

SUPPLEMENTARY MATERIAL

Mechanistic, Energetic and Structural Studies of Carbon Nanotubes Functionalized with Penicillamine

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28 Cartesian coordinates, sum of electronic and zero-point energies (E), sum of
 29 electronic and thermal enthalpies (H) and Gibbs free energies (G) for the calculated
 30 structures.

31 1- In water

32

33 NTCOOH

34	C	-4.899397000	-2.146763000	-2.963260000
35	C	-4.899166000	-3.159030000	-2.035517000
36	C	-3.701830000	-3.494569000	-1.325958000
37	C	-3.702526000	-3.765140000	0.098873000
38	C	-2.476948000	-3.627792000	0.803484000
39	C	-2.477128000	-2.991279000	2.090512000
40	C	-1.230843000	-2.488745000	2.593937000
41	C	-1.229466000	-1.221036000	3.237048000
42	C	0.000006000	-0.519475000	3.365658000
43	C	-0.000004000	0.898416000	3.135210000
44	C	1.223742000	1.539153000	2.814654000
45	C	1.217941000	2.599525000	1.865479000
46	C	2.485670000	3.009147000	1.295816000
47	C	2.501168000	3.306701000	-0.121748000
48	C	3.730174000	3.187182000	-0.823237000
49	C	3.717802000	2.529042000	-2.105523000
50	C	4.912255000	2.021834000	-2.720980000
51	C	4.903886000	0.804858000	-3.350516000
52	C	-4.899296000	-3.711905000	0.879486000
53	C	-4.898040000	-3.101484000	2.111953000
54	C	-3.701864000	-2.519002000	2.631367000
55	C	-3.700494000	-1.221244000	3.290362000
56	C	-2.471666000	-0.511777000	3.354440000
57	C	-2.468250000	0.906911000	3.146812000
58	C	-1.223757000	1.539137000	2.814653000
59	C	-1.217971000	2.599508000	1.865478000
60	C	-0.000017000	2.995770000	1.286633000
61	C	-0.000020000	3.656055000	-0.097954000
62	C	1.270296000	3.230081000	-0.831771000
63	C	1.245788000	2.510334000	-2.026632000
64	C	2.484381000	1.996171000	-2.555492000
65	C	2.477073000	0.724238000	-3.220878000
66	C	3.701670000	0.025941000	-3.411470000
67	C	3.700996000	-1.408149000	-3.231191000
68	C	4.899435000	-2.146697000	-2.963257000
69	C	4.899217000	-3.158965000	-2.035514000
70	C	-4.888960000	-0.458031000	3.474312000
71	C	-4.882382000	0.909828000	3.291018000
72	C	-3.689025000	1.588159000	2.913349000
73	C	-3.688632000	2.679330000	1.941361000
74	C	-2.485704000	3.009113000	1.295814000

75	C	-2.501205000	3.306667000	-0.121750000
76	C	-1.270331000	3.230063000	-0.831772000
77	C	-1.245813000	2.510318000	-2.026633000
78	C	-0.000009000	2.000709000	-2.543015000
79	C	0.000000000	0.742457000	-3.175533000
80	C	1.235482000	0.025977000	-3.325768000
81	C	1.233238000	-1.380793000	-3.168892000
82	C	2.475149000	-2.040505000	-2.892150000
83	C	2.475281000	-3.103411000	-1.925460000
84	C	3.701885000	-3.494520000	-1.325956000
85	C	3.702584000	-3.765090000	0.098875000
86	C	4.899353000	-3.711838000	0.879489000
87	C	4.898088000	-3.101417000	2.111956000
88	C	-4.909600000	3.093561000	1.300156000
89	C	-4.931161000	3.326640000	-0.047879000
90	C	-3.730209000	3.187133000	-0.823240000
91	C	-3.717828000	2.528992000	-2.105526000
92	C	-2.484398000	1.996138000	-2.555495000
93	C	-2.477073000	0.724205000	-3.220880000
94	C	-1.235473000	0.025960000	-3.325769000
95	C	-1.233210000	-1.380809000	-3.168893000
96	C	0.000018000	-2.043028000	-2.883300000
97	C	0.000025000	-3.096650000	-1.926869000
98	C	1.233262000	-3.446715000	-1.298424000
99	C	1.231975000	-3.718328000	0.095465000
100	C	2.477004000	-3.627759000	0.803485000
101	C	2.477174000	-2.991245000	2.090513000
102	C	3.701903000	-2.518951000	2.631369000
103	C	3.700515000	-1.221194000	3.290364000
104	C	4.888971000	-0.457965000	3.474315000
105	C	4.882375000	0.909894000	3.291022000
106	C	-4.912272000	2.021768000	-2.720984000
107	C	-4.903887000	0.804792000	-3.350520000
108	C	-3.701661000	0.025892000	-3.411472000
109	C	-3.700967000	-1.408199000	-3.231193000
110	C	-2.475113000	-2.040538000	-2.892152000
111	C	-2.475231000	-3.103444000	-1.925461000
112	C	-1.233208000	-3.446731000	-1.298425000
113	C	-1.231917000	-3.718345000	0.095464000
114	C	0.000028000	-3.638324000	0.808584000
115	C	0.000023000	-3.001603000	2.092374000
116	C	1.230883000	-2.488728000	2.593938000
117	C	1.229488000	-1.221019000	3.237049000
118	C	2.471678000	-0.511743000	3.354442000
119	C	2.468243000	0.906945000	3.146815000
120	C	3.689009000	1.588209000	2.913352000
121	C	3.688602000	2.679381000	1.941364000
122	C	4.909565000	3.093628000	1.300160000
123	C	4.931124000	3.326706000	-0.047875000
124	H	-5.883959000	3.482254000	-0.542682000

