

Supplementary Information

Carboxylic Acids as Anchoring Component on Aluminum Oxide for the Alignment Relay Technique of Single-Walled Carbon Nanotubes

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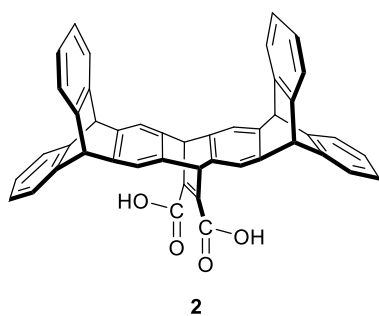
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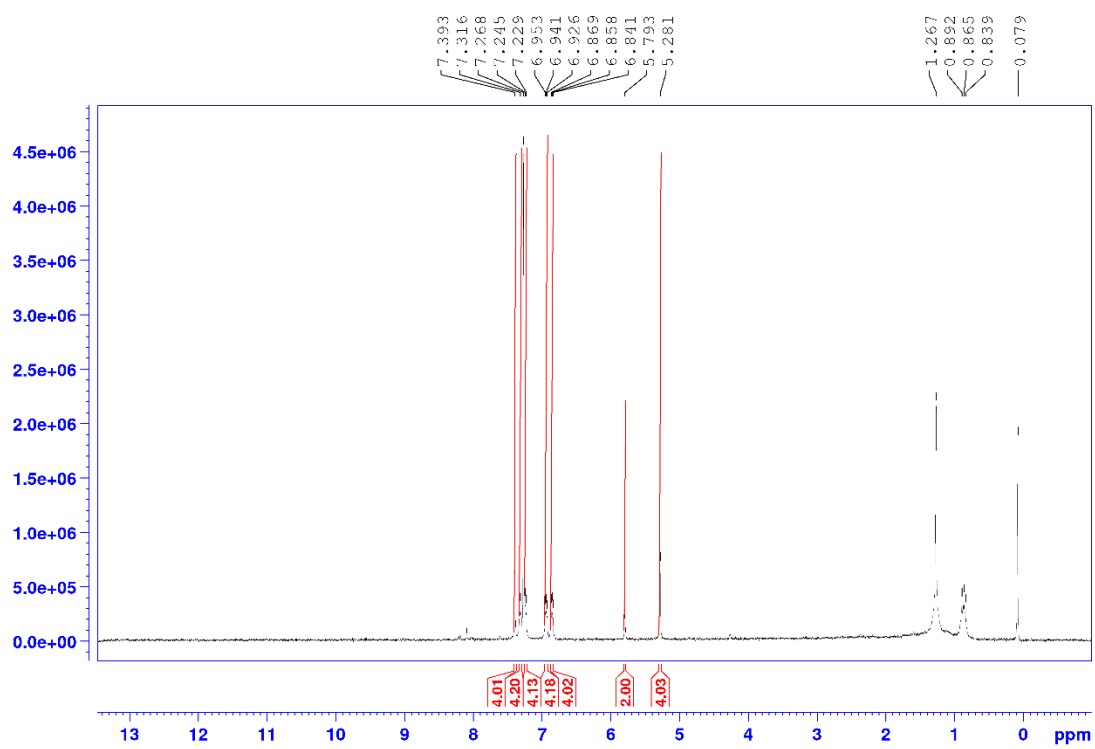
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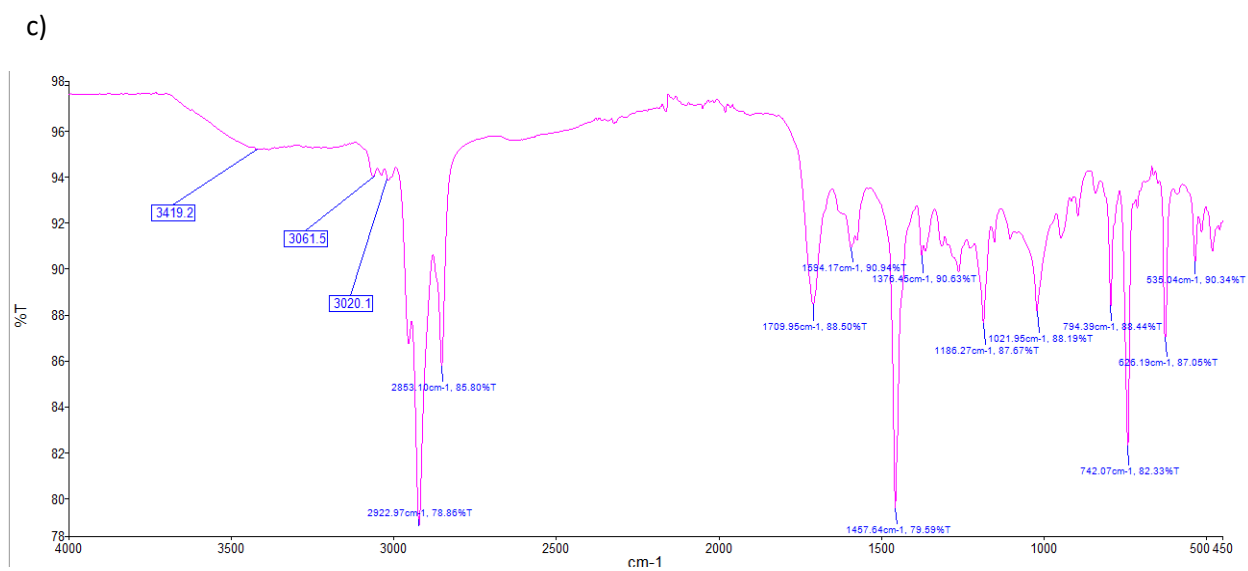
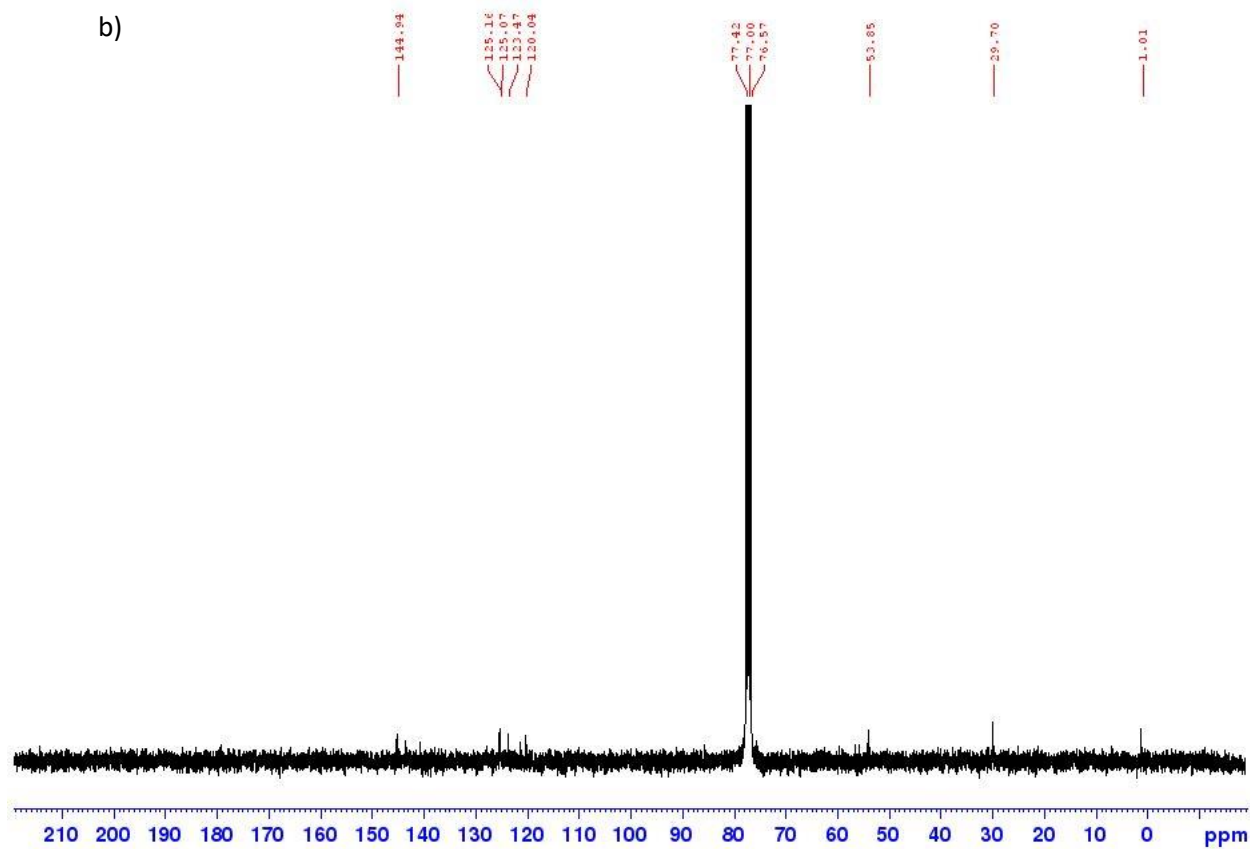
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Spectra for compound 2

a)





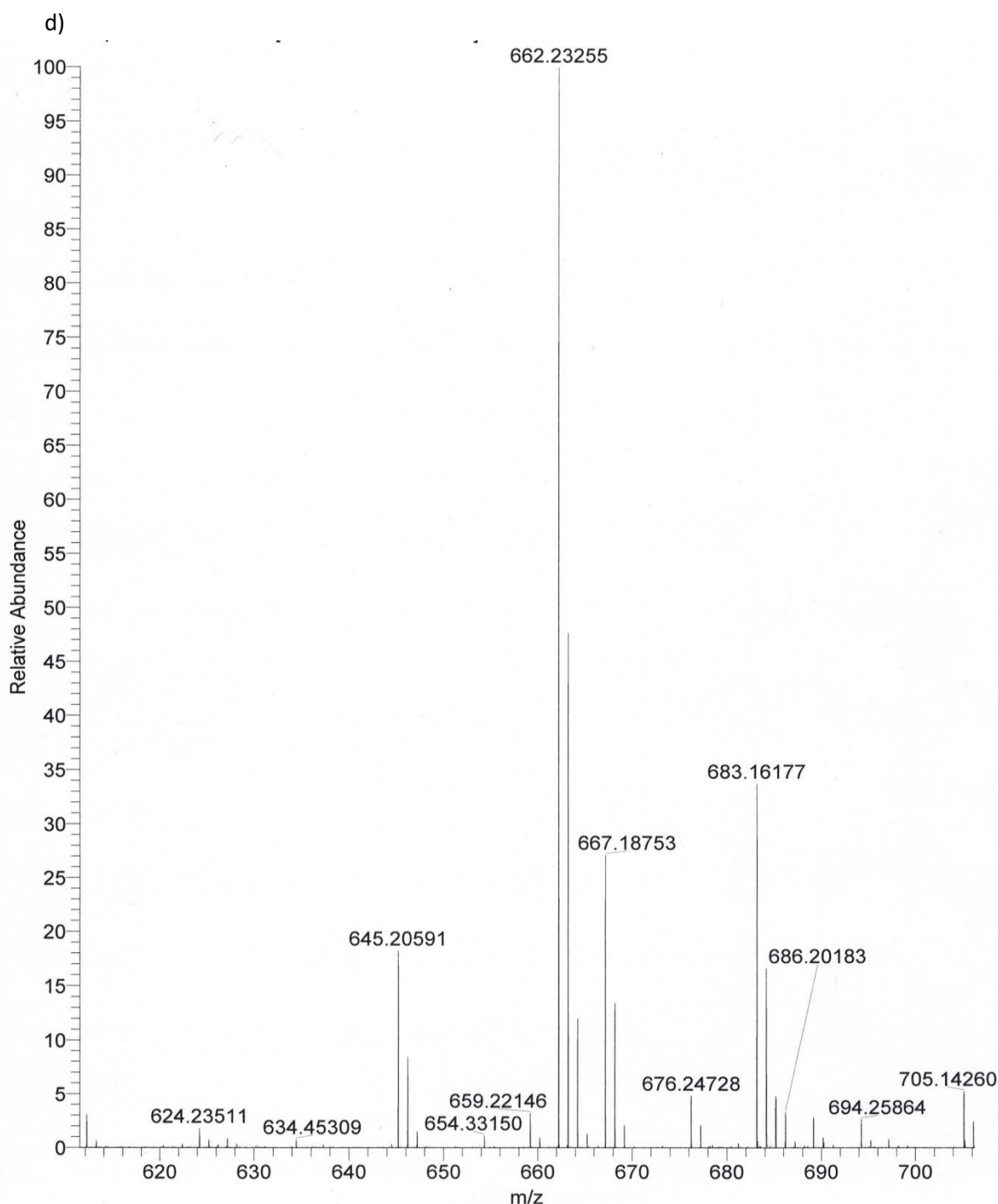
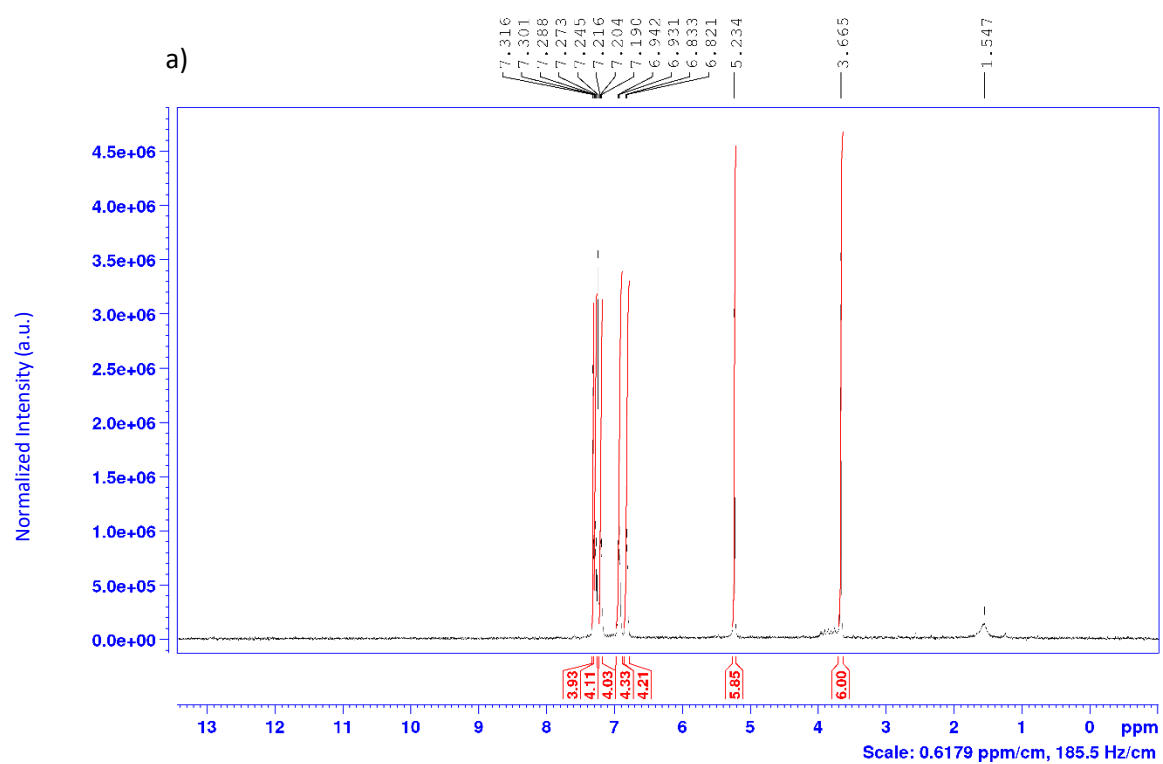
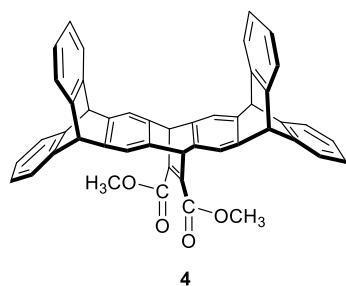


Figure S1 – a) ^1H NMR (300 MHz, CDCl_3 , 7.26 ppm): δ 7.42 (br s, 4 H), 7.39-7.35 (m, 4 H), 7.32-7.29 (m, 4 H), 6.95-6.92 (d, 4 H, $J = 4.7$ Hz), 6.86-6.84 (d, 4 H, $J = 4.7$ Hz), 5.79 (s, 2 H), 5.28 (s, 4 H). 1.27 (water), 0.86 (hexanes), 0.07 (TMS) b) ^{13}C NMR (75.5 MHz, CDCl_3 , 77.0 ppm): 167.8, 144.9, 143.3, 140.6, 125.2, 125.1, 123.5, 123.0, 53.9, 29.7. (low sample concentration) c) FTIR neat (cm^{-1}): 3419 (-OH), 3061-3020 (C-H, sp^2), 2922-2853 (C-H, sp^3), 1709 (C=O). d) HR ESI MS of compound 2 in anionic mode. Performed in 1:1 MeOH: H_2O + 0.1% NH_4OH . Calculated for $\text{C}_{46}\text{H}_{29}\text{O}_4$ [M-H] $^-$ - 643.19039, found 643.19135; e) HR ESI MS of compound 2 in cationic mode. Performed in 1:1 MeOH: H_2O + 0.1% Formic Acid. Calculated for $\text{C}_{46}\text{H}_{29}\text{O}_4$ [M+H] $^+$ + 645.20604, found 645.20591; calculated for $\text{C}_{46}\text{H}_{29}\text{O}_4$ [M+ NH_4] $^+$ + 662.24504, found 662.23255.

