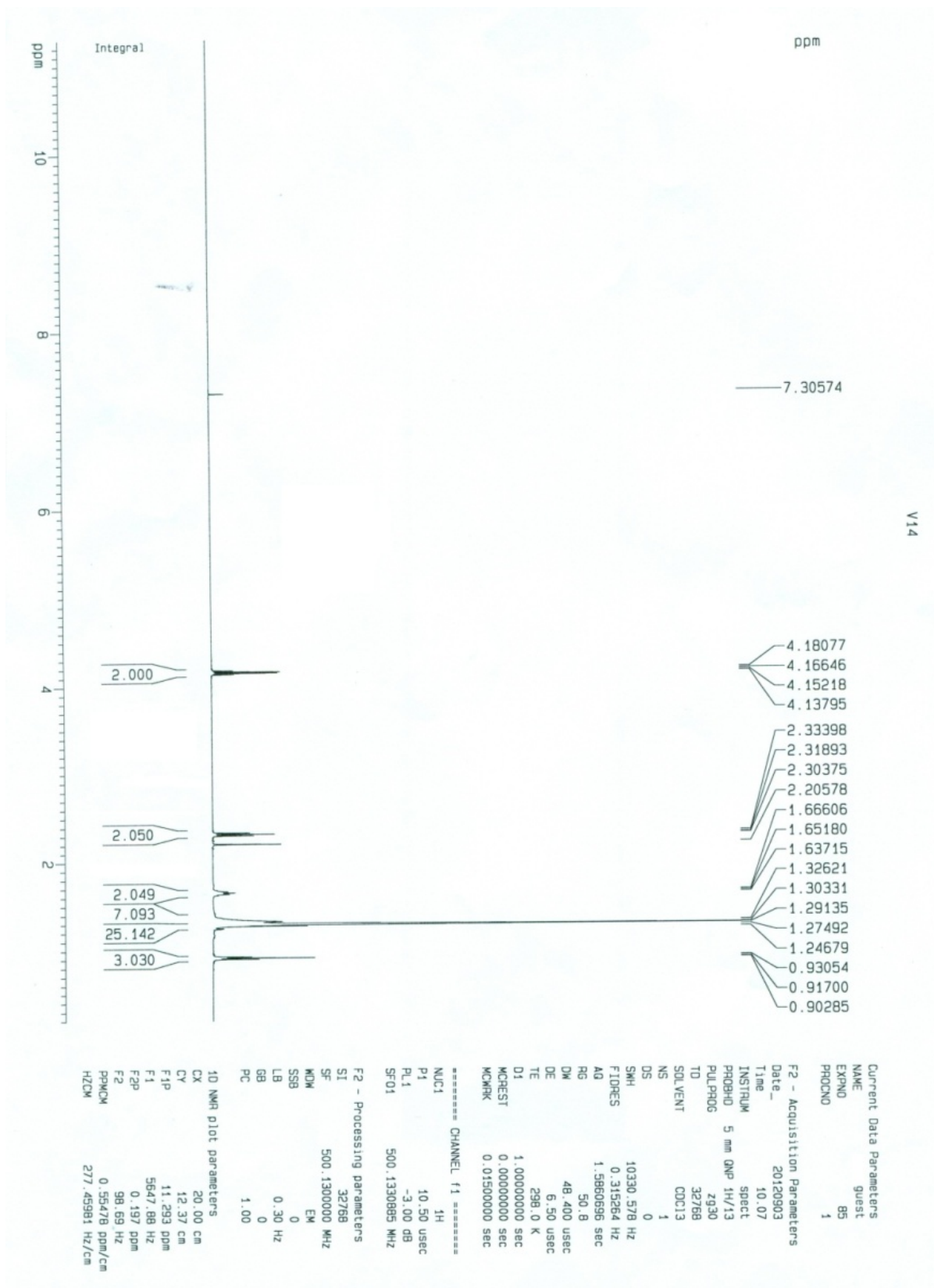


Fig 5S: ¹H NMR of the ethyl stearate