125	H	-5.845021000	3.077940000	1.848607000
126	H	-5.831150000	1.435294000	3.292029000
127	H	-5.842218000	-0.958489000	3.606105000
128	H	-5.846665000	-2.932183000	2.610281000
129	H	-5.847791000	-4.005204000	0.442516000
130	H	-5.846336000	-3.598386000	-1.741249000
131	H	-5.845753000	-1.816509000	-3.377808000
132	H	-5.844169000	0.378695000	-3.683872000
133	H	-5.857450000	2.532289000	-2.570510000
134	H	5.844174000	0.378773000	-3.683868000
135	H	5.857425000	2.532367000	-2.570506000
136	H	5.883920000	3.482332000	-0.542678000
137	H	5.844985000	3.078019000	1.848612000
138	H	5.831136000	1.435373000	3.292034000
139	H	5.842236000	-0.958410000	3.606109000
140	H	5.846710000	-2.932103000	2.610285000
141	H	5.847852000	-4.005125000	0.442520000
142	H	5.846393000	-3.598307000	-1.741246000
143	H	5.845787000	-1.816431000	-3.377804000
144	C	-0.000032000	5.211032000	-0.062834000
145	O	-0.000119000	5.899911000	-1.061235000
146	O	-0.000187000	5.712920000	1.182516000
147	H	-0.000297000	6.684006000	1.103421000
148	E=-3630,141426000,H=-3630,09431000,G=-3630,20669700 a.u.			
149				
150	PCA			
151	C	-0.414380000	0.596098000	-0.596400000
152	C	-1.590579000	-0.141967000	0.042263000
153	C	0.965825000	0.210924000	0.048526000
154	O	-2.175354000	-1.011821000	-0.800087000
155	N	-0.770427000	2.015424000	-0.553214000
156	S	1.155922000	-1.654534000	0.028771000
157	O	-1.997558000	0.061330000	1.169933000
158	C	1.074388000	0.617047000	1.526058000
159	C	2.104483000	0.846269000	-0.762275000
160	H	-0.371385000	0.299192000	-1.648553000
161	H	-2.920630000	-1.421038000	-0.324234000
162	H	-0.064411000	2.578750000	-1.017816000
163	H	-0.835667000	2.331235000	0.410890000
164	H	1.118880000	-1.821718000	-1.309144000
165	H	2.053228000	0.335317000	1.923781000
166	H	0.295825000	0.155896000	2.135859000
167	H	0.981901000	1.703620000	1.618707000
168	H	3.074121000	0.547690000	-0.356833000
169	H	2.046585000	1.939310000	-0.713273000
170	H	2.064669000	0.550032000	-1.815014000
171	E=-800.417185000,H=-800.40523600,G=-800.45318800a.u.			
172	NTCOOH/PCA1R			
173	C	-4.192949000	-4.208062000	3.142135000
174	C	-5.242459000	-3.953744000	2.293787000