Spectra for compound 4



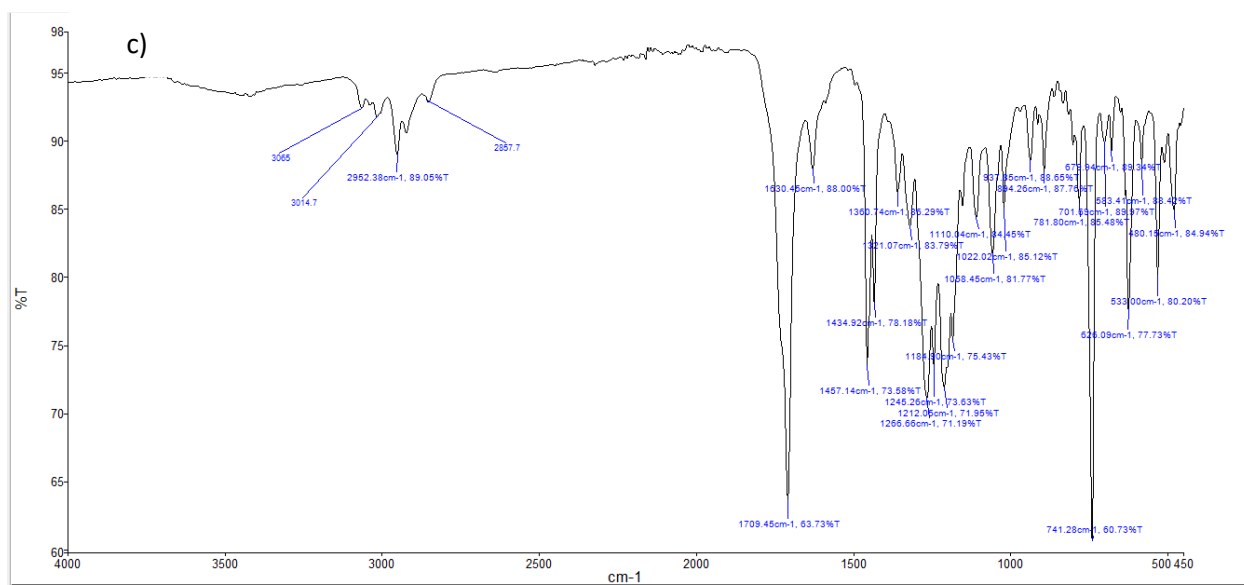
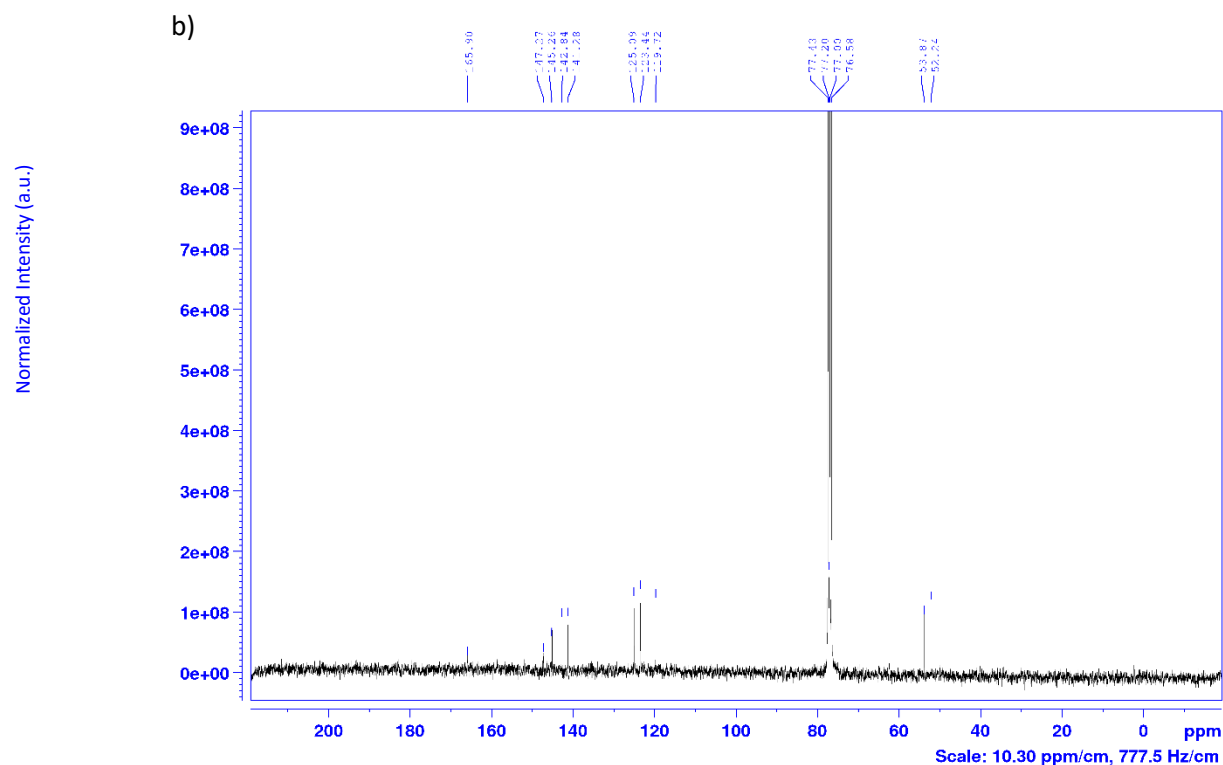


Figure S2 – a) ^1H NMR (300 MHz, CDCl_3 , 7.26 ppm): δ = 7.32 – 7.30 (br s, 4 H), 7.28 (t, 4 H, J = 3.7 Hz), 7.20 (t, 4 H, J = 3.7 Hz), 6.94 (t, 4 H, J = 3.5 Hz), 6.82 (t, 4 H, J = 3.5 Hz), 5.24 – 5.22 (br s, 6 H), 3.66 (s, 6 H), 1.54 (water). b) ^{13}C NMR (75.5 MHz, CDCl_3 , 77.0 ppm): 165.9, 147.3, 142.8, 141.3, 125.1, 123.4, 123.4, 119.7, 76.6, 53.9, 52.2. c) FTIR neat (cm^{-1}): 3065-3014 (C-H, sp^2), 2952-2857 (C-H, sp^3), 1709 (C=O).

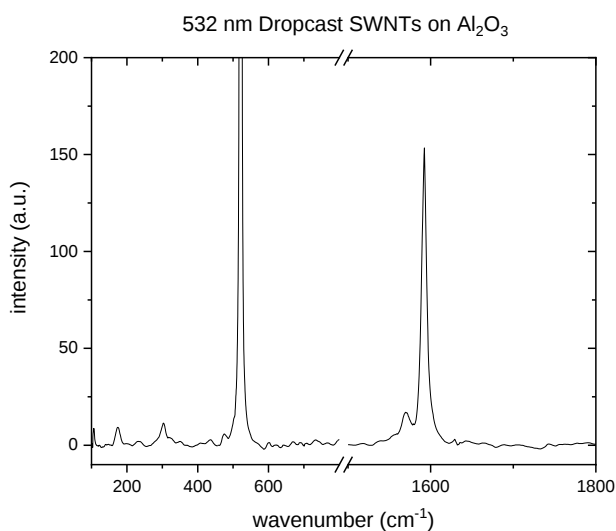
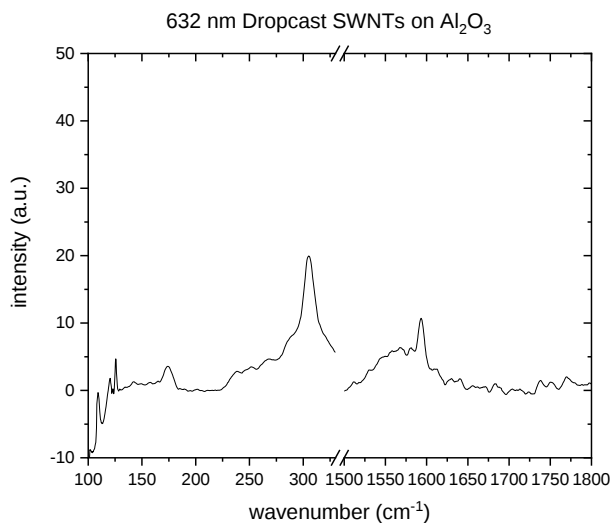


Figure S3 – a) Red ($\lambda = 632$ nm) laser wavelength spectrum of the NanoIntegris Inc. 90% pure single-walled carbon nanotubes dropcast on the TMA-ALD Al_2O_3 treated silicon wafer, b) Green ($\lambda = 532$ nm) laser wavelength spectrum of the NanoIntegris Inc. 90% pure single-walled carbon nanotubes dropcast on the TMA-ALD Al_2O_3 treated silicon wafer. The silicon peaks dominate the spectrum and are used for calibration purposes.

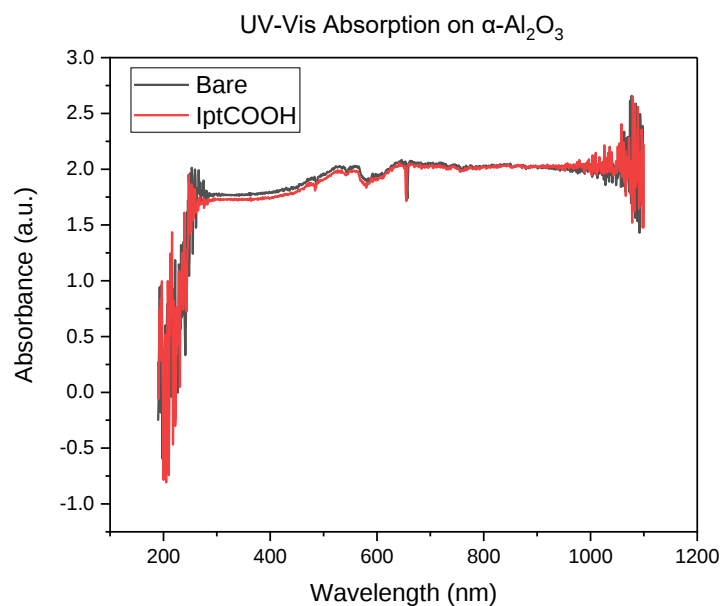


Figure S4 – UV-vis absorption spectra of sapphire substrate (bare) and with molecule 2 and SWCNTs (ART treatment).

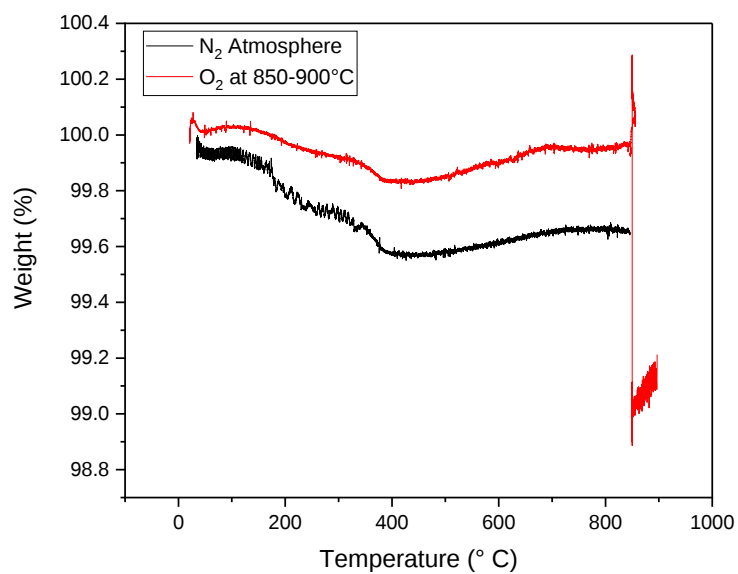


Figure S5 – Thermal gravimetric analysis in both nitrogen and oxygen atmosphere on a silicon surface functionalized with molecule 1.

The SEM and/or AFM tiff images were processed for length and angle using ImageJ software. Gwyddion software was used for processing .ibw files and converting to tiff in some occasions. Measurement scales were in μm . Standard deviation was calculated from all the angles using excel STDEV.P. If the SD of the binned data is taken instead, the SD will be significantly lower, so all the individual angles were considered in the calculation in this work. The process is outlined in Figure S6 The AFM was either a Asylum MFB-3D Origin (Tanaguchi Lab, National Institute for Materials Science) or Bruker Dimension FastScan (QNFAB, Waterloo). Density was calculated based on counting the SWCNTs/Area of the image, and then dividing to get units of $1\ \mu\text{m}^2$. Ex. 25 SWCNTs/ $100\ \mu\text{m}^2 = 0.25\ \text{SWCNTs}/\ \mu\text{m}^2$. The results of density per image are then averaged for total number of images.