175	C	-5.332753000	-2.702903000	1.603367000
176	C	-5.702814000	-2.621965000	0.203142000
177	C	-5.328429000	-1.457335000	-0.518062000
178	C	-4.809786000	-1.595658000	-1.849824000
179	C	-4.062034000	-0.500794000	-2.398878000
180	C	-2.883413000	-0.796980000	-3.136209000
181	C	-1.918769000	0.229201000	-3.327055000
182	C	-0.529055000	-0.114177000	-3.206288000
183	C	0.408780000	0.916231000	-2.942247000
184	C	1.506177000	0.643903000	-2.078685000
185	C	2.248833000	1.769928000	-1.549570000
186	C	2.651647000	1.694503000	-0.160951000
187	C	2.889099000	2.906597000	0.540563000
188	C	2.345512000	3.038508000	1.869696000
189	C	2.188682000	4.312652000	2.513425000
190	C	1.055515000	4.590993000	3.232058000
191	C	-5.999867000	-3.786483000	-0.571353000
192	C	-5.502721000	-3.917716000	-1.847134000
193	C	-4.688830000	-2.891588000	-2.416832000
194	C	-3.482014000	-3.194848000	-3.172260000
195	C	-2.504727000	-2.171834000	-3.298281000
196	C	-1.115176000	-2.511492000	-3.200729000
197	C	-0.178221000	-1.459372000	-2.927966000
198	C	0.923699000	-1.720264000	-2.064734000
199	C	1.643494000	-0.640864000	-1.524209000
200	C	2.384555000	-0.819695000	-0.193448000
201	C	2.332409000	0.509212000	0.559354000
202	C	1.723518000	0.645182000	1.807941000
203	C	1.565147000	1.965029000	2.365981000
204	C	0.382417000	2.257115000	3.125033000
205	C	0.016181000	3.611730000	3.359331000
206	C	-1.385398000	3.958296000	3.288762000
207	C	-1.832515000	5.302171000	3.070983000
208	C	-2.883404000	5.556282000	2.224326000
209	C	-3.043091000	-4.529428000	-3.406153000
210	C	-1.703769000	-4.853643000	-3.329106000
211	C	-0.731530000	-3.863047000	-3.013382000
212	C	0.398986000	-4.136943000	-2.128083000
213	C	1.056102000	-3.056203000	-1.517293000
214	C	1.444309000	-3.159078000	-0.125846000
215	C	1.722248000	-1.953885000	0.577879000
216	C	1.121251000	-1.772997000	1.823370000
217	C	0.967705000	-0.446849000	2.368416000
218	C	-0.200560000	-0.150972000	3.096427000
219	C	-0.584499000	1.218958000	3.291482000
220	C	-1.957978000	1.557063000	3.242158000
221	C	-2.318206000	2.924555000	3.008540000
222	C	-3.421040000	3.191671000	2.127180000
223	C	-3.550203000	4.483218000	1.550995000
224	C	-3.920579000	4.565469000	0.151111000

225	C	-3.642233000	5.723212000	-0.640194000
226	C	-3.147019000	5.589865000	-1.916439000
227	C	0.552425000	-5.428850000	-1.511225000
228	C	0.873489000	-5.521545000	-0.184390000
229	C	1.086532000	-4.331686000	0.590684000
230	C	0.550096000	-4.177092000	1.919920000
231	C	0.365979000	-2.857180000	2.400120000
232	C	-0.811911000	-2.551477000	3.161133000
233	C	-1.180082000	-1.179311000	3.309671000
234	C	-2.552319000	-0.836843000	3.260257000
235	C	-2.917658000	0.522815000	3.017930000
236	C	-4.010533000	0.787498000	2.145822000
237	C	-4.100339000	2.075905000	1.537526000
238	C	-4.469079000	2.155948000	0.168548000
239	C	-4.136668000	3.351103000	-0.552945000
240	C	-3.618572000	3.213193000	-1.884983000
241	C	-2.909367000	4.294905000	-2.469970000
242	C	-1.703067000	3.989228000	-3.225349000
243	C	-0.692562000	4.961659000	-3.473804000
244	C	0.643355000	4.624691000	-3.393604000
245	C	-0.181082000	-5.221328000	2.581372000
246	C	-1.308528000	-4.927558000	3.302602000
247	C	-1.767816000	-3.574025000	3.414332000
248	C	-3.169150000	-3.225999000	3.343551000
249	C	-3.511030000	-1.880381000	3.044474000
250	C	-4.612947000	-1.613537000	2.162094000
251	C	-4.693993000	-0.317909000	1.554902000
252	C	-5.061876000	-0.235348000	0.185891000
253	C	-4.743547000	0.949573000	-0.539764000
254	C	-4.224723000	0.811334000	-1.868656000
255	C	-3.470287000	1.888349000	-2.416465000
256	C	-2.292486000	1.589625000	-3.153953000
257	C	-1.316677000	2.626809000	-3.333633000
258	C	0.070903000	2.280412000	-3.233433000
259	C	1.040949000	3.299166000	-3.060241000
260	C	2.170952000	3.024356000	-2.175046000
261	C	2.917279000	4.100786000	-1.576637000
262	C	3.254833000	4.048151000	-0.251747000
263	H	0.829325000	-6.488921000	0.304707000
264	H	0.268482000	-6.326352000	-2.049738000
265	H	-1.423379000	-5.900776000	-3.363574000
266	H	-3.766274000	-5.333255000	-3.491922000
267	H	-5.606007000	-4.873044000	-2.350766000
268	H	-6.479700000	-4.641368000	-0.107180000
269	H	-5.917947000	-4.763865000	2.040155000
270	H	-4.070063000	-5.210699000	3.537202000
271	H	-1.922070000	-5.741323000	3.674294000
272	H	0.073883000	-6.259863000	2.399170000
273	H	0.895076000	5.602549000	3.589481000
274	H	2.899411000	5.108716000	2.318679000

275	H	3.673844000	4.928821000	0.223339000
276	H	3.085236000	5.019245000	-2.128349000
277	H	1.380054000	5.419358000	-3.439504000
278	H	-0.957765000	6.008771000	-3.572883000
279	H	-2.794204000	6.475901000	-2.433482000
280	H	-3.664611000	6.709385000	-0.189095000
281	H	-3.103433000	6.584712000	1.958237000
282	H	-1.253345000	6.136420000	3.451959000
283	C	3.903080000	-1.151856000	-0.349322000
284	O	4.554895000	-1.598492000	0.583264000
285	O	4.392310000	-0.850235000	-1.536022000
286	H	5.417564000	-0.963822000	-1.527646000
287	C	7.666899000	-0.928858000	-0.226874000
288	C	7.095230000	0.272524000	0.526555000
289	C	9.240343000	-0.920688000	-0.228971000
290	O	6.568754000	1.201431000	-0.291428000
291	N	7.061347000	-1.024984000	-1.564969000
292	S	9.786475000	-1.049438000	1.569328000
293	O	7.135233000	0.395481000	1.732765000
294	C	9.810097000	0.361289000	-0.854491000
295	C	9.755658000	-2.160875000	-0.976969000
296	H	7.336558000	-1.804133000	0.337661000
297	H	6.230736000	1.927562000	0.262366000
298	H	7.342575000	-1.891870000	-2.015702000
299	H	7.361228000	-0.258453000	-2.164112000
300	H	11.031387000	-1.480170000	1.283545000
301	H	10.902575000	0.328723000	-0.853984000
302	H	9.499219000	1.255783000	-0.309267000
303	H	9.487652000	0.462172000	-1.897546000
304	H	10.844796000	-2.222116000	-0.904848000
305	H	9.511769000	-2.102860000	-2.042685000
306	H	9.332718000	-3.082976000	-0.568442000
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308				
309	TS _{k1}			
310	C	5.058597000	-3.420958000	-2.807358000
311	C	5.923540000	-3.051702000	-1.806686000
312	C	5.713305000	-1.840229000	-1.073430000
313	C	5.867707000	-1.776080000	0.367338000
314	C	5.213055000	-0.723748000	1.061023000
315	C	4.544157000	-1.011570000	2.298453000
316	C	3.557038000	-0.079197000	2.762808000
317	C	2.349565000	-0.596642000	3.305079000
318	C	1.212093000	0.251826000	3.380007000
319	C	-0.071363000	-0.298850000	3.043389000
320	C	-1.121746000	0.581138000	2.683156000
321	C	-2.034771000	0.183607000	1.664700000
322	C	-2.859630000	1.217723000	1.068444000
323	C	-3.026744000	1.164864000	-0.369373000
324	C	-3.351983000	2.365244000	-1.055795000