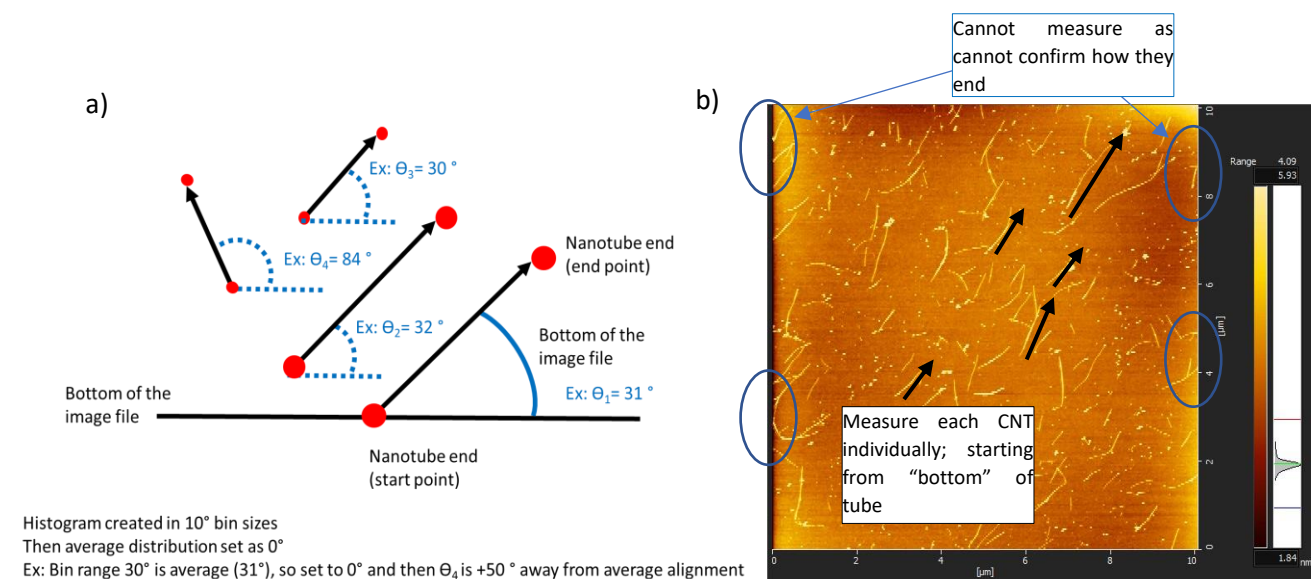
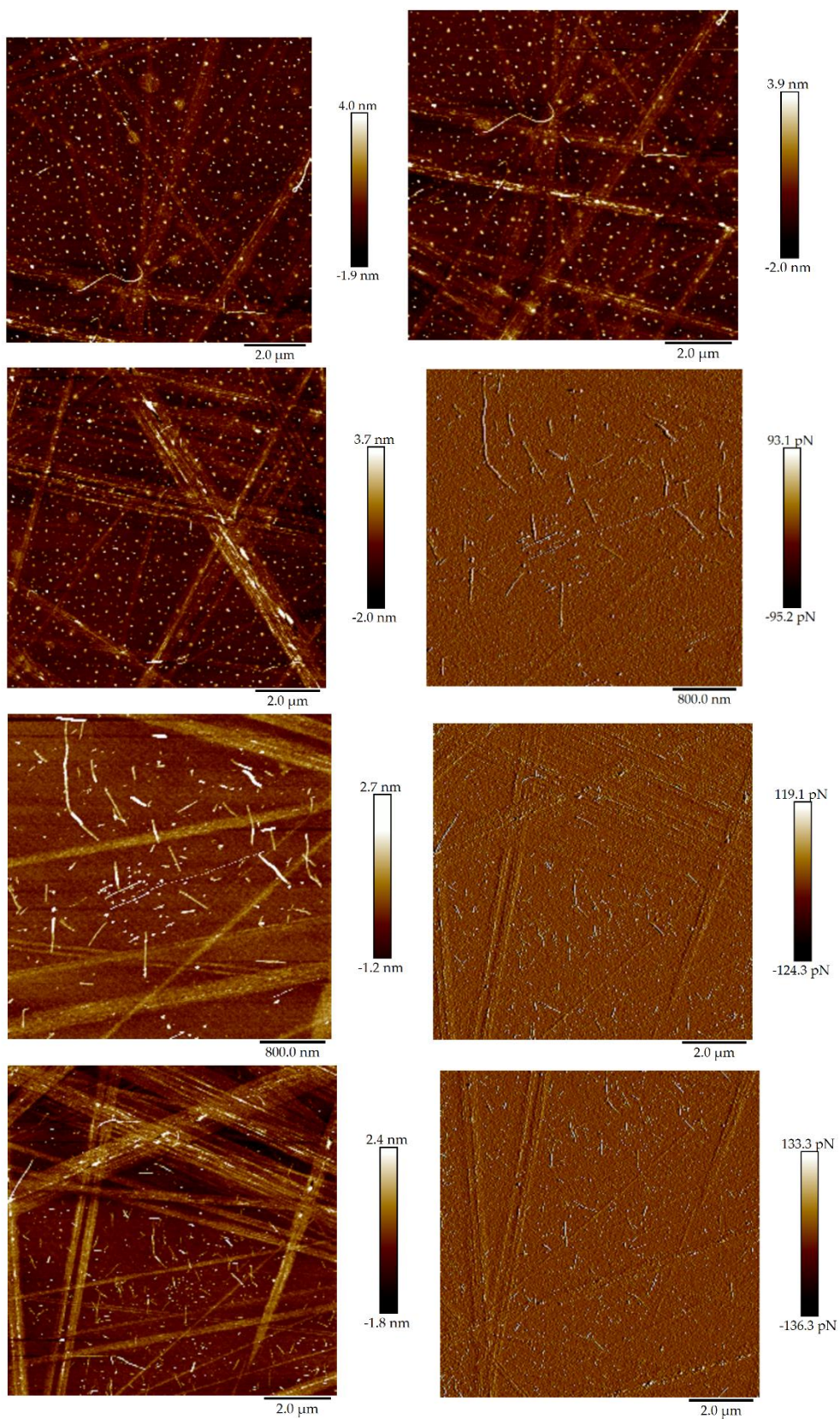
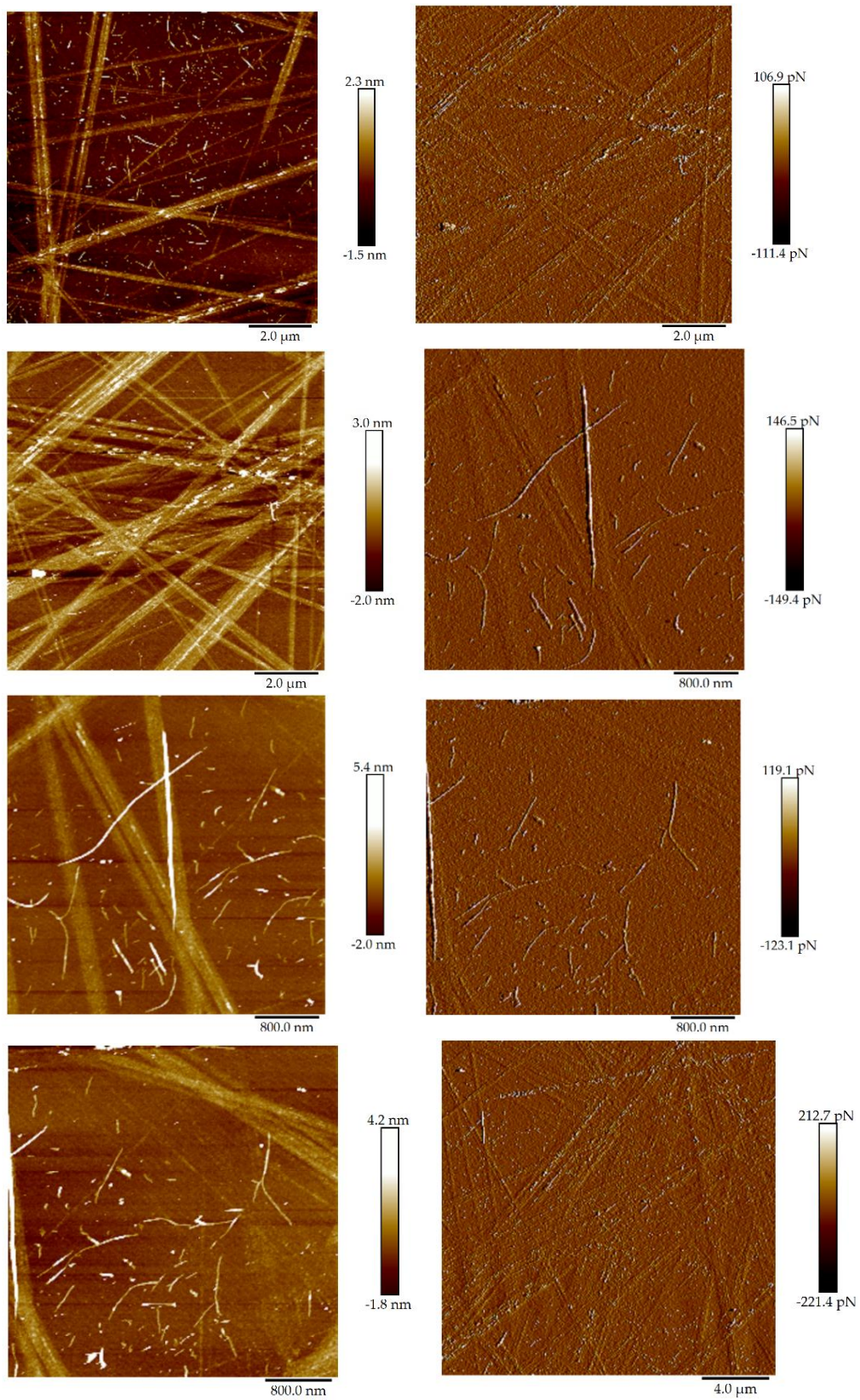
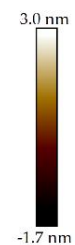
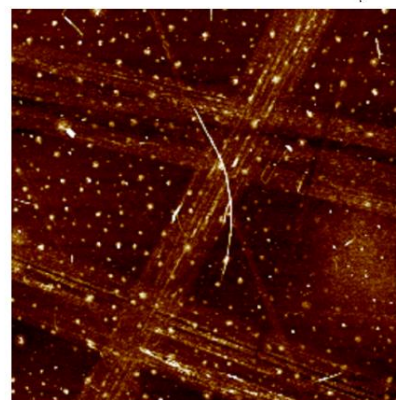
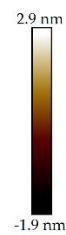
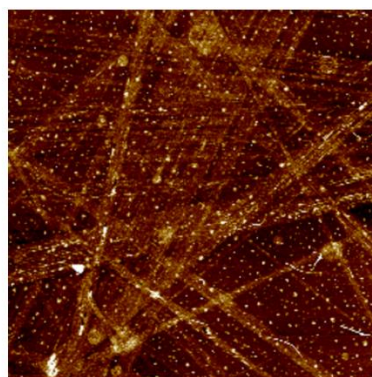
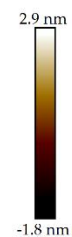
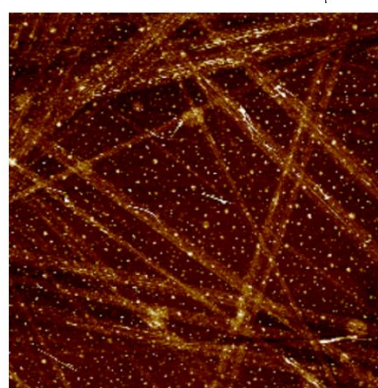
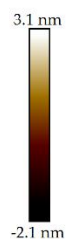
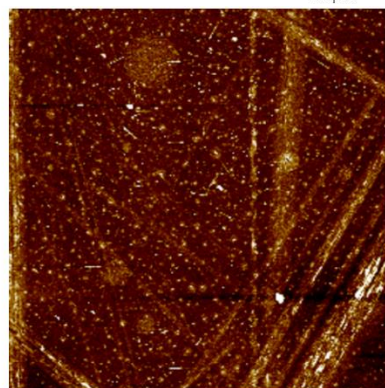
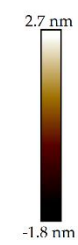
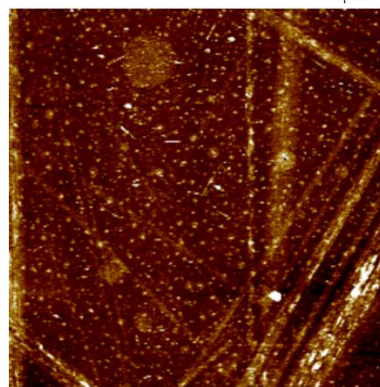
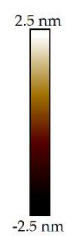
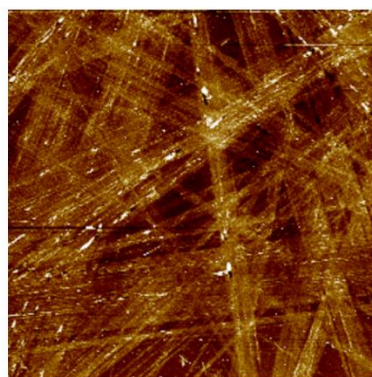
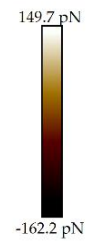
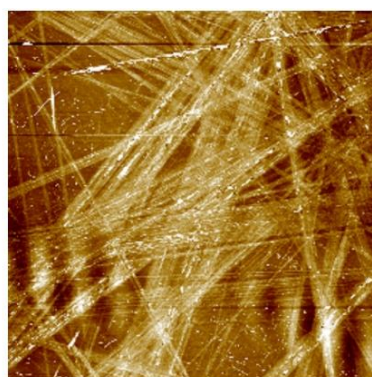


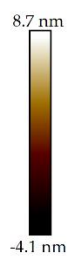
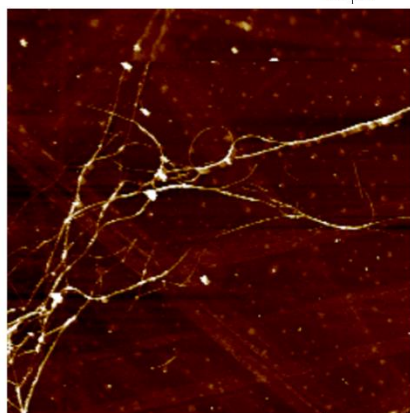
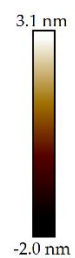
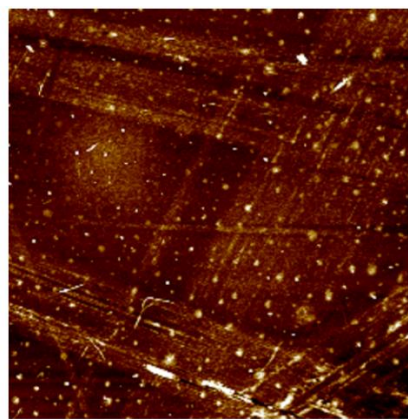
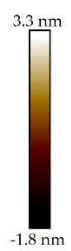
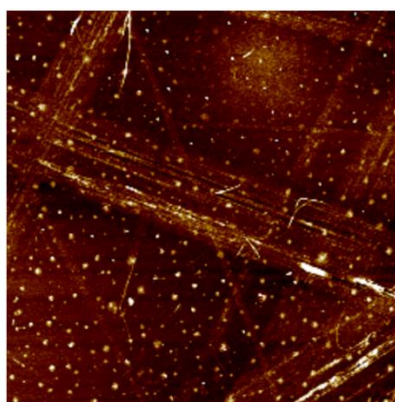
Figure S6 – a) Diagram to illustrate how the angles and lengths were tabulated on ImageJ b) Sample AFM image to represent data analysis of CNTs with indications as to what kinds of tubes were not considered in the calculation.

SiO₂ with Compound 2 (AFM images) with 5CB, ART

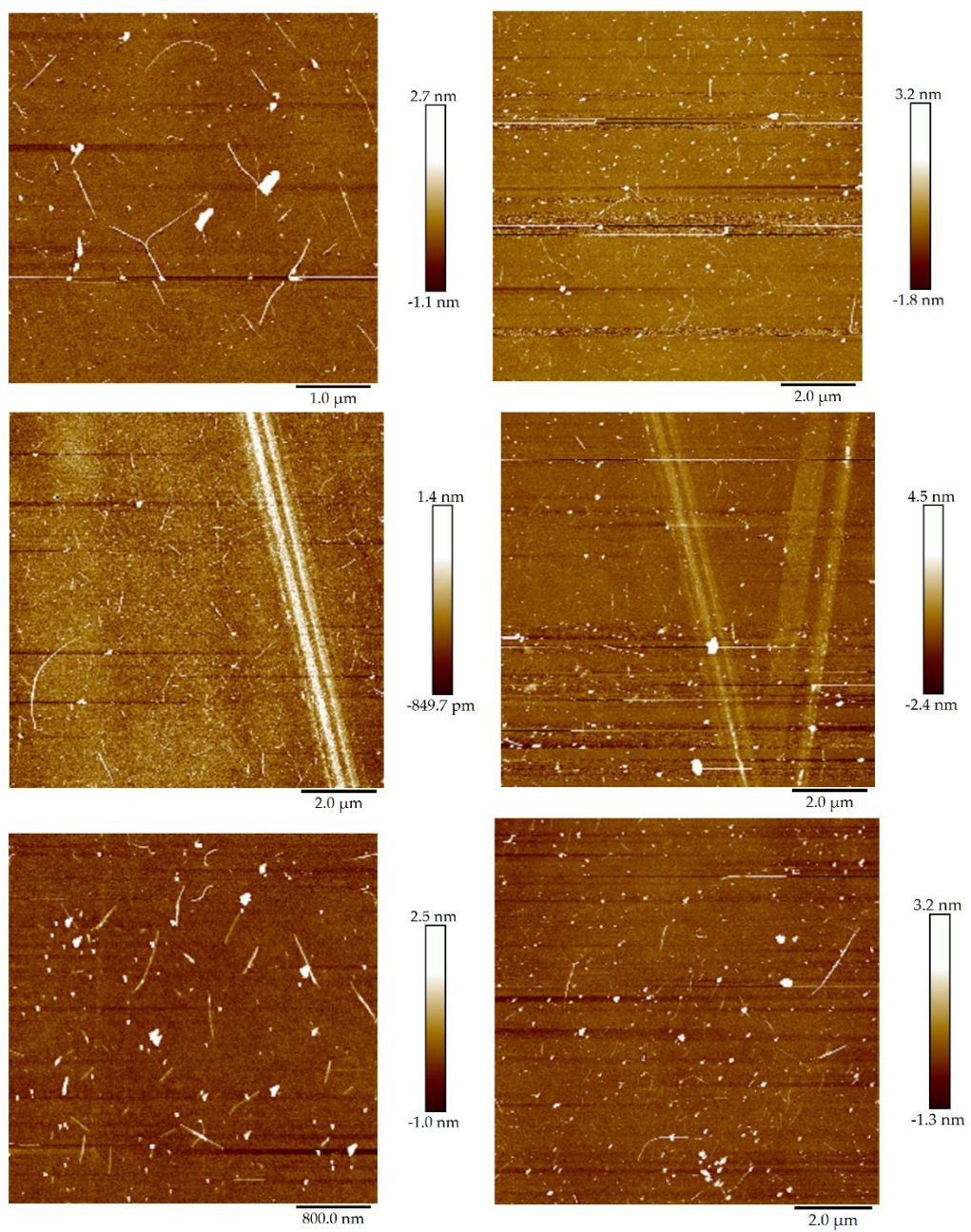


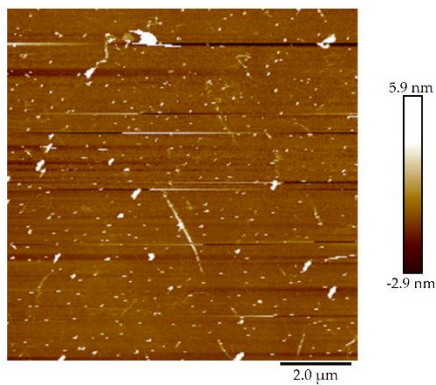
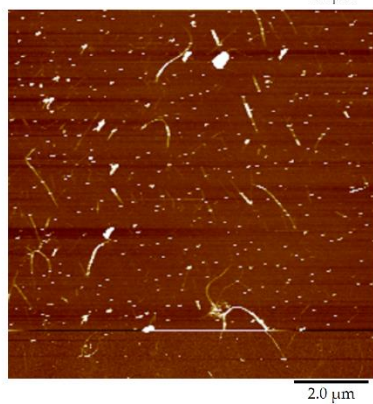
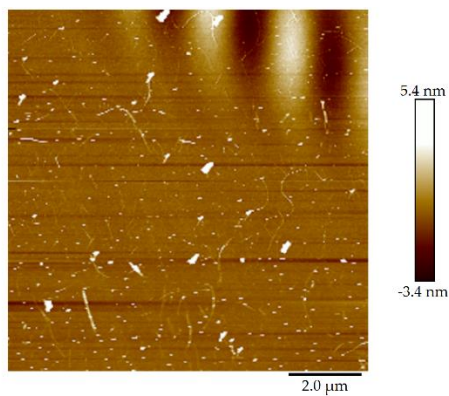
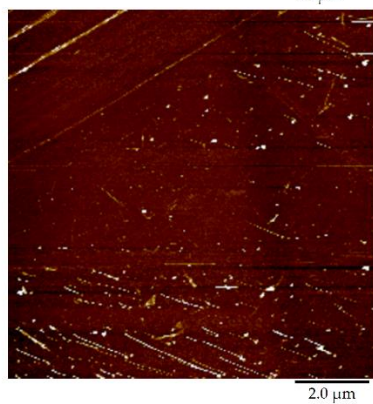
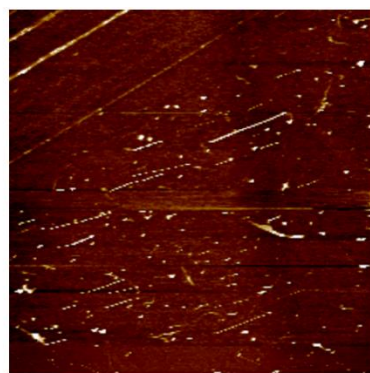
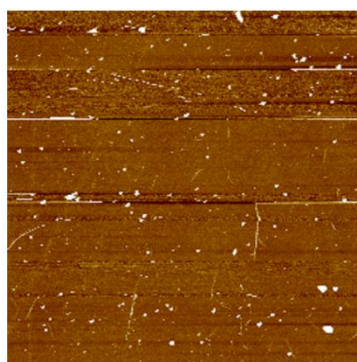