325	C	-2.667988000	2.644720000	-2.290689000
326	C	-2.635113000	3.957218000	-2.873433000
327	C	-1.474460000	4.443950000	-3.414273000
328	C	6.238804000	-2.919416000	1.141413000
329	C	5.597725000	-3.193534000	2.327026000
330	C	4.557452000	-2.338379000	2.803003000
331	C	3.322033000	-2.867239000	3.362692000
332	C	2.181928000	-2.020094000	3.367972000
333	C	0.895661000	-2.568282000	3.053033000
334	C	-0.154033000	-1.664922000	2.671382000
335	C	-1.070962000	-2.051551000	1.654934000
336	C	-1.898949000	-1.078999000	1.056793000
337	C	-2.405954000	-1.293086000	-0.382576000
338	C	-2.443727000	0.072136000	-1.071333000
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430	O	-7.278338000	-1.209449000	-2.329651000
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695	O	4.085720000	0.250211000	-2.892165000
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697	H	5.406782000	-0.914853000	-1.309733000
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963	H	-2.556013000	-5.420379000	3.909868000
964	H	-4.637859000	-4.978294000	3.312216000
965	H	-6.088706000	-4.724837000	1.393599000
966	H	-6.128986000	-4.798764000	-0.825933000
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969	O	4.310172000	-1.665206000	-2.061516000
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971	H	7.500696000	-1.886428000	-2.836372000
972	C	6.920609000	-1.031369000	0.741165000
973	C	6.100088000	-0.392153000	-0.374229000
974	C	8.355532000	-0.438755000	0.920830000

975	O	4.723660000	-0.566021000	-0.118963000
976	N	6.813303000	-2.464829000	0.482891000
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979	C	9.249395000	-0.581176000	-0.320884000
980	C	9.025332000	-1.116761000	2.125847000
981	H	6.372924000	-0.830881000	1.669372000
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1265	H	-7.161217000	-3.821808000	-0.299911000
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1271	C	5.213678000	-2.983765000	-0.690303000
1272	C	5.212222000	-2.997615000	0.759928000
1273	C	4.747228000	-1.838541000	1.436267000
1274	C	3.891877000	-1.991505000	2.579147000

1275	C	3.106190000	-0.862767000	2.988262000
1276	C	1.758451000	-1.089382000	3.378342000
1277	C	0.852713000	0.006093000	3.382975000
1278	C	-0.478075000	-0.211438000	2.889443000
1279	C	-1.242856000	0.906306000	2.467681000
1280	C	-2.097943000	0.768080000	1.339449000
1281	C	-2.593244000	1.976360000	0.713226000
1282	C	-2.619325000	1.998880000	-0.733794000
1283	C	-2.582677000	3.256853000	-1.393772000
1284	C	-1.702797000	3.400475000	-2.528534000
1285	C	-1.294595000	4.684224000	-3.025538000
1286	C	0.003329000	4.896042000	-3.410581000
1287	C	5.213859000	-4.217064000	1.506515000
1288	C	4.393899000	-4.362219000	2.601088000
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1290	C	2.156000000	-3.528395000	3.411079000
1291	C	1.254400000	-2.432505000	3.350287000
1292	C	-0.082763000	-2.648192000	2.880637000
1293	C	-0.840635000	-1.509334000	2.446909000
1294	C	-1.698013000	-1.637393000	1.318648000
1295	C	-2.186779000	-0.477334000	0.688030000
1296	C	-2.552571000	-0.524460000	-0.801616000
1297	C	-2.206761000	0.824541000	-1.423908000
1298	C	-1.288594000	0.962827000	-2.465543000
1299	C	-0.897976000	2.287804000	-2.877268000
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1302	C	2.323647000	4.059642000	-2.886780000
1303	C	2.792158000	5.349375000	-2.474413000
1304	C	3.602749000	5.474576000	-1.373297000
1305	C	1.578780000	-4.830183000	3.438916000
1306	C	0.286146000	-5.035710000	3.002263000
1307	C	-0.498388000	-3.952614000	2.514265000
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1309	C	-1.777020000	-2.930129000	0.670181000
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1311	C	-1.795387000	-1.679743000	-1.448095000
1312	C	-0.881584000	-1.493814000	-2.487140000
1313	C	-0.495887000	-0.163935000	-2.887196000
1314	C	0.839950000	0.062595000	-3.271538000
1315	C	1.358068000	1.401719000	-3.272837000
1316	C	2.692267000	1.618525000	-2.853268000
1317	C	3.075678000	2.938261000	-2.446310000
1318	C	3.928332000	3.070407000	-1.297899000
1319	C	3.995043000	4.319098000	-0.624652000
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1321	C	3.603341000	5.447308000	1.593452000
1322	C	2.783510000	5.299522000	2.687616000
1323	C	-1.457439000	-5.334043000	0.636115000
1324	C	-1.430829000	-5.338086000	-0.731589000