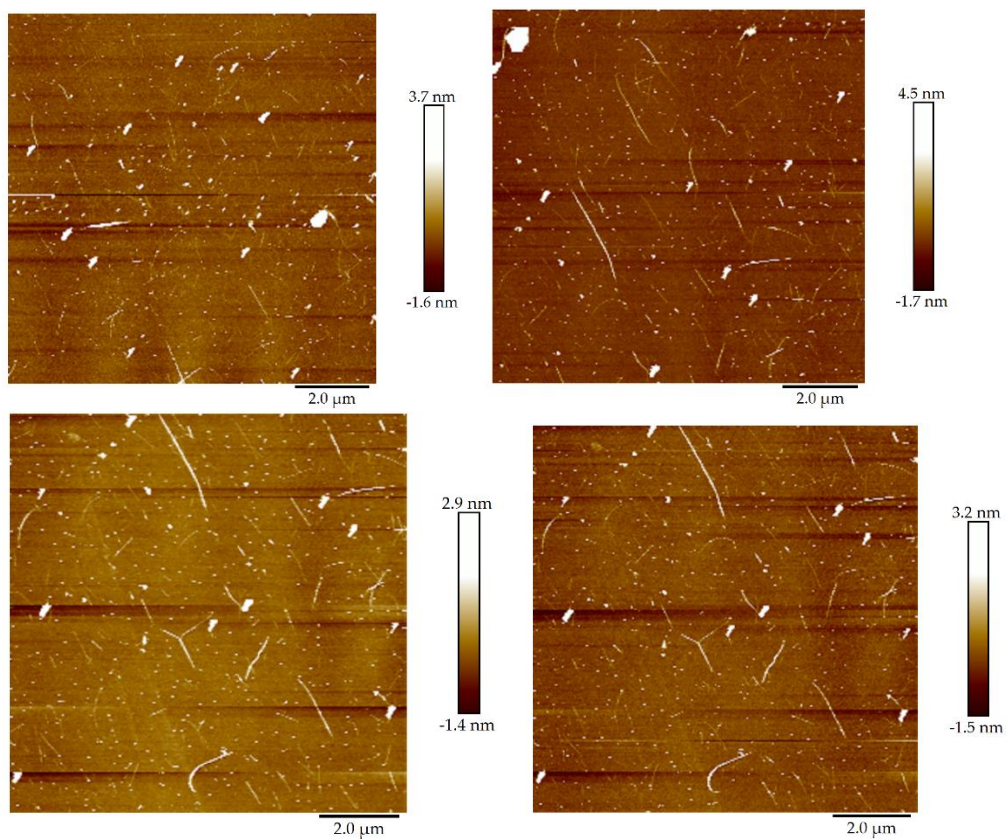




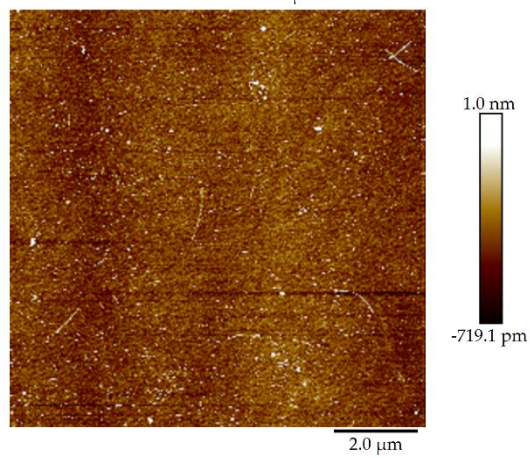
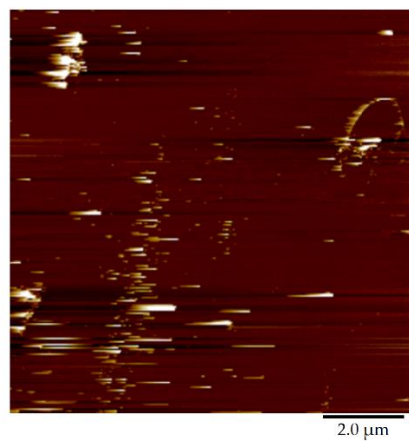
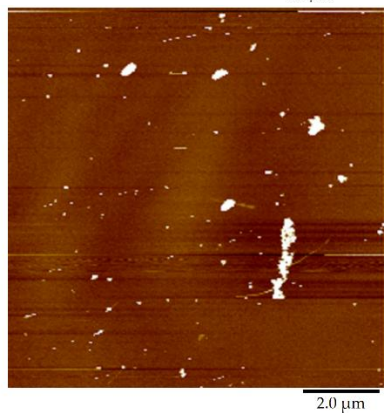
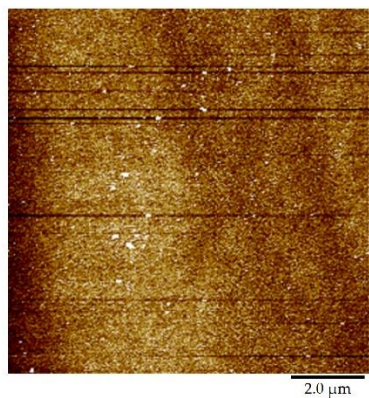
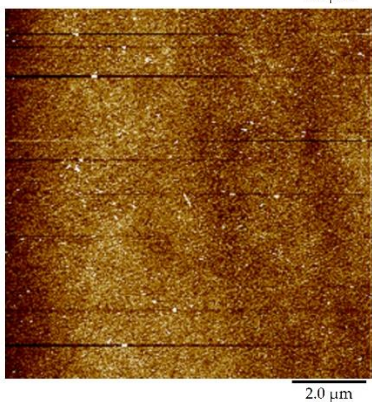
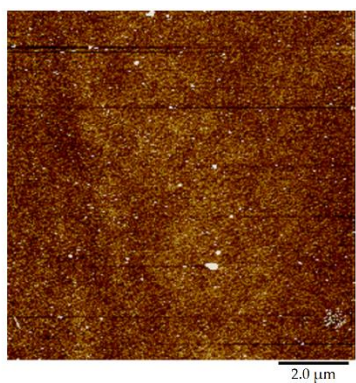
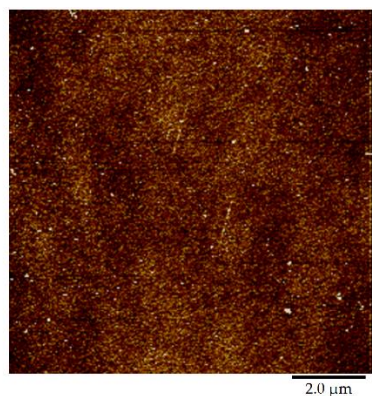
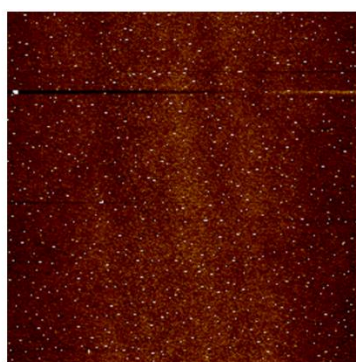
ALD-Al₂O₃ with Compound 2 (AFM images) with 5CB, ART

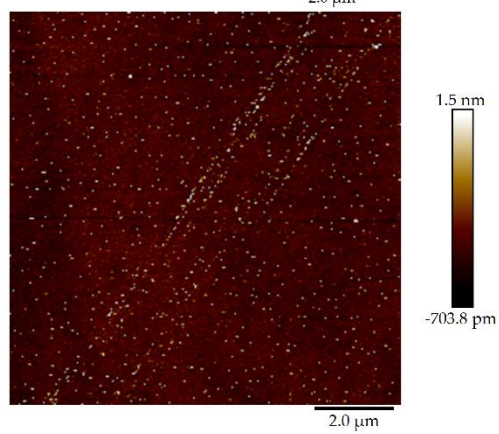
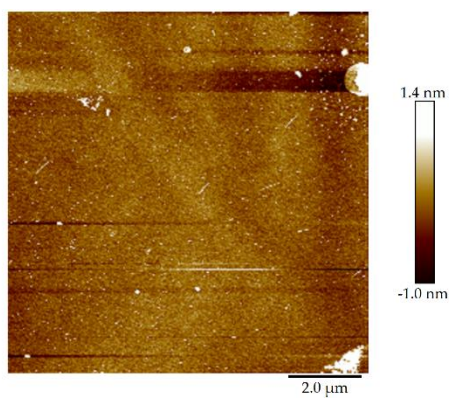
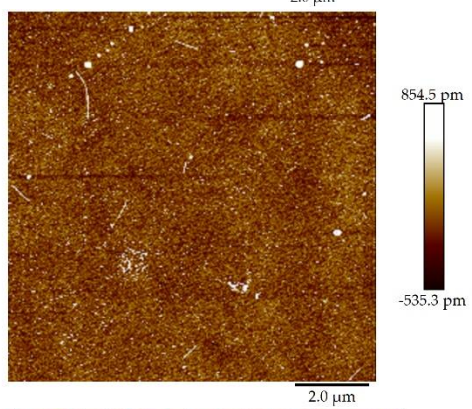
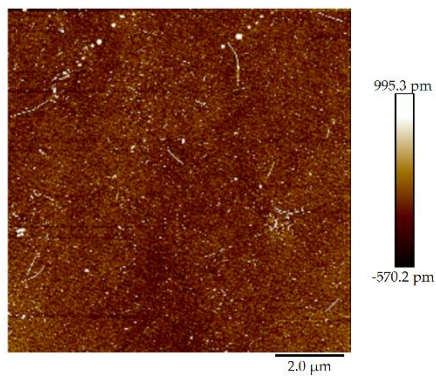
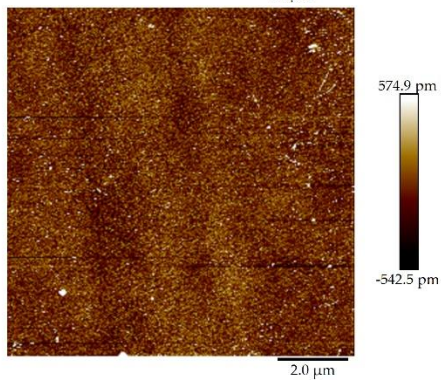
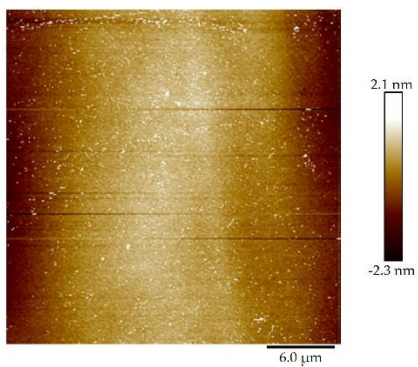
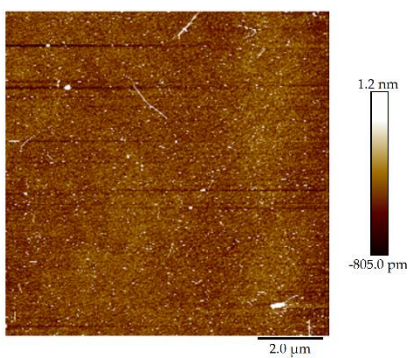




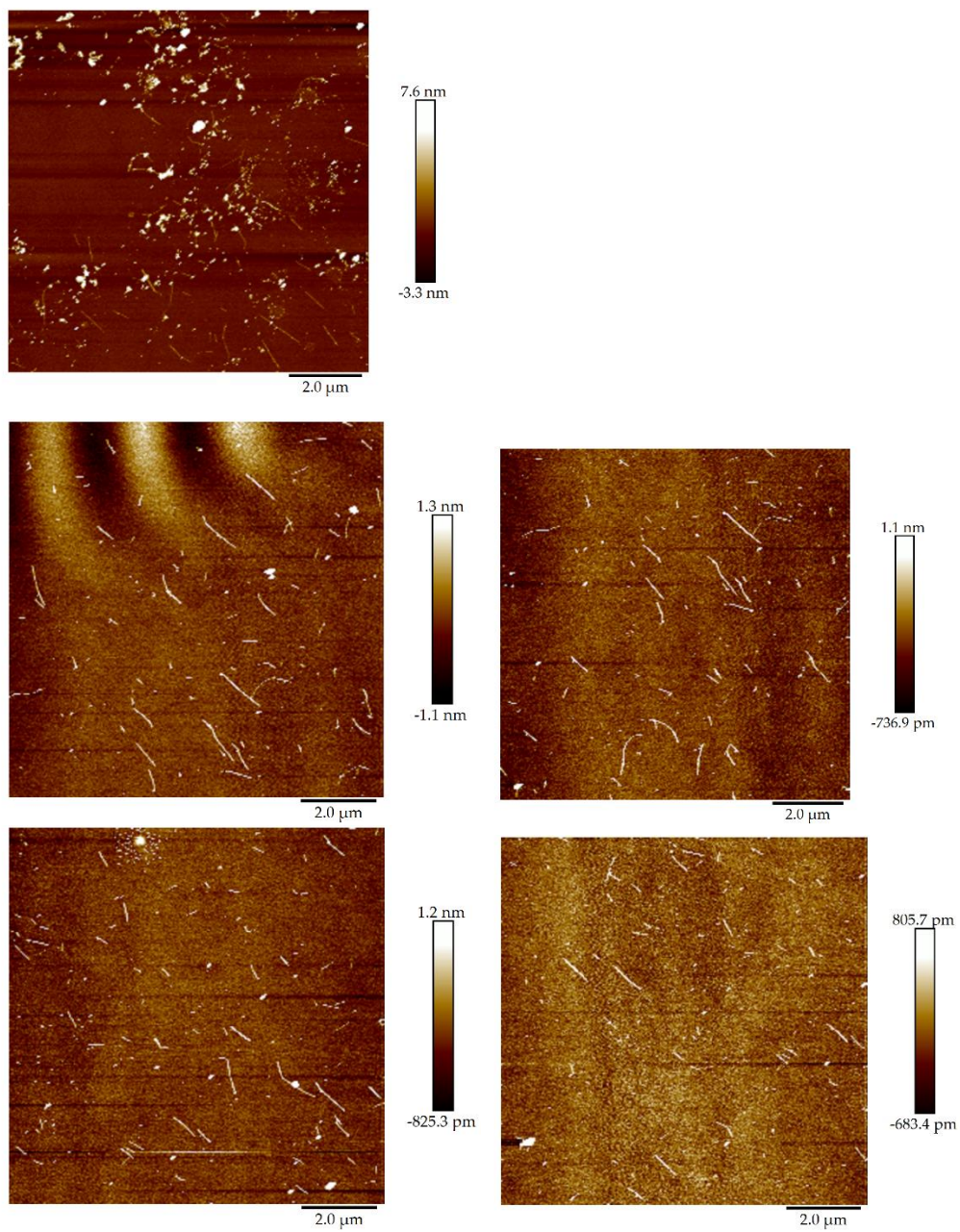


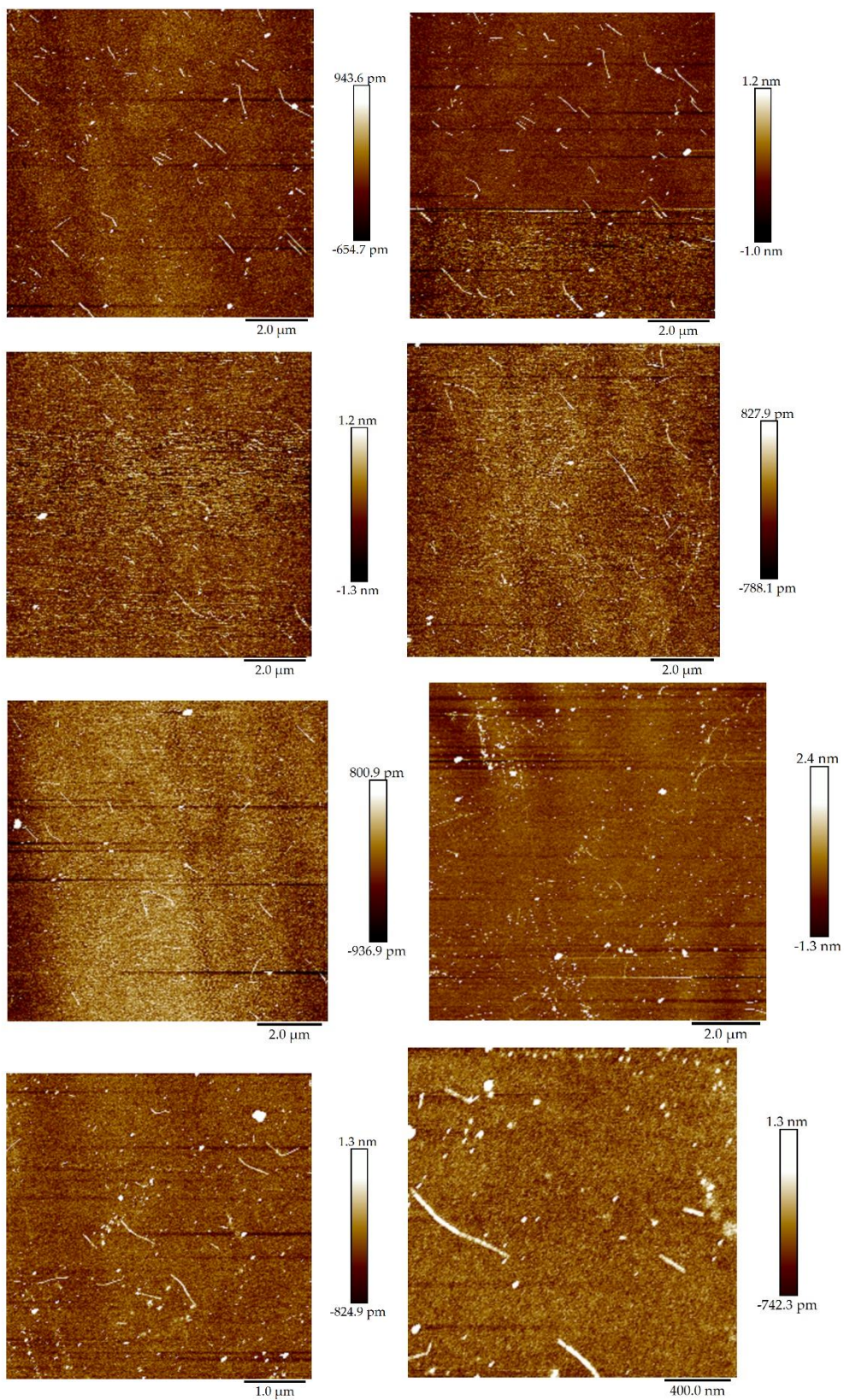
SiO₂ with Compound 2 (AFM images) with 8CB, ART

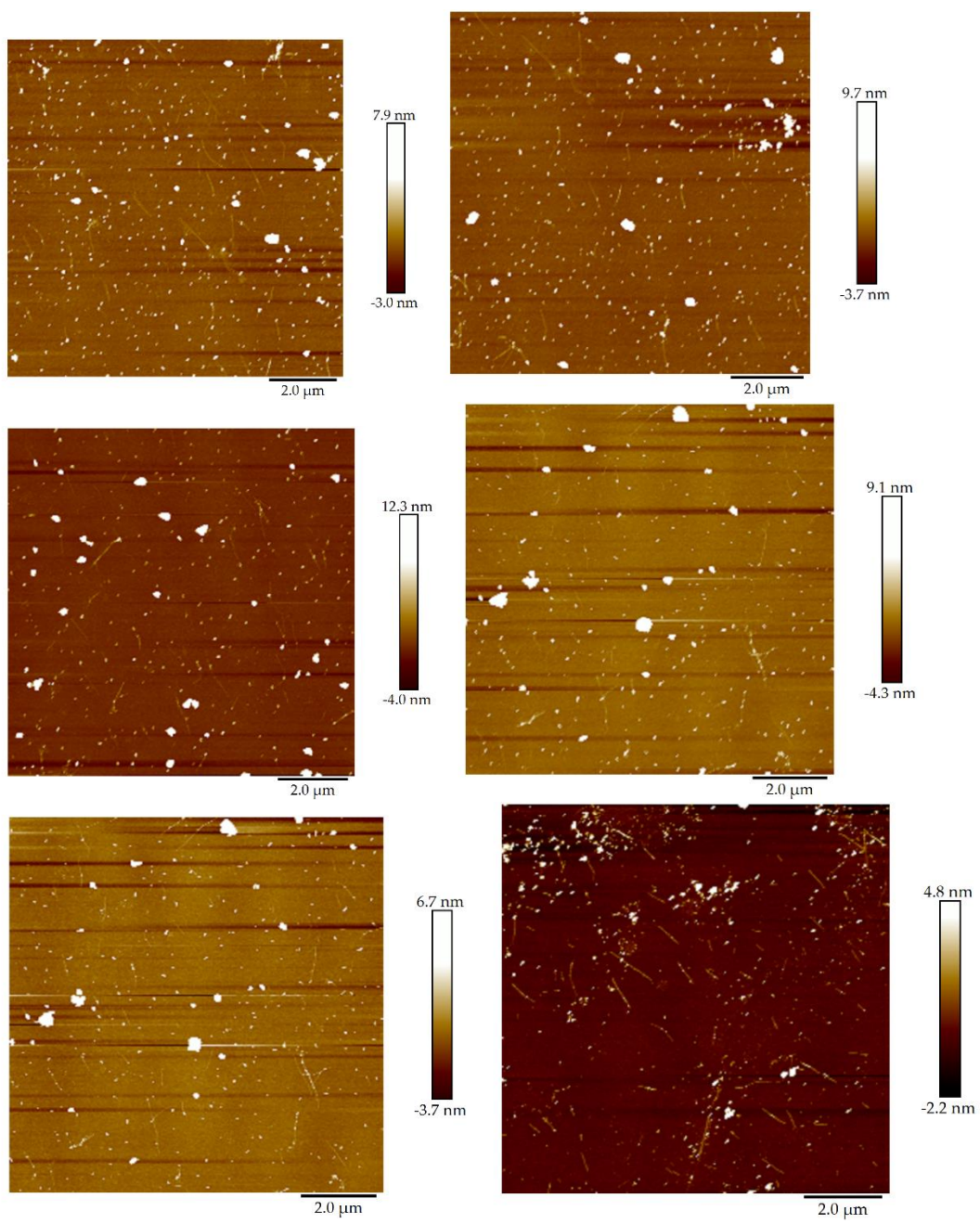




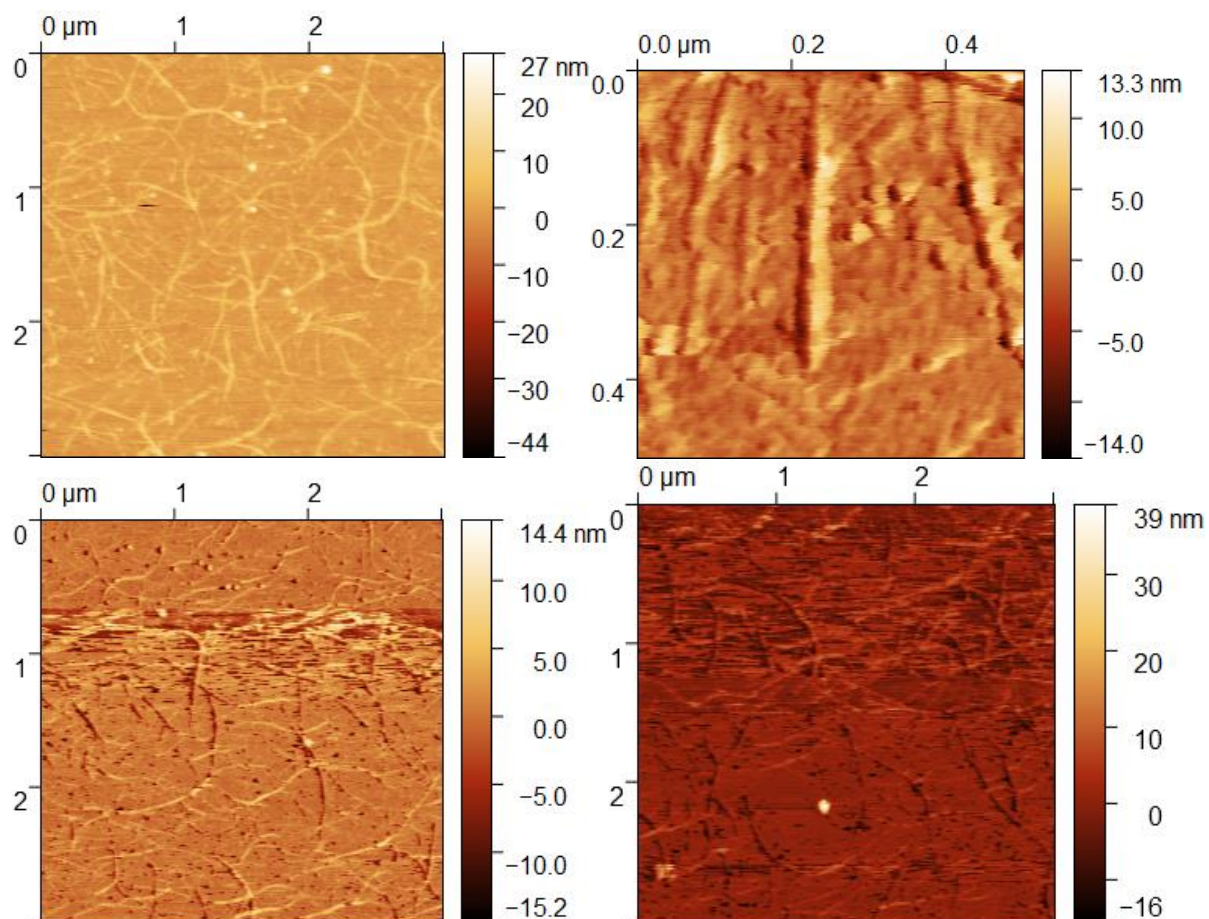
ALD- Al_2O_3 with Compound 2 (AFM images) with 8CB, ART



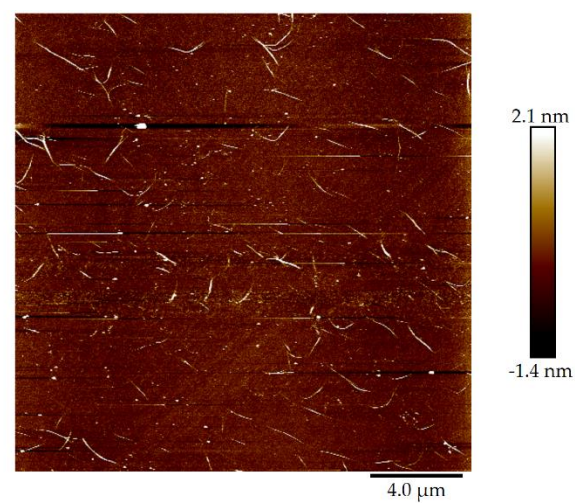
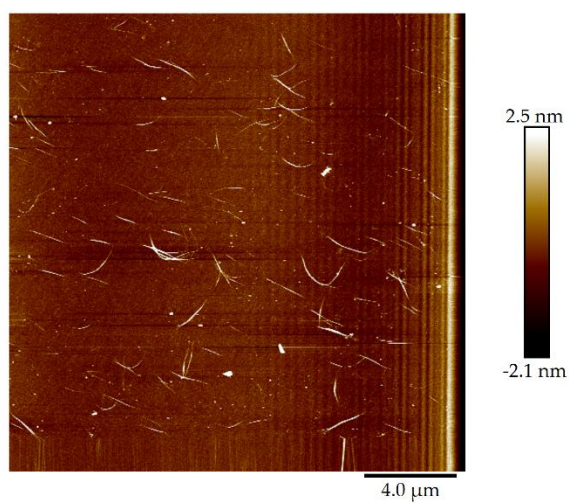
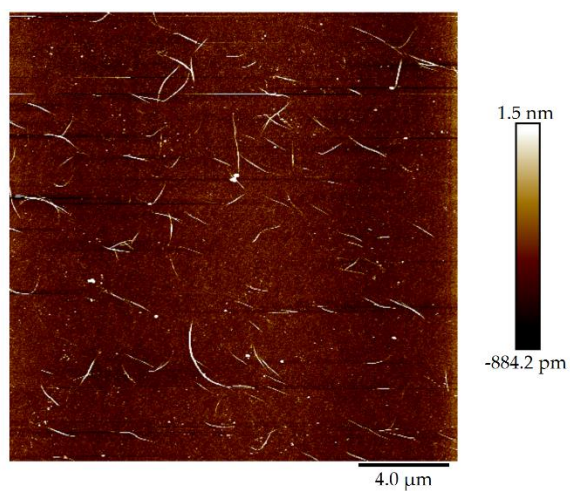
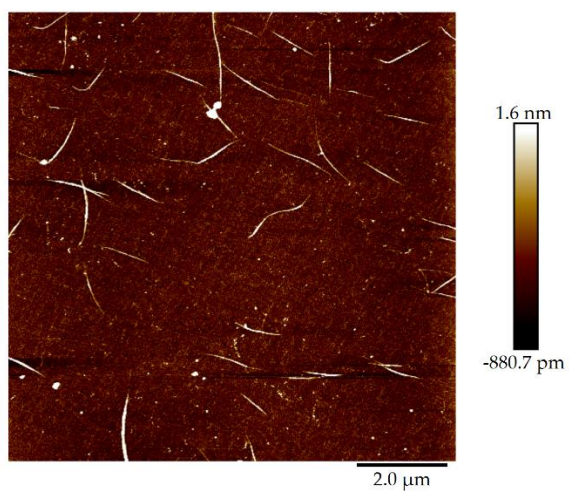


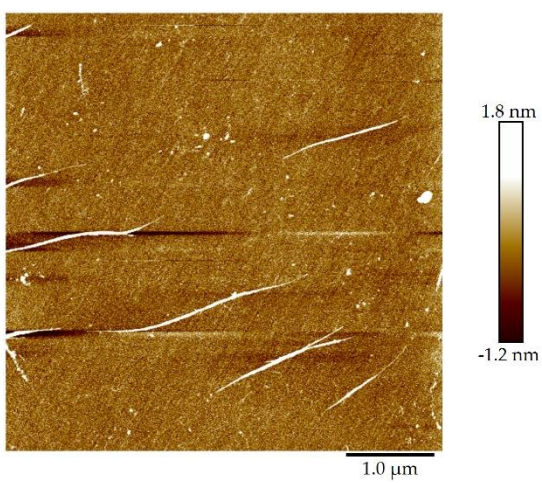
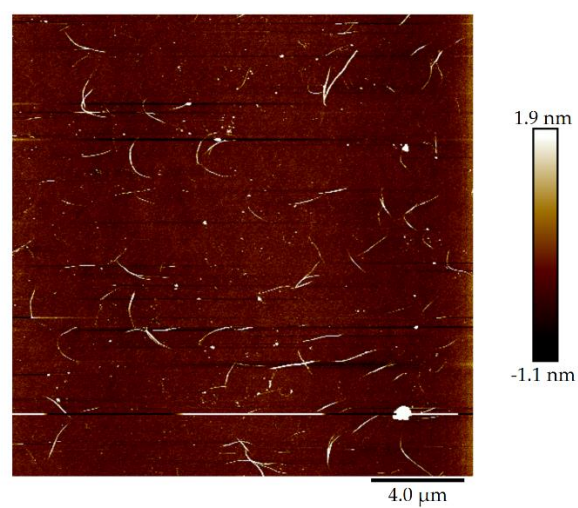
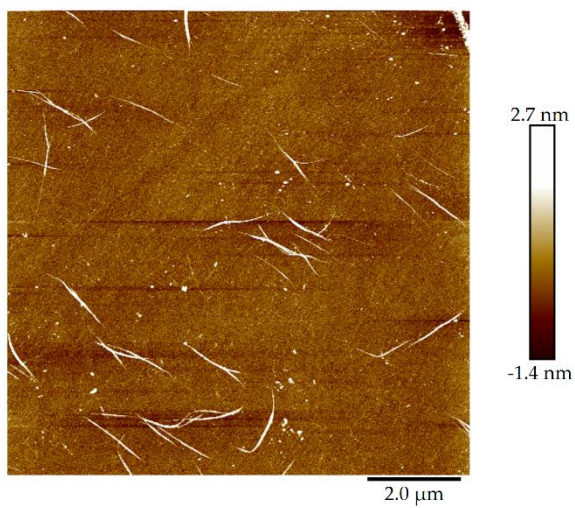
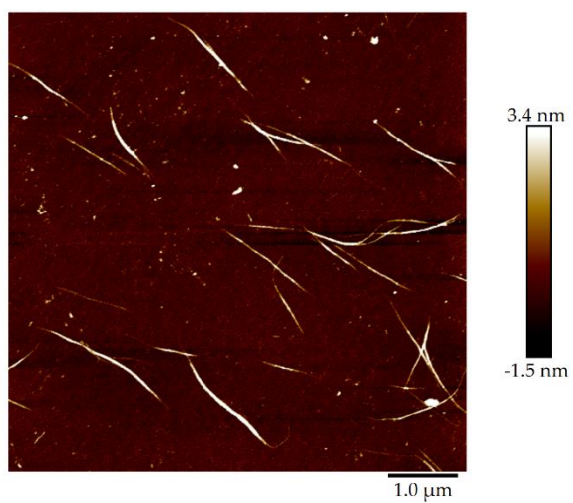
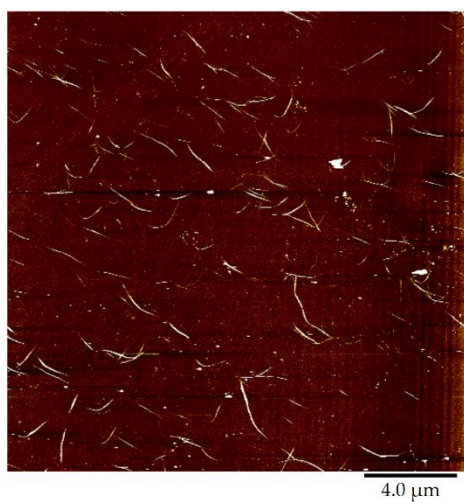


α -Al₂O₃ with Compound 1 (AFM images) with 5CB, ART



α -Al₂O₃ with Compound 2 (AFM images) with 5CB, ART





Theoretical calculations for the iptycene and SWCNT interactions

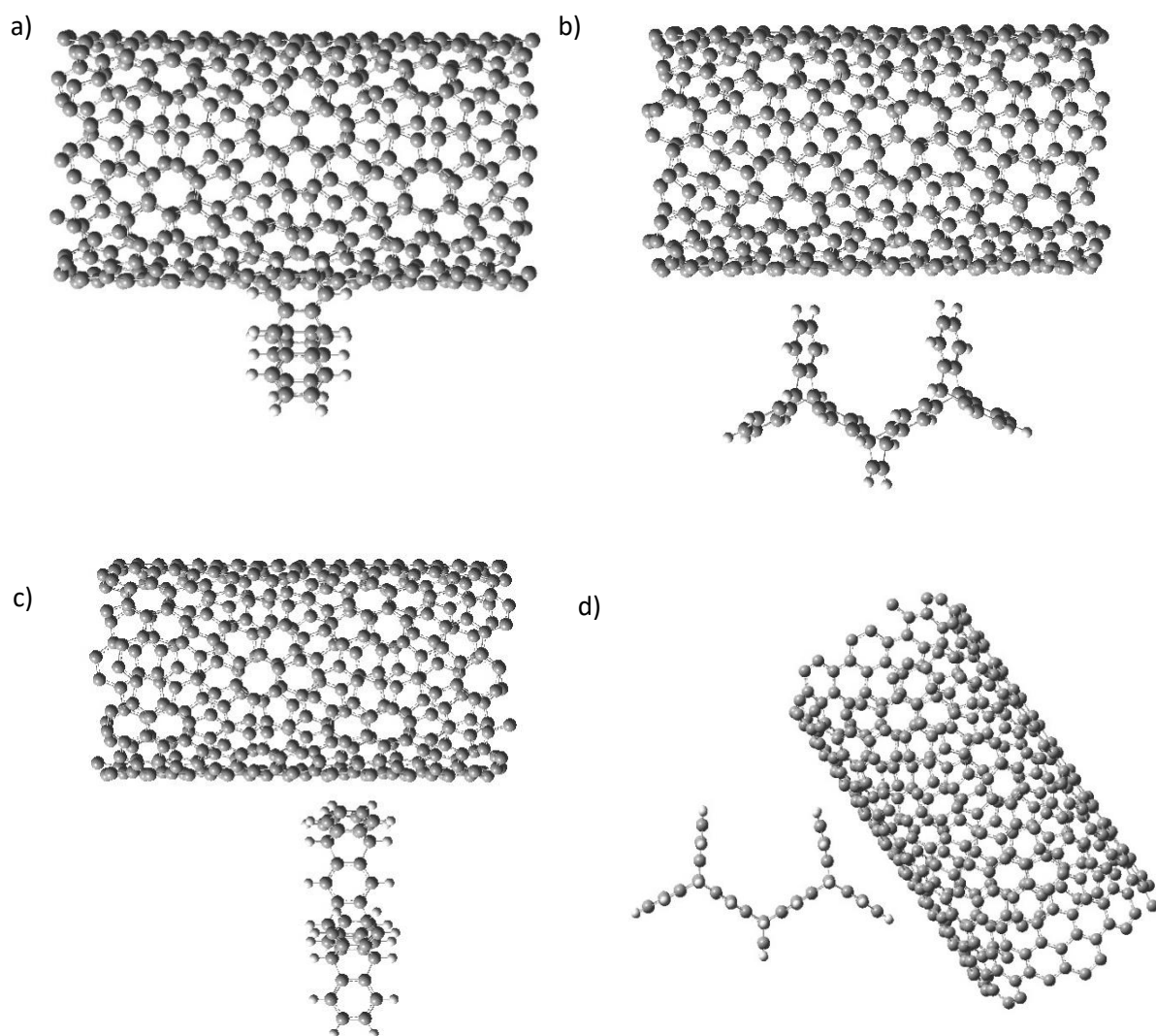


Figure S7 - a) complimentary side view figure to 8a in the main text, b) complimentary side view figure to 8b in the main text, c) complimentary side view figure to 8c in the main text, d) interaction between the side pockets of the iptycene perpendicular to the length of the SWCNT – very unlikely to occur given the iptycenes are bonded to the surface .

Table S1. Computed energies for model C₁₀₀ + triptycene and (12,7) SWCNT + iptycene systems.