1325	C	-1.350809000	-4.100054000	-1.455142000
1326	C	-0.477862000	-3.931757000	-2.589333000
1327	C	-0.081446000	-2.612032000	-2.919387000
1328	C	1.272592000	-2.375532000	-3.332720000
1329	C	1.764696000	-1.035273000	-3.294297000
1330	C	3.098456000	-0.814220000	-2.875285000
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1332	C	4.329736000	0.627770000	-1.322686000
1333	C	4.350640000	1.875411000	-0.628980000
1334	C	4.355888000	1.862171000	0.790825000
1335	C	3.932675000	3.047562000	1.479982000
1336	C	3.077006000	2.894782000	2.622485000
1337	C	2.318504000	4.005887000	3.075306000
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1346	C	4.743483000	-1.812746000	-1.341923000
1347	C	4.756623000	-0.557443000	-0.650789000
1348	C	4.761117000	-0.568138000	0.769100000
1349	C	4.349441000	0.606033000	1.464949000
1350	C	3.493369000	0.453104000	2.603648000
1351	C	2.701210000	1.565270000	3.009704000
1352	C	1.354028000	1.336057000	3.399773000
1353	C	0.441579000	2.443546000	3.393142000
1354	C	-0.894282000	2.222068000	2.922728000
1355	C	-1.711400000	3.327428000	2.577435000
1356	C	-2.588292000	3.191470000	1.417452000
1357	C	-3.073505000	4.353847000	0.719449000
1358	C	-3.057789000	4.389558000	-0.647907000
1359	H	-1.331113000	-6.282409000	-1.256130000
1360	H	-1.387175000	-6.275983000	1.168762000
1361	H	-0.067237000	-6.055557000	2.896307000
1362	H	2.196984000	-5.694962000	3.654363000
1363	H	4.293769000	-5.344575000	3.050303000
1364	H	5.734988000	-5.088462000	1.124964000
1365	H	5.744340000	-5.065594000	-1.097469000
1366	H	4.318205000	-5.285577000	-3.040099000
1367	H	2.246812000	-5.623059000	-3.750927000
1368	H	-0.044167000	-6.024204000	-3.066184000
1369	H	0.323219000	5.905452000	-3.646097000
1370	H	-1.972746000	5.528682000	-2.965852000
1371	H	-3.274599000	5.323217000	-1.155726000
1372	H	-3.311097000	5.258252000	1.268510000
1373	H	-1.984460000	5.449940000	2.995191000
1374	H	0.276077000	5.829970000	3.755137000

1375	H	2.372074000	6.188183000	3.154284000
1376	H	3.813490000	6.447109000	1.229234000
1377	H	3.818017000	6.467275000	-0.992521000
1378	H	2.391741000	6.245994000	-2.935041000
1379	C	-4.080800000	-0.753635000	-1.116254000
1380	O	-4.469541000	-0.777448000	-2.270703000
1381	O	-4.973508000	1.669468000	-3.743544000
1382	H	-4.695834000	2.279443000	-3.046900000
1383	C	-7.783650000	-1.255831000	0.921164000
1384	C	-7.621109000	-0.147073000	1.962158000
1385	C	-6.881772000	-1.034136000	-0.363040000
1386	O	-6.838212000	-0.517466000	2.990755000
1387	N	-9.216357000	-1.347429000	0.659487000
1388	S	-5.118852000	-0.938070000	0.317416000
1389	O	-8.150945000	0.943560000	1.888812000
1390	C	-7.234515000	0.265012000	-1.099748000
1391	C	-7.016838000	-2.263344000	-1.274223000
1392	H	-7.461576000	-2.194196000	1.382316000
1393	H	-6.769158000	0.242030000	3.597423000
1394	H	-9.417178000	-2.077205000	-0.017091000
1395	H	-9.561290000	-0.466973000	0.286431000
1396	H	-4.669954000	0.808186000	-3.415223000
1397	H	-6.575063000	0.431280000	-1.952022000
1398	H	-7.179147000	1.130164000	-0.436597000
1399	H	-8.258396000	0.195925000	-1.482772000
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1414	C	1.232018000	-2.377139000	-2.749990000
1415	C	1.229890000	-1.066096000	-3.298558000
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1420	C	-2.487959000	3.006744000	-1.056346000
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1422	C	-3.731020000	3.027497000	1.070644000
1423	C	-3.717378000	2.278289000	2.302210000
1424	C	-4.911300000	1.728962000	2.880779000