System	Conformation	E _{absolute} (Hartree)	E _{relative} (Hartree)	E _{relative} (kJ mol ⁻¹)
C ₁₀₀ + triptycene [PM7]	#1 (grab)	1.83594	0	0.0
	#2 (transverse)	1.84112	0.00518	13.6
C ₁₀₀ + triptycene [DFT]	#1 (grab)	-4582.07527	0	0.0
	#2 (transverse)	-4582.07310	0.00217	5.7
(12,7) SWCNT + iptycene [PM7]	#1 (centre grab)	7.15342	0	0
	#2 (side grab)	7.18849	0.03506	92.1
	#3 (transverse)	7.20990	0.05645	148.3

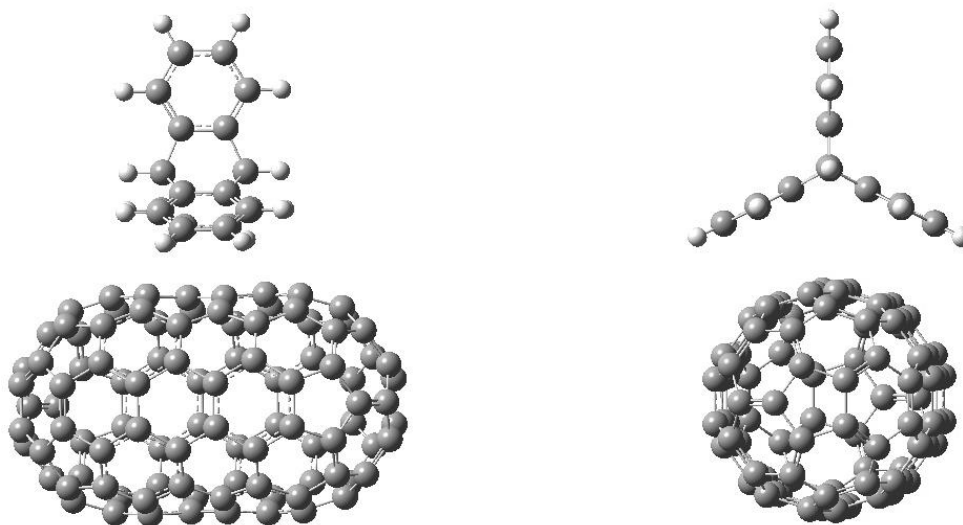
Optimized (x,y,z) atomic coordinates for C₁₀₀ + triptycene model system

Conformation #1 – 0.0 kJ mol⁻¹

C	-1.35560100	5.10322400	-2.36949600
C	-0.18745100	4.31931300	-2.74320800
C	-1.35524200	5.83460800	-1.19711500
C	0.92282000	4.31250600	-1.93674500
C	1.61594700	3.05331000	-1.69832800
C	0.04613700	-0.59954400	-3.13568000
C	1.17587000	-0.60589000	-2.30711000
C	1.23271000	1.86660100	-2.32174600
C	0.06151200	1.87298100	-3.17739800
C	-0.63914600	3.06774200	-3.33776400
C	2.03956900	0.62554200	-0.36491100
C	1.60798000	0.63589500	-1.69754000
C	2.05993900	-3.04287200	0.33242400
C	2.10792100	-1.84500800	-0.37891500
C	1.66080200	-1.83462600	-1.75877300
C	1.19780400	-3.02378200	-2.32008000
C	-3.64594200	5.09111500	-0.70524000
C	-3.63445800	4.31383200	-1.93601900
C	-2.53609700	5.82854400	-0.33915100
C	-2.52466000	4.31998300	-2.74288500
C	-2.07499800	3.06768700	-3.33715200
C	-3.89558500	-0.60541600	-2.30848600
C	-2.76272200	-0.59933900	-3.13426900
C	-2.77671400	1.87329000	-3.17614600
C	-3.94972400	1.86648500	-2.32165200
C	-4.32827200	3.05461500	-1.69741000
C	-0.65711300	0.64893000	-3.35565600
C	-2.05880400	0.64901400	-3.35466000

C	0.03678300	-3.01770200	-3.16500600
C	-0.63197100	-1.82338700	-3.43192200
C	-2.08311700	-1.82289200	-3.43073200
C	-2.75036800	-3.01783400	-3.16355000
C	-2.77089100	5.07050600	1.98729400
C	-3.93207600	4.28676400	1.59153700
C	-2.08489900	5.81783100	1.04899900
C	-4.35603400	4.29666000	0.28659100
C	-4.77139400	3.04404300	-0.33167800
C	-4.33015300	-0.63581400	1.69947200
C	-4.76262600	-0.62560600	0.36591600
C	-4.82553500	1.84558500	0.37913500
C	-4.37761600	1.83521200	1.75952600
C	-3.91076300	3.02416400	2.31895700
C	-4.33029600	0.63621200	-1.69911100
C	-4.76260700	0.62604700	-0.36550200
C	-3.91135400	-3.02381200	-2.31864600
C	-4.37801800	-1.83481100	-1.75915800
C	-4.82577000	-1.84513800	-0.37871200
C	-4.77166400	-3.04360100	0.33209600
C	0.06056500	5.06932500	1.98683300
C	-0.66953900	4.27603500	2.96544600
C	-0.62522700	5.81711000	1.04887200
C	-2.04168800	4.27647800	2.96547300
C	-2.74967500	3.01806700	3.16371800
C	-0.65677500	-0.64890500	3.35556500
C	-2.05846300	-0.64884700	3.35474400
C	-2.08251400	1.82305800	3.43081800
C	-0.63137200	1.82340500	3.43182900
C	0.03747200	3.01765000	3.16483300
C	-3.89524200	0.60576900	2.30879300
C	-2.76228000	0.59957700	3.13443700
C	-4.32837600	-3.05421700	1.69777400
C	-3.94963100	-1.86612500	2.32196800
C	-2.77651800	-1.87304900	3.17631800
C	-2.07490400	-3.06751600	3.33724000
C	0.93536200	5.08946300	-0.70542200
C	1.64612300	4.29511100	0.28633200
C	-0.17409500	5.82718800	-0.33935200
C	1.22166600	4.28552600	1.59146600
C	1.19838800	3.02361200	2.31976500
C	2.03955000	-0.62579100	0.36449400
C	1.60811400	-0.63609900	1.69717200
C	1.66119300	1.83441200	1.75839900
C	2.10814800	1.84475100	0.37849000
C	2.06020400	3.04262000	-0.33283900
C	0.04657200	0.59949600	3.13549900
C	1.17620000	0.60572700	2.30679000
C	-0.63905300	-3.06771500	3.33767500
C	0.06170400	-1.87302600	3.17722000
C	1.23279800	-1.86676500	2.32142700
C	1.61584400	-3.05351400	1.69796700
C	-1.35583100	-5.10312600	2.36950000
C	-0.18755600	-4.31933300	2.74306900
C	0.92261800	-4.31264000	1.93647200
C	-1.35569000	-5.83451400	1.19712100

C	-3.64637400	-5.09078800	0.70552300
C	-3.63466100	-4.31350400	1.93630000
C	-2.52476500	-4.31976600	2.74303100
C	-2.53664900	-5.82833000	0.33929900
C	-2.77165000	-5.07027200	-1.98712000
C	-3.93270700	-4.28641000	-1.59122200
C	-4.35650700	-4.29626100	-0.28622300
C	-2.08561900	-5.81766600	-1.04890600
C	0.05981000	-5.06938000	-1.98700400
C	-0.67033400	-4.27601600	-2.96553100
C	-2.04248400	-4.27631800	-2.96539000
C	-0.62594500	-5.81709400	-1.04895700
C	0.93493200	-5.08960200	0.70514800
C	1.64565500	-4.29532400	-0.28669500
C	1.22104000	-4.28569800	-1.59178000
C	-0.17464600	-5.82721500	0.33921400
C	6.03215300	1.30527700	0.13414000
C	6.03199000	-1.30569400	-0.13414100
H	6.02785900	-2.40471300	-0.24747100
H	6.02815900	2.40429700	0.24747100
C	9.81849200	-0.69176600	-0.07183700
C	9.81857800	0.69088300	0.07179300
C	8.61381300	1.40239500	0.14558700
C	7.42504500	0.70225400	0.07285300
C	7.42495800	-0.70284300	-0.07287100
C	8.61363900	-1.40313000	-0.14561700
H	8.62078000	2.48330400	0.25777600
H	8.62047100	-2.48404000	-0.25780600
C	5.35174000	0.57775600	1.27718100
C	4.80113600	1.17012800	2.39813900
C	4.25777500	0.34928500	3.39465400
C	4.26719700	-1.03427300	3.25731300
C	4.81589700	-1.63559200	2.11736700
C	5.35558800	-0.82665800	1.13511300
H	4.79226200	2.25104400	2.51251700
H	4.81699100	-2.71792100	2.01460100
C	4.26727200	1.03407200	-3.25728600
C	4.81607200	1.63532600	-2.11735400
C	5.35567600	0.82632400	-1.13510600
C	5.35165100	-0.57809000	-1.27717300
C	4.80095400	-1.17039500	-2.39812100
C	4.25767200	-0.34948500	-3.39462400
H	4.81730900	2.71765400	-2.01459200
H	4.79194600	-2.25131000	-2.51249800
H	10.76144100	1.23120000	0.12796700
H	10.76128700	-1.23220000	-0.12802000
H	3.84351700	1.66098800	-4.03952000
H	3.82540500	-0.80412400	-4.28381300
H	3.82558600	0.80397700	4.28385400
H	3.84338400	-1.66113700	4.03955600

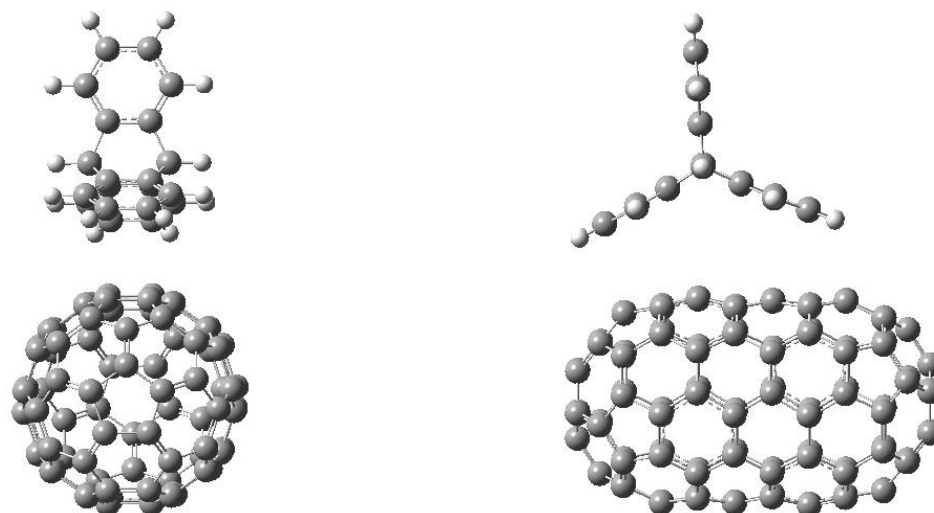


Conformation #2 – 5.6 kJ mol⁻¹

C	-3.14713100	-4.43828600	2.29077200
C	-1.69655800	-4.31824200	2.27919700
C	-3.81298000	-4.92290000	1.18107600
C	-0.98476500	-4.69624500	1.16868700
C	0.11794000	-3.85792000	0.71791500
C	0.91057500	-0.12982400	2.54304100
C	1.63637300	-0.51556600	1.40679100
C	0.52618000	-2.72399000	1.41920900
C	-0.22343600	-2.32634900	2.59537900
C	-1.32574100	-3.09196300	2.97386600
C	1.24856200	-1.72010600	-0.70082700
C	1.24855400	-1.72008400	0.70092800
C	2.77953500	1.61316700	-1.39390600
C	2.46346800	0.43086300	-0.72565100
C	2.46346000	0.43088600	0.72569800
C	2.77951800	1.61321200	1.39391800
C	-5.52467400	-3.17466900	1.41575700
C	-4.81126400	-2.66289900	2.57696500
C	-5.03888100	-4.27152900	0.72992700
C	-3.65903100	-3.27527200	3.00126700
C	-2.53148200	-2.45110200	3.41751400
C	-2.62868200	1.75072800	2.97553600
C	-1.45138000	1.12522600	3.40965600
C	-2.60671500	-1.05968400	3.47212300
C	-3.82532300	-0.41207600	3.02288900
C	-4.87132400	-1.20697500	2.55526000
C	-0.20442900	-0.94821200	2.97772300
C	-1.38220000	-0.32283200	3.41024800
C	2.03760900	2.00925500	2.55707300
C	0.99235300	1.21380700	3.02550300
C	-0.22694900	1.86191600	3.47257200
C	-0.30355000	3.25331000	3.41684000

C	-5.52465700	-3.17471500	-1.41569300
C	-6.02386500	-2.01814600	-0.68606100
C	-5.03887200	-4.27155300	-0.72982100
C	-6.02387300	-2.01812400	0.68608300
C	-5.61645900	-0.81091800	1.39352700
C	-4.08760300	2.52590000	-0.70103900
C	-4.08761200	2.52592200	0.70093900
C	-5.29861300	0.37113100	0.72561800
C	-5.29860400	0.37110700	-0.72566400
C	-5.61644200	-0.81096200	-1.39353900
C	-3.74258400	0.93160000	2.53981700
C	-4.47016000	1.31821800	1.40551600
C	-1.50916800	3.89395600	2.97268800
C	-2.61169800	3.12884800	2.59374400
C	-3.36488900	3.52919300	1.41958400
C	-2.95588400	4.66267800	0.71782200
C	-3.14710300	-4.43836000	-2.29063700
C	-3.65899400	-3.27536800	-3.00117600
C	-3.81296500	-4.92293800	-1.18093400
C	-4.81123300	-2.66298200	-2.57690800
C	-4.87129300	-1.20705700	-2.55525000
C	-1.45133900	1.12511700	-3.40967900
C	-2.62864600	1.75063300	-2.97559300
C	-3.82528600	-0.41217300	-3.02289200
C	-2.60667300	-1.05979500	-3.47209100
C	-2.53144000	-2.45121200	-3.41743600
C	-4.47014300	1.31817300	-1.40558200
C	-3.74255300	0.93151800	-2.53986200
C	-2.95587500	4.66265500	-0.71797800
C	-3.36487100	3.52914700	-1.41970800
C	-2.61166600	3.12876500	-2.59384600
C	-1.50913200	3.89386000	-2.97280100
C	-1.67770100	-5.21927500	0.00008900
C	-0.98475100	-4.69628200	-1.16851700
C	-3.05530200	-5.32544900	0.00008200
C	-1.69653000	-4.31831500	-2.27904900
C	-1.32570500	-3.09205900	-2.97375300
C	1.63639000	-0.51561100	-1.40672300
C	0.91060600	-0.12990600	-2.54299500
C	-0.22340400	-2.32643200	-2.59527600
C	0.52619600	-2.72403500	-1.41908400
C	0.11794800	-3.85794200	-0.71775900
C	-1.38215800	-0.32294100	-3.41022400
C	-0.20439300	-0.94830800	-2.97766500
C	-0.30350900	3.25320000	-3.41691700
C	-0.22690700	1.86180400	-3.47260400
C	0.99239000	1.21371000	-3.02550000
C	2.03764000	2.00917300	-2.55708200
C	0.31194700	5.24088000	-2.29065900
C	0.82395200	4.07799900	-3.00135900
C	1.97617700	3.46540600	-2.57802900
C	0.97744500	5.72619900	-1.18105300
C	-1.15787900	6.02210000	-0.00008900
C	-1.85094000	5.49928000	-1.16861400
C	-1.13868600	5.12059300	-2.27859600
C	0.21981400	6.12882400	-0.00008200

C	0.31191900	5.24095300	2.29052500
C	-1.13871400	5.12066700	2.27844900
C	-1.85095400	5.49931800	1.16844500
C	0.97743000	5.72623700	1.18091100
C	2.68777500	3.97785400	1.41598000
C	1.97614500	3.46548900	2.57797300
C	0.82391600	4.07809600	3.00126800
C	2.20317100	5.07491500	0.72975300
C	2.68779300	3.97780800	-1.41604400
C	3.18292800	2.82127000	-0.68594500
C	3.18291900	2.82129200	0.68592400
C	2.20317900	5.07489100	-0.72985900
C	6.28770900	-1.76833300	-1.31222300
C	6.28769900	-1.76837900	1.31222200
H	6.28386000	-1.76652700	2.41674000
H	6.28387800	-1.76644000	-2.41674100
C	9.74719700	-3.31061600	0.69502200
C	9.74720200	-3.31059100	-0.69505200
C	8.64684700	-2.81990600	-1.41039500
C	7.56125300	-2.33585300	-0.70638700
C	7.56124700	-2.33587800	0.70637600
C	8.64683700	-2.81995600	1.41037500
H	8.65315000	-2.82271400	-2.49706900
H	8.65313200	-2.82280300	2.49704800
C	6.16690400	-0.38509100	-0.70537500
C	6.12095900	0.80364200	-1.41013100
C	6.09570400	2.00701400	-0.69548000
C	6.09569900	2.00698900	0.69561400
C	6.12094900	0.80359200	1.41022100
C	6.16689900	-0.38511600	0.70542300
H	6.11382200	0.80995600	-2.49675000
H	6.11380400	0.80986700	2.49684000
C	3.36856500	-4.16963800	-0.69536200
C	4.26975500	-3.37164900	-1.41018000
C	5.17911400	-2.60492200	-0.70558900
C	5.17910800	-2.60494800	0.70554900
C	4.26974400	-3.37170000	1.41010600
C	3.36856000	-4.16966400	0.69525200
H	4.25938900	-3.36992100	-2.49674400
H	4.25937000	-3.37001100	2.49667000
H	10.60830000	-3.69459100	-1.23826100
H	10.60829000	-3.69463500	1.23822500
H	6.07196300	2.95055000	-1.23775700
H	6.07195900	2.95050600	1.23792400
H	2.66294100	-4.79709700	-1.23782000
H	2.66293300	-4.79714300	1.23768300



Optimized (x,y,z) atomic coordinates for (12,7)SWCNT + iptycene model system
Conformation #1 – 0.0 kJ mol⁻¹