1425	C	-4.902513000	0.469377000	3.420012000
1426	C	4.901089000	-3.719266000	-1.129400000
1427	C	4.899421000	-3.021168000	-2.314444000
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1429	C	3.700536000	-1.061707000	-3.353696000
1430	C	2.471547000	-0.349952000	-3.365589000
1431	C	2.467828000	1.049739000	-3.055533000
1432	C	1.223469000	1.656072000	-2.677479000
1433	C	1.217916000	2.645289000	-1.654888000
1434	C	-0.001362000	3.004363000	-1.050772000
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1436	C	-1.271873000	3.067130000	1.080875000
1437	C	-1.245013000	2.264653000	2.222749000
1438	C	-2.483756000	1.714418000	2.712567000
1439	C	-2.476102000	0.398569000	3.285584000
1440	C	-3.700415000	-0.311720000	3.425097000
1441	C	-3.699435000	-1.728951000	3.140095000
1442	C	-4.897543000	-2.446487000	2.819701000
1443	C	-4.897000000	-3.386621000	1.818855000
1444	C	4.888710000	-0.286750000	-3.485282000
1445	C	4.881997000	1.063702000	-3.202789000
1446	C	3.688818000	1.712127000	-2.774760000
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1448	C	2.485227000	3.009312000	-1.056841000
1449	C	2.500138000	3.198823000	0.378004000
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1451	C	1.243638000	2.265699000	2.222456000
1452	C	-0.000398000	1.722452000	2.703954000
1453	C	0.000260000	0.420702000	3.243326000
1454	C	-1.234364000	-0.305007000	3.341060000
1455	C	-1.231669000	-1.696318000	3.080078000
1456	C	-2.473386000	-2.334173000	2.755635000
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1458	C	-3.699690000	-3.668968000	1.086902000
1459	C	-3.700432000	-3.832746000	-0.354210000
1460	C	-4.897186000	-3.724159000	-1.128688000
1461	C	-4.896378000	-3.026094000	-2.313748000
1462	C	4.908975000	3.093508000	-1.054030000
1463	C	4.929512000	3.226006000	0.307743000
1464	C	3.728672000	3.030974000	1.069961000
1465	C	3.715986000	2.281730000	2.301525000
1466	C	2.482981000	1.716697000	2.712119000
1467	C	2.476665000	0.400895000	3.285220000
1468	C	1.235595000	-0.303846000	3.340891000
1469	C	1.234199000	-1.695155000	3.079922000
1470	C	0.001548000	-2.335678000	2.747728000
1471	C	0.001953000	-3.315594000	1.715285000
1472	C	-1.231120000	-3.619353000	1.063148000
1473	C	-1.229920000	-3.785598000	-0.347145000
1474	C	-2.474913000	-3.644407000	-1.046568000