C	12.29536900	2.35648700	-5.56483600
C	4.78054700	2.12930100	-5.68493500
C	7.43274800	2.98004200	-5.12204600
C	8.75890700	3.36860700	-4.79124400
C	9.86404800	2.67432700	-5.35196300
C	11.41125300	4.05986100	-4.04142300
C	11.19018500	3.08124800	-5.04399800
C	-1.40776500	2.34416800	-5.54976000
C	-0.08189700	2.77143300	-5.27006300
C	1.02272700	2.01309500	-5.74060900
C	2.56937000	3.55190700	-4.61338900
C	2.34925800	2.45612700	-5.48627900
C	3.89638000	3.89962500	-4.24056800
C	5.00146700	3.27291100	-4.87561200
C	6.54857400	4.50042400	-3.41605600
C	6.32763800	3.64171200	-4.52298700
C	7.87466600	4.74920200	-2.97019800
C	8.97987100	4.28872600	-3.73473000
C	10.52665200	5.13568100	-2.02546300
C	10.30599800	4.56266600	-3.30394400
C	11.85251100	5.27094100	-1.53256100
C	-8.92303300	2.11525900	-5.66669000
C	-6.27084600	2.97248400	-5.11358000
C	-4.94469100	3.36480800	-4.78725400
C	-3.83954300	2.66413500	-5.34012300
C	-2.29245100	4.06452300	-4.04540600
C	-2.51334100	3.07480700	-5.03684000
C	-0.96630200	4.36749600	-3.63472600
C	0.13893400	3.81580800	-4.33631500
C	1.68591600	4.86980300	-2.74673700
C	1.46516900	4.14204700	-3.94360300
C	3.01190200	5.06585000	-2.27513400

C	4.11725700	4.69423700	-3.08626500
C	5.66353000	5.34171600	-1.29164300
C	5.44330400	4.91712000	-2.62690000
C	6.98922700	5.41968400	-0.78611400
C	8.09516800	5.24881300	-1.66128600
C	9.64021100	5.45290700	0.23669200
C	9.42085000	5.35555300	-1.16121800
C	10.96547300	5.40805200	0.74739400
C	12.07203500	5.44731700	-0.14252800
C	-12.68043500	1.99837000	-5.72097700
C	-11.13350500	3.54965200	-4.61130900
C	-11.35438600	2.44402600	-5.47181200
C	-9.80733000	3.90198200	-4.24211900
C	-8.70213200	3.26790600	-4.87040000
C	-7.15501900	4.51205600	-3.42482700
C	-7.37606200	3.64080700	-4.52200900
C	-5.82891900	4.76587800	-2.98200200
C	-4.72372400	4.29680000	-3.74117100
C	-3.17701000	5.16322800	-2.04180300
C	-3.39759000	4.57569600	-3.31368500
C	-1.85113700	5.30405100	-1.55054000
C	-0.74548400	5.02617400	-2.39814100
C	0.80026900	5.46554900	-0.54112400
C	0.58035700	5.19491200	-1.91592700
C	2.12577400	5.48517600	-0.02946500
C	3.23193200	5.41395700	-0.91788300
C	4.77621900	5.40128700	0.99155200
C	4.55753600	5.46285800	-0.40850500
C	6.10123500	5.29819800	1.49438800
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H	-2.13896500	9.32536300	-0.10327600
C	-1.15730100	8.32929500	-2.47376500
C	1.56781200	9.31844100	-0.10427100
C	1.68871900	8.33114000	-2.47558400
C	0.97038000	8.70117300	1.14256400
C	-1.15595200	8.39010600	2.29194500
C	-0.43853300	8.09940000	-3.64123900
H	-2.24354400	8.31763600	-2.47134400
C	0.93634800	10.72057200	-0.12149200
H	2.67063000	9.32747300	-0.10441400
C	0.96892600	8.10006400	-3.64225800
H	2.77477900	8.32206800	-2.47497500
C	1.69013300	8.38910400	2.28987700
C	-0.43593700	8.18955000	3.46403800
H	-2.24231600	8.37848000	2.29123600
C	-1.04775700	8.06152500	-5.02874500
C	1.57593200	8.06191900	-5.03084000
C	0.97162300	8.18890400	3.46292300
H	2.77605700	8.37695600	2.28755500
C	-1.04274400	8.18821100	4.85322700
C	-0.44159300	6.90389300	-5.79166100
C	-0.44366300	9.28717800	-5.70520800
H	-2.15235400	8.05342400	-5.02243800

C	0.97036900	9.28720700	-5.70664600
C	0.96891800	6.90404800	-5.79277700
H	2.68067100	8.05394100	-5.02657100
C	1.58094900	8.18697400	4.85090900
C	-0.43686700	9.43107400	5.49579000
C	-0.43579200	7.05128800	5.64607300
H	-2.14754700	8.17985200	4.84895500
C	-1.14643600	5.97490600	-6.53557000
C	-1.14821000	10.32803700	-6.27610300
C	1.67364500	10.32772100	-6.27973900
C	1.67281200	5.97504700	-6.53761800
C	0.97458800	7.05004800	5.64422500
C	0.97725500	9.43026800	5.49482700
H	2.68545000	8.17794700	4.84475900
C	-1.13970800	10.48718900	6.04012200
C	-1.13986300	6.14308100	6.41599000
C	-0.43278300	5.04580400	-7.30214500
H	-2.23324300	5.97215500	-6.54156700
C	-0.43271300	11.38371100	-6.85809600
H	-2.23478400	10.33516600	-6.27767700
C	0.95688000	11.38344800	-6.86005800
H	2.76034600	10.33438200	-6.28456000
C	0.95835100	5.04560400	-7.30292900
H	2.76014500	5.97176900	-6.54500800
C	1.67945900	6.14020600	6.41138300
C	1.68204800	10.48542600	6.03849600
C	-0.42263400	11.55763800	6.59242300
H	-2.22639400	10.49491400	6.04363300
C	-0.42551900	5.23389800	7.20523000
H	-2.22700300	6.13972200	6.42243200
H	-0.97586500	4.32036700	-7.90491000
H	-0.97659000	12.20978500	-7.31176300
H	1.49977600	12.20920700	-7.31557600
H	1.50086700	4.31895400	-7.90531600
C	0.96567200	5.23243000	7.20287400
H	2.76636900	6.13508900	6.41513300
C	0.96694300	11.55674600	6.59170600
H	2.76852600	10.49174600	6.04094700
H	-0.96519800	12.39582300	7.02494200
H	-0.96787700	4.52330000	7.82622000
H	1.50879900	4.52109300	7.82241900
H	1.51105400	12.39409700	7.02373000
H	1.58701700	11.57392000	-0.13223300
H	-1.05674700	11.57309300	-0.13147000



Conformation #2 – 92.1 kJ mol⁻¹

C	12.49600000	-1.57647300	-3.69234700
C	5.57336400	1.34755200	-3.95029700
C	8.21997000	0.78437200	-3.08246700
C	9.52144200	0.45461300	-2.61712900
C	10.36164400	-0.38796700	-3.39294200
C	12.07775700	-0.30805600	-1.63805300
C	11.67372200	-0.69428500	-2.94162200
C	-0.01628600	4.01412800	-3.79152300
C	1.30917000	3.73334300	-3.36010000
C	2.11036200	2.80525000	-4.07642000
C	3.91379500	3.07865900	-2.43177000
C	3.44477700	2.54845100	-3.66055100
C	5.19301400	2.69983900	-1.94293400
C	6.07077000	1.94008000	-2.76167200
C	7.70314500	1.83491200	-0.93003200
C	7.36130300	1.58612400	-2.28383500
C	8.93329700	1.34722400	-0.41225700
C	9.89461300	0.77277200	-1.28627100
C	11.34309000	0.25977900	0.62950800
C	11.13669800	0.31154000	-0.77272900
C	12.52276700	-0.33994500	1.14704400
C	-6.93928700	6.93425100	-4.04786900
C	-4.28864900	6.38010800	-3.18653100
C	-2.98503700	6.05508000	-2.72387900
C	-2.14850300	5.20438900	-3.49491500
C	-0.42434500	5.30235600	-1.74890100
C	-0.83421700	4.90270500	-3.04634100
C	0.83190200	4.87247500	-1.24271000
C	1.74878100	4.19958200	-2.09385200
C	3.29462100	3.90245700	-0.20879900
C	3.01666700	3.79549500	-1.59549700
C	4.50073500	3.36144300	0.31243700
C	5.50315700	2.87816700	-0.57042400
C	6.86239100	2.16734700	1.34742900
C	6.72132300	2.36389300	-0.05012900

C	8.01837600	1.51496500	1.85458200
C	9.10704800	1.22301400	0.98983700
C	10.28205900	0.10276500	2.83253200
C	10.27470000	0.59681000	1.50301500
C	11.39076900	-0.65484700	3.29721600
C	12.56118000	-0.76465600	2.49968400
C	-10.40278200	8.39139500	-4.17281500
C	-8.59185500	8.68113800	-2.53959100
C	-9.06662400	8.13824900	-3.76087400
C	-7.31024400	8.30744700	-2.05275500
C	-6.43634400	7.53914200	-2.86777400
C	-4.79545100	7.45283500	-1.04262500
C	-5.14370800	7.19008600	-2.39222500
C	-3.56290600	6.97045200	-0.52570900
C	-2.60570200	6.38688200	-1.39808000
C	-1.14833600	5.89373800	0.51592400
C	-1.36118100	5.93104000	-0.88568200
C	0.03382100	5.29911300	1.03452400
C	1.07746000	4.90794000	0.15361600
C	2.34798800	3.99984900	2.04923700
C	2.27144800	4.33982200	0.67429400
C	3.48093700	3.29619300	2.53960100
C	4.60937400	3.09285500	1.70089400
C	5.70055000	1.78601800	3.47076700
C	5.75372500	2.41459700	2.20039900
C	6.78850100	0.98211800	3.90579000
C	7.99516100	0.95286400	3.15654700
C	8.92444200	-0.71490200	4.70121100
C	9.09322700	0.17177000	3.60714600
C	9.97416200	-1.60422000	5.05663700
C	11.24783100	-1.48356800	4.43925500
C	12.30589600	-2.35421400	4.81562700
C	-9.20065600	9.52798700	-0.32240100
C	-9.48495700	9.40670700	-1.70658100
C	-7.99214600	8.99228700	0.19890000
C	-6.99372500	8.49989000	-0.68366100
C	-5.62560200	7.80880500	1.23501600
C	-5.77315500	7.99094800	-0.16372600
C	-4.46730700	7.16155900	1.74356400
C	-3.38273400	6.86073900	0.87686400
C	-2.19905400	5.75953400	2.72557300
C	-2.21263200	6.23973600	1.39101900
C	-1.08831800	5.00667500	3.19281700
C	0.07848500	4.88885800	2.39112800
C	1.08983900	3.40389200	4.06547000
C	1.20010100	4.15981200	2.87054600
C	2.15858500	2.55713100	4.46538400
C	3.39868800	2.60274600	3.77401300
C	4.25989800	0.78268000	5.17995700
C	4.47688200	1.77708100	4.19223400
C	5.29427100	-0.14077800	5.49016200
C	6.59501200	0.04025200	4.94844200
C	7.33633400	-2.04813600	6.00667600
C	7.63683800	-0.86674200	5.28173600
C	8.34623600	-3.02690600	6.20983500
C	9.69111200	-2.74640300	5.84847600

C	10.35001900	-5.02083000	6.49970700
C	10.70593700	-3.71405700	6.07841300
C	-9.00153400	8.95010600	2.43115700
C	-7.87696100	8.73800200	1.58944400
C	-6.77752600	7.44955100	3.36762400
C	-6.73028500	8.06491300	2.09064700
C	-5.68754000	6.65019300	3.80590300
C	-4.48450600	6.61309700	3.05139300
C	-3.54797400	4.96127300	4.60888100
C	-3.38427100	5.83659400	3.50490200
C	-2.49669700	4.07568200	4.96861900
C	-1.22584700	4.18978300	4.34403900
C	-0.42606000	2.23251000	5.59321300
C	-0.16600800	3.32310200	4.72446700
C	0.59542500	1.27985600	5.85419000
C	1.91932600	1.51312000	5.39510900
C	2.61646500	-0.67490200	6.26565900
C	2.94702200	0.57442700	5.68113900
C	3.61854200	-1.67143400	6.41347400
C	4.97797700	-1.35795000	6.14589800
C	5.61202900	-3.68877500	6.58879800
C	5.98361900	-2.34636900	6.32170300
C	6.60621700	-4.70366600	6.61536800
C	7.98155600	-4.35342700	6.55459400
C	8.59602500	-6.73115000	6.54526500
C	8.97652400	-5.36638300	6.61043300
C	9.59432900	-7.73777200	6.44921200
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C	-9.07793400	8.26953400	3.67318700
C	-8.21030300	6.46405600	5.09384800
C	-7.99782300	7.44814100	4.09482100
C	-7.17440800	5.54376700	5.40867700
C	-5.87629500	5.71915200	4.85912600
C	-5.12998700	3.64171600	5.93547200
C	-4.83291700	4.81563600	5.19692700
C	-4.11914700	2.66506400	6.14400400
C	-2.77597300	2.94172800	5.77349400
C	-2.11414900	0.67416000	6.44500600
C	-1.76011600	1.97640100	6.00861300
C	-1.11732800	-0.33443800	6.53572800
C	0.25231600	0.00214700	6.36542900
C	0.87145200	-2.36329200	6.59455900
C	1.25130300	-1.00119900	6.48487000
C	1.86612900	-3.37751300	6.56244300
C	3.24184500	-3.02572700	6.60220800
C	3.86249100	-5.39102200	6.37612700
C	4.23590200	-4.04111800	6.59935800
C	4.86692900	-6.38443500	6.22325200
C	6.22837000	-6.06310800	6.47094200
C	6.89457800	-8.33039400	5.80277600
C	7.22930800	-7.06384400	6.34626500
C	7.92022100	-9.27752800	5.53801500
C	9.24745900	-9.03050500	5.97986400
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C	-3.48702000	0.32981900	6.56571000
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C	-1.49857200	-1.70018400	6.56597200
C	-0.86165600	-4.03087800	6.12625000
C	-0.50266400	-2.71188100	6.50464300
C	0.15152200	-5.00527600	5.91850600
C	1.49900000	-4.71402800	6.26112200
C	2.20185200	-6.90162700	5.39432600
C	2.50749600	-5.69862400	6.08053600
C	3.24117900	-7.81848400	5.08119200
C	4.54590200	-7.62108000	5.60744900
C	5.35381100	-9.57791800	4.36272400
C	5.57814600	-8.55373600	5.31798200
C	6.42895100	-10.41614700	3.96204100
C	7.67417100	-10.34948800	4.64242600
C	-11.59205400	3.33304300	6.55666100
C	-11.21269600	4.69393200	6.43118000
C	-10.59765500	2.31848600	6.53039800
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C	-8.22763400	1.65515900	6.56308600
C	-7.59839300	-0.69196700	6.20834100
C	-6.23589700	-0.36812600	6.44639500
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C	-4.54845500	-3.59215200	5.53876500
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C	-2.47079900	-5.42853600	4.91765300
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C	-0.13725600	-6.17107600	5.16412700
C	0.73309200	-7.99067100	3.76317600
C	0.90988500	-7.07099500	4.82829100
C	1.82794400	-8.78538900	3.32854100
C	3.04002400	-8.79185800	4.06931300
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C	4.12485400	-9.60870400	3.65101800
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C	6.33759500	-11.14698400	2.74991500
C	7.53334700	-12.24742300	0.90865600
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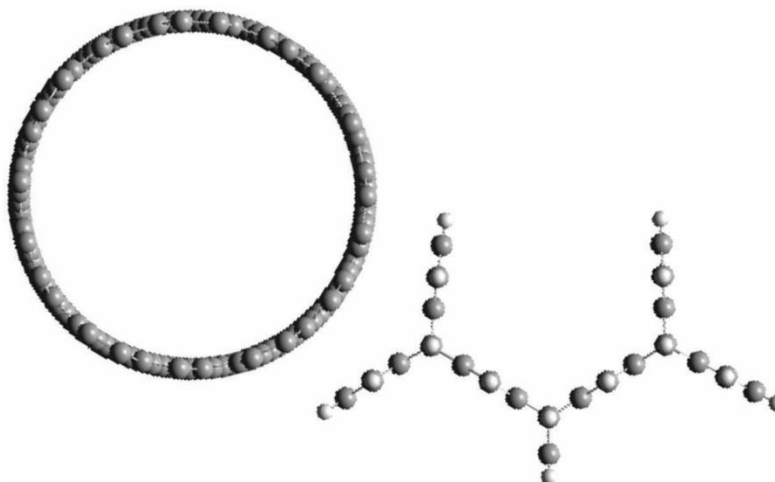
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C	-13.88845300	-0.63476700	4.57390000
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C	-10.65093100	-3.12248400	3.35276600
C	-9.43531500	-3.12139100	4.08792200
C	-8.42083600	-4.62263900	2.43027300
C	-8.35257000	-3.94259500	3.67305300
C	-7.28245500	-5.32109900	1.94511500
C	-6.14394300	-5.49021000	2.77769300
C	-4.95689100	-6.60967600	0.94219900
C	-5.01684800	-6.21364500	2.30286500
C	-3.76907100	-7.19858400	0.43101300
C	-2.71462600	-7.55417600	1.31404400
C	-1.34289500	-8.26425300	-0.59515100
C	-1.53886300	-8.16957500	0.80637500
C	-0.10458400	-8.74107000	-1.10339600
C	0.86325600	-9.28863900	-0.21952700
C	2.42131100	-9.58491100	-2.09445400
C	2.08959700	-9.79205100	-0.73114300
C	3.70831600	-9.95342500	-2.57094500
C	4.59218700	-10.68796100	-1.73578900
C	6.32773500	-10.58928300	-3.47048000
C	5.86787500	-11.08165900	-2.22233300
C	7.65888900	-10.85938600	-3.88781800
C	-14.04501100	-1.50957300	3.46849600
C	-12.95040900	-2.83391200	1.71375800
C	-12.94181600	-2.28585400	3.02186600
C	-11.78887700	-3.48085200	1.21255200
C	-10.68975000	-3.73741600	2.07525400
C	-9.41561500	-4.66393500	0.19139800
C	-9.53982300	-4.41030500	1.58131100
C	-8.20371900	-5.19941800	-0.32217700
C	-7.19053900	-5.64631400	0.56762600
C	-5.72954200	-6.15847900	-1.33873900
C	-5.99069200	-6.20853900	0.05435600
C	-4.46776400	-6.58288000	-1.83542200
C	-3.54046900	-7.22081200	-0.96866700

C	-1.89612600	-7.32518200	-2.78966900
C	-2.29027600	-7.67121900	-1.47192500
C	-0.58740100	-7.64530700	-3.24119900
C	0.25863400	-8.46386100	-2.44613700
C	2.07273900	-8.19034400	-4.07873400
C	1.55662800	-8.80790000	-2.91086700
C	3.42249500	-8.41865600	-4.45944900
C	4.19678000	-9.39753000	-3.78081600
C	6.15718300	-8.79706800	-5.13257200
C	5.53750900	-9.64625500	-4.18050600
C	7.54003100	-8.95152000	-5.42077400
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C	-13.83990600	-2.64177900	-0.56123700
C	-14.02936700	-2.53266100	0.84012900
C	-12.60410100	-3.12392000	-1.07040100
C	-11.63207600	-3.66243900	-0.18527000
C	-10.08275800	-3.97813200	-2.06432600
C	-10.40813500	-4.17117700	-0.69744600
C	-8.79800500	-4.35165800	-2.54298100
C	-7.91036000	-5.07754600	-1.70440700
C	-6.18281100	-4.99693200	-3.44806500
C	-6.63690600	-5.47622000	-2.19275800
C	-4.85359900	-5.27136900	-3.86885400
C	-4.04321200	-6.16940200	-3.12403400
C	-2.15603100	-5.73257300	-4.63354000
C	-2.72404400	-6.46624400	-3.56086300
C	-0.78936600	-5.92330400	-4.97261900
C	-0.04480700	-6.96840400	-4.36330500
C	1.97470900	-6.23583600	-5.55325900
C	1.31367500	-7.17744700	-4.72379500
C	3.36985800	-6.36263100	-5.79123500
C	4.06358800	-7.52174800	-5.35163300
C	6.18039900	-6.57025300	-6.15461400
C	5.45289400	-7.66169100	-5.61515600
C	7.59337800	-6.65666100	-6.27776300
C	8.25428400	-7.89000800	-6.03273300
C	10.42816600	-6.80902900	-6.40304700
C	9.66405500	-7.98373700	-6.18408400
C	-14.40336800	-1.72546600	-2.76281600
C	-14.79151200	-2.05789200	-1.43970800
C	-13.09675800	-2.05030500	-3.21705100
C	-12.24704100	-2.86065400	-2.41754400
C	-10.44065500	-2.60410700	-4.06135600
C	-10.95122900	-3.20955500	-2.88470800
C	-9.09261800	-2.83650400	-4.44592000
C	-8.31513300	-3.80823200	-3.76081100
C	-6.36107100	-3.22195100	-5.12785000
C	-6.97640000	-4.06116900	-4.16415700
C	-4.97959200	-3.37947400	-5.42080500
C	-4.26134500	-4.48352100	-4.88865100
C	-2.19081200	-3.63622300	-5.90152100
C	-2.88697600	-4.65699200	-5.20521000
C	-0.78575300	-3.74064800	-6.08606900
C	-0.10991700	-4.94035800	-5.73676200
C	2.03930600	-3.91550100	-6.33794400
C	1.29040100	-5.05525200	-5.94838700

C	3.45670400	-3.99169500	-6.40346000
C	4.10889100	-5.24508400	-6.25648600
C	6.29455300	-4.13620100	-6.41187800
C	5.52442100	-5.32562700	-6.35099700
C	7.71240100	-4.21052900	-6.35447700
C	8.36144600	-5.47262100	-6.41796100
C	10.53925400	-4.37796100	-6.11844600
C	9.78029200	-5.54493800	-6.38982000
C	-13.30675700	-0.34625200	-4.96523600
C	-12.55940900	-1.38511000	-4.34860700
C	-10.54553600	-0.66494400	-5.55545800
C	-11.20261000	-1.59792000	-4.71320400
C	-9.15150900	-0.79426500	-5.79856200
C	-8.45564500	-1.94882800	-5.35037700
C	-6.34259300	-1.00581600	-6.17301300
C	-7.06770400	-2.09159300	-5.61884700
C	-4.93021900	-1.09360900	-6.30182200
C	-4.26816100	-2.32432600	-6.04704300
C	-2.09605000	-1.24742900	-6.43873500
C	-2.85914300	-2.41976600	-6.20401500
C	-0.67700500	-1.31931600	-6.44582200
C	-0.02886000	-2.58262300	-6.39873300
C	2.15862100	-1.46816900	-6.33699800
C	1.38975800	-2.65590100	-6.43510500
C	3.57251600	-1.55086700	-6.22176200
C	4.22711900	-2.80107800	-6.38483700
C	6.38579900	-1.74762100	-5.87306300
C	5.64333700	-2.87882000	-6.29844700
C	7.78258400	-1.86723200	-5.64174800
C	8.46405800	-3.05946200	-6.00559400
C	10.55091500	-2.16220400	-5.07228000
C	9.86603500	-3.16797900	-5.80099500
C	11.92008800	-2.34261800	-4.73779100
C	-13.30834000	1.82471200	-6.10126000
C	-12.63098900	0.62867400	-5.74260800
C	-10.48446600	1.64714800	-6.36438200
C	-11.23157500	0.51149100	-5.95962000
C	-9.06749100	1.57021600	-6.43586000
C	-8.41456500	0.31829700	-6.27888400
C	-6.22961700	1.42544200	-6.45586400
C	-6.99946100	0.23676400	-6.37916200
C	-4.81149200	1.35168700	-6.40436900
C	-4.16288300	0.08894200	-6.45777200
C	-1.98357300	1.18654000	-6.17976400
C	-2.74390600	0.01687300	-6.43549800
C	-0.57638500	1.08935900	-6.00796500
C	0.08854600	-0.13862100	-6.26860900
C	2.21806900	0.85183600	-5.55099800
C	1.49939900	-0.22786400	-6.12488500
C	3.60312200	0.70617100	-5.26859000
C	4.30388900	-0.44351200	-5.72139600
C	6.34268100	0.34824000	-4.60455900
C	5.69510100	-0.57554200	-5.46404700
C	7.69536300	0.13140300	-4.22703100
C	8.44966000	-0.90074900	-4.84633500
C	9.81084200	-1.09874100	-4.48976600

C	-12.55297700	2.97947600	-6.42934200
C	-10.36515000	4.09429800	-6.38935100
C	-11.13454800	2.90573300	-6.47157400
C	-8.95075200	4.01267800	-6.27983300
C	-8.29689400	2.76088300	-6.43305000
C	-6.13595200	3.81945400	-5.94223600
C	-6.88028800	2.68396200	-6.35240300
C	-4.73797900	3.70220300	-5.71616300
C	-4.05833600	2.50621900	-6.07085200
C	-1.96705800	3.41290900	-5.15668400
C	-2.65542800	2.39972800	-5.87167100
C	-0.59588400	3.23510000	-4.82631400
C	0.12801500	2.13781400	-5.36279600
C	1.50600200	1.97694200	-5.05581800
C	4.22958400	1.58390700	-4.34764400
C	-10.30197400	6.42238800	-5.62764600
C	-11.02346100	5.33680100	-6.18697300
C	-8.91572900	6.27946500	-5.35022600
C	-8.21702700	5.12515300	-5.79430800
C	-6.17308100	5.92833400	-4.69518700
C	-6.82462800	4.99571200	-5.54211100
C	-4.81870100	5.71536100	-4.32183300
C	-4.06723400	4.67673500	-4.93398600
C	-2.70449800	4.48240500	-4.58169600
C	-8.28479200	7.16678000	-4.44120500
C	6.79495100	10.72040300	-2.42925100
C	6.82504400	12.22468100	-2.63372000
C	8.07597300	10.13461800	-2.43176100
C	7.72030100	12.74023000	-1.52086200
C	7.61516000	12.44024500	-3.91888900
H	5.82525900	12.68955600	-2.64918300
C	5.65226600	9.95584900	-2.23596600
C	9.19333800	11.14169700	-2.63878100
C	8.24583700	8.77000800	-2.24047700
C	9.00169700	12.15443100	-1.52373400
C	7.35796300	13.67677900	-0.56274100
C	5.82222400	8.59179700	-2.04226300
H	4.66487400	10.40692000	-2.23058900
C	8.83497400	11.88234400	-3.92151900
H	10.19895400	10.68948600	-2.65865500
C	7.10364200	8.00590300	-2.04396800
H	9.23310400	8.31805700	-2.23906600
C	9.95063200	12.49187700	-0.56870700
C	8.30714300	14.01342300	0.39393400
H	6.36955100	14.12562300	-0.55721800
C	4.69913000	7.59511200	-1.80079100
C	7.08530400	6.50447700	-1.80276000
C	9.58766700	13.42831000	0.39089800
H	10.93693100	12.03830700	-0.56779600
C	8.09471800	15.00504200	1.52279300
C	5.06633800	6.93811400	-0.48505100
C	4.88735100	6.55042800	-2.88212800
H	3.69280600	8.05030000	-1.79924900
C	6.17058700	5.96329200	-2.88274800
C	6.35033100	6.35226700	-0.48583800
H	8.08834300	6.04104200	-1.80309700

C	10.48084300	13.91498300	1.51702300
C	9.22051200	16.01247600	1.38337000
C	8.41089200	14.23272300	2.79027500
H	7.08977500	15.46312700	1.52411200
C	4.29675800	6.94680100	0.66340100
C	3.95813100	6.21300300	-3.84870000
C	6.52170200	5.03878900	-3.84896800
C	6.86295100	5.77792700	0.66246400
C	9.69514800	13.64614200	2.78720500
C	10.50477900	15.42577400	1.38017200
H	11.48501900	13.45527300	1.51346300
C	9.07188800	17.38161500	1.26795300
C	7.56897400	14.07835400	3.87526700
C	4.82332200	6.37841900	1.82998300
H	3.30771800	7.39724500	0.67103100
C	4.32060700	5.28863300	-4.83631500
H	2.96878100	6.66231400	-3.85442500
C	5.58478200	4.70883800	-4.83602200
H	7.50862400	4.58199800	-3.85497500
C	6.08936800	5.80288100	1.82967600
H	7.85231900	5.32776600	0.66907300
C	10.13405500	12.90691700	3.86923000
C	11.63654900	16.20995900	1.26143400
C	10.21988800	18.17535600	1.14804200
H	8.08656000	17.83950100	1.26935400
C	8.01513400	13.32903300	4.97155400
H	6.57866900	14.52526100	3.88321500
H	4.23366500	6.39299100	2.74462000
H	3.60315100	5.02577900	-5.61118800
H	5.85370100	3.99167000	-5.60987000
H	6.48880200	5.37038600	2.74479700
C	9.27986700	12.75150500	4.96859400
H	11.12030800	12.45124200	3.87251300
C	11.48451000	17.59761600	1.14479300
H	12.62771900	15.76488800	1.25773000
H	10.11586600	19.25435700	1.05655800
H	7.36114800	13.19914000	5.83112500
H	9.61332200	12.17081800	5.82586500
H	12.36786200	18.22552900	1.05071600
H	9.55524800	11.90984900	-4.71821000
H	7.16214200	13.00448000	-4.71291200



Conformation #3 – 148.3 kJ mol⁻¹

C	12.13219200	3.86794600	-4.43395600
C	4.62226900	3.49447300	-4.44233300
C	7.27589800	4.18214200	-3.69391800
C	8.60494700	4.47497500	-3.28528000
C	9.70366400	4.03357200	-4.06997900
C	11.26730200	4.95053700	-2.41309200
C	11.03166400	4.35125200	-3.67683300
C	-1.56198300	3.48904800	-4.09537800
C	-0.23526900	3.83551300	-3.72257400
C	0.86747800	3.30400800	-4.44337100
C	2.42267100	4.42579900	-2.90903500
C	2.19311100	3.67326000	-4.08905200
C	3.75286300	4.66639400	-2.47357300
C	4.84902500	4.31313700	-3.30632700
C	6.41978600	5.03187100	-1.56114300
C	6.17896700	4.58018800	-2.88382600
C	7.75475800	5.15489300	-1.09005200
C	8.84316800	5.00128500	-1.98993700
C	10.42805300	5.27858600	-0.13448500
C	10.17727300	5.15300100	-1.52476700
C	11.76619900	5.27894500	0.34354800
C	-9.07179200	3.11308900	-4.10165500
C	-6.41858500	3.81007100	-3.36032400
C	-5.08970300	4.10790900	-2.95467000
C	-3.99066500	3.65794900	-3.73408800
C	-2.42788600	4.59415100	-2.08723400
C	-2.66288000	3.98056000	-3.34412900
C	-1.09487300	4.77975800	-1.63138900
C	-0.00303600	4.51958200	-2.50208000
C	1.57487400	5.03146900	-0.69118300
C	1.32902900	4.73299000	-2.05574900
C	2.91143200	5.09645500	-0.21324800
C	3.99762000	5.04192200	-1.12791000
C	5.58751200	5.10285800	0.74242800
C	5.33279200	5.13594100	-0.65238600
C	6.92684900	5.04497100	1.21347800

C	8.00759100	5.20116500	0.30473100
C	9.60761200	4.80951000	2.12617800
C	9.34627100	5.17224000	0.78011900
C	10.94879000	4.63399300	2.56159000
C	12.02610800	4.99339800	1.70824600
C	-12.82651000	2.92135200	-4.10149500
C	-11.27226600	4.06090700	-2.57946800
C	-11.50110100	3.29495400	-3.75105500
C	-9.94137900	4.30689800	-2.14656000
C	-8.84574800	3.94457100	-2.97515100
C	-7.27556200	4.68358700	-1.23748100
C	-7.51597000	4.21682700	-2.55508000
C	-5.94074900	4.81238400	-0.76757500
C	-4.85213600	4.64887800	-1.66530900
C	-3.26787400	4.94781600	0.18728400
C	-3.51814000	4.80641200	-1.20154600
C	-1.92986200	4.95398000	0.66560300
C	-0.84671700	5.00009300	-0.25243000
C	0.74871800	4.84401400	1.60798500
C	0.49050400	5.03557100	0.22656400
C	2.08907100	4.72904800	2.06557500
C	3.16792200	4.98366700	1.17719900
C	4.77123300	4.38363300	2.93795200
C	4.50779200	4.89708900	1.64229200
C	6.11291100	4.15573600	3.34672900
C	7.18936600	4.60615200	2.53640600
C	8.79675400	3.59796700	4.09552800
C	8.53072500	4.40407200	2.95927100
C	10.13867300	3.27197100	4.43034600
C	11.21439100	3.89404900	3.74201200
C	12.55635500	3.58970200	4.09653700
C	-12.12081800	4.69144100	-0.36901300
C	-12.36609200	4.37754400	-1.73018900
C	-10.78438600	4.76209700	0.10867500
C	-9.69844100	4.69786200	-0.80500600
C	-8.10852000	4.78035100	1.06475900
C	-8.36280800	4.79772700	-0.33039900
C	-6.76927300	4.72817400	1.53687000
C	-5.68842700	4.87452800	0.62674200
C	-4.08868600	4.50408900	2.45296700
C	-4.34977400	4.85143400	1.10277100
C	-2.74767200	4.33388900	2.89063600
C	-1.67013800	4.68412300	2.03359400
C	-0.06438500	3.88369700	3.71045100
C	-0.32937200	4.54116700	2.48205900
C	1.27754700	3.60688200	4.08695400
C	2.35336400	4.14261900	3.32962600
C	3.96137000	2.95968400	4.76003400
C	3.69520000	3.88985500	3.72299600
C	5.30291900	2.59365600	5.05191700
C	6.37909700	3.28624500	4.43521500
C	7.98508200	1.78952700	5.53586300
C	7.72091100	2.93962000	4.74907900
C	9.32536400	1.35681100	5.72446000
C	10.40356700	2.16866600	5.28137900
C	12.00376600	0.44482000	5.98777600

C	11.74426800	1.74966600	5.49598700
C	-11.60728600	4.42040300	2.39115000
C	-10.52817800	4.66532900	1.50026800
C	-8.92515100	4.08583600	3.26811500
C	-9.18839800	4.58444200	1.96670400
C	-7.58351300	3.86310000	3.67984900
C	-6.50707900	4.30458100	2.86478000
C	-4.89969300	3.31463400	4.43567200
C	-5.16567100	4.10774000	3.29024900
C	-3.55785900	2.99292000	4.77456000
C	-2.48205600	3.60745900	4.07945700
C	-0.87455500	2.26529700	5.36225000
C	-1.14009200	3.30768500	4.43777500
C	0.46657200	1.86451100	5.60687200
C	1.54343600	2.61900700	5.06929700
C	3.14719900	1.00242300	5.98902700
C	2.88485300	2.23495300	5.33802700
C	4.48646700	0.54706500	6.12353000
C	5.56630600	1.40044400	5.77192700
C	7.16229300	-0.39723100	6.27404100
C	6.90611100	0.95558500	5.93384400
C	8.49875500	-0.87969800	6.28872500
C	9.58322400	0.02587600	6.14114400
C	11.16823500	-1.84924500	6.19495400
C	10.92043500	-0.45278100	6.18491200
C	12.50109900	-2.32975300	6.08673500
C	-12.41890300	3.32105700	4.42491300
C	-11.34304900	3.84844800	3.66185900
C	-9.73515300	2.68235600	5.10605900
C	-10.00124200	3.60062900	4.05839500
C	-8.39346800	2.32011100	5.40234700
C	-7.31744400	3.00602100	4.77819800
C	-5.71117400	1.52238500	5.89621200
C	-5.97560500	2.66346400	5.09633600
C	-4.37080500	1.09229800	6.09003700
C	-3.29274400	1.89942300	5.63806900
C	-1.69228200	0.18420900	6.36427200
C	-1.95196700	1.48326900	5.85769800
C	-0.35423800	-0.28765800	6.44257400
C	0.72771400	0.59668000	6.18656100
C	2.31881800	-1.25124700	6.47756100
C	2.06629800	0.13217600	6.29319000
C	3.65365300	-1.73637500	6.43363600
C	4.74083500	-0.82329300	6.38628800
C	6.31944800	-2.69739700	6.22300000
C	6.07650500	-1.30801100	6.37164500
C	7.65037800	-3.16673200	6.05723000
C	8.74422900	-2.27491700	6.21932800
C	10.30793100	-4.06731400	5.60857800
C	10.07604200	-2.75068700	6.08217400
C	11.63447800	-4.49246800	5.32818300
C	12.73566600	-3.67079900	5.68881300
C	-12.15296200	2.34443200	5.41850000
C	-10.54903000	0.73891500	6.35682500
C	-10.81149300	1.96386900	5.69191300
C	-9.20964900	0.28554200	6.49689100

C	-8.12988800	1.13519100	6.13600000
C	-6.53345600	-0.65613300	6.65884900
C	-6.79008400	0.69267300	6.30328200
C	-5.19683900	-1.13803700	6.67934400
C	-4.11262500	-0.23377500	6.52183300
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