1475	C	-2.475547000	-2.916322000	-2.283940000
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1477	C	-3.699619000	-1.065433000	-3.353135000
1478	C	-4.888596000	-0.291660000	-3.484474000
1479	C	-4.883188000	1.058779000	-3.201890000
1480	C	4.910534000	1.733583000	2.879925000
1481	C	4.903033000	0.474032000	3.419258000
1482	C	3.701677000	-0.308212000	3.424583000
1483	C	3.702009000	-1.725444000	3.139614000
1484	C	2.476486000	-2.331829000	2.755317000
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1486	C	1.235228000	-3.618159000	1.062972000
1487	C	1.233997000	-3.784379000	-0.347325000
1488	C	0.001923000	-3.653953000	-1.052331000
1489	C	0.001476000	-2.924591000	-2.285792000
1490	C	-1.229681000	-2.378383000	-2.749818000
1491	C	-1.228953000	-1.067336000	-3.298373000
1492	C	-2.471345000	-0.352447000	-3.365196000
1493	C	-2.468983000	1.047220000	-3.055058000
1494	C	-3.690582000	1.708371000	-2.774036000
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1496	C	-4.911787000	3.088648000	-1.053129000
1497	C	-4.932199000	3.221268000	0.308630000
1498	H	5.882025000	3.342802000	0.813541000
1499	H	5.845183000	3.116737000	-1.600683000
1500	H	5.830217000	1.588981000	-3.168520000
1501	H	5.841692000	-0.775791000	-3.655670000
1502	H	5.847863000	-2.815423000	-2.799210000
1503	H	5.849800000	-4.042592000	-0.714851000
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1505	H	5.846957000	-2.142825000	3.256803000
1506	H	5.843782000	0.025675000	3.720554000
1507	H	5.855180000	2.254463000	2.766986000
1508	H	-5.842784000	0.020092000	3.721417000
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1510	H	-5.884732000	3.337167000	0.814598000
1511	H	-5.848116000	3.110927000	-1.599616000
1512	H	-5.831923000	1.583113000	-3.167437000
1513	H	-5.841117000	-0.781645000	-3.654737000
1514	H	-5.845090000	-2.821292000	-2.798381000
1515	H	-5.845517000	-4.048406000	-0.713990000
1516	H	-5.843937000	-3.803222000	1.492408000
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1518	C	-0.002142000	5.107084000	0.524330000
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1526	C	0.965671000	0.211041000	0.048639000
1527	O	-2.173835000	-1.013997000	-0.799436000
1528	N	-0.770706000	2.015061000	-0.554346000
1529	S	1.156491000	-1.654182000	0.029324000
1530	O	-1.998427000	0.062730000	1.168897000
1531	C	1.073434000	0.617554000	1.526115000
1532	C	2.104467000	0.846632000	-0.761815000
1533	H	-0.371058000	0.298438000	-1.648926000
1534	H	-2.918564000	-1.423393000	-0.322931000
1535	H	-0.063374000	2.578991000	-1.016145000
1536	H	-0.840297000	2.330224000	0.409649000
1537	H	1.117899000	-1.821457000	-1.308561000
1538	H	2.052106000	0.336056000	1.924426000
1539	H	0.294593000	0.156450000	2.135572000
1540	H	0.980608000	1.704134000	1.618434000
1541	H	3.074041000	0.548334000	-0.356036000
1542	H	2.046387000	1.939710000	-0.713121000
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1549	C	2.457537000	4.791581000	2.111953000
1550	C	3.114620000	4.998287000	0.835373000
1551	C	3.678787000	3.868305000	0.186156000
1552	C	3.505823000	3.717141000	-1.230946000
1553	C	3.701271000	2.414010000	-1.798453000
1554	C	2.788726000	1.972217000	-2.794603000
1555	C	2.692737000	0.580688000	-3.067285000
1556	C	1.387949000	0.019099000	-3.277821000
1557	C	1.209523000	-1.377554000	-3.105629000
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1561	C	-0.340951000	-4.577262000	-0.013781000
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1566	C	2.670378000	5.989084000	-1.342490000
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1568	C	1.847597000	4.249973000	-2.973088000
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1571	C	0.257939000	0.875083000	-3.236760000
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1573	C	-1.001196000	-0.925766000	-2.170593000
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1577	C	-0.303549000	-3.096990000	1.931026000
1578	C	0.603744000	-2.651574000	2.950256000
1579	C	1.629088000	-3.525867000	3.405647000
1580	C	2.934437000	-2.962945000	3.667287000
1581	C	4.121754000	-3.764256000	3.696366000
1582	C	5.281673000	-3.308192000	3.119986000
1583	C	0.778563000	5.064781000	-3.444589000
1584	C	-0.465453000	4.520411000	-3.688712000
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1590	C	-2.028354000	0.178843000	1.079822000
1591	C	-1.264518000	-0.812685000	1.792783000
1592	C	-0.355617000	-0.375775000	2.777423000
1593	C	0.701463000	-1.248953000	3.200527000
1594	C	1.975236000	-0.696258000	3.476825000
1595	C	3.113451000	-1.566976000	3.475327000
1596	C	4.329347000	-1.088955000	2.878115000
1597	C	5.323410000	-2.024723000	2.487347000
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1602	C	-3.582388000	3.398929000	-1.240589000
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1663	N	-7.404787000	-2.491756000	0.081479000
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1666	C	-9.177773000	-0.397971000	-1.374784000
1667	C	-6.958670000	0.518398000	-0.610516000
1668	H	-7.353237000	-1.024683000	1.546543000
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1672	H	-8.318547000	1.386658000	1.797084000
1673	H	-9.344158000	0.507795000	-1.964444000
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2173	C	2.714321000	1.787973000	2.952420000
2174	C	1.392872000	1.456294000	3.355825000

2175	C	0.394053000	2.486001000	3.341603000
2176	C	-0.921621000	2.150573000	2.883473000
2177	C	-1.824032000	3.182102000	2.524135000
2178	C	-2.687908000	2.960700000	1.369713000
2179	C	-3.268867000	4.065963000	0.656485000
2180	C	-3.261100000	4.079656000	-0.710628000
2181	H	-0.688471000	-6.414383000	-1.179295000
2182	H	-0.737133000	-6.378287000	1.248234000
2183	H	0.570441000	-6.028598000	2.970631000
2184	H	2.803726000	-5.474690000	3.712043000
2185	H	4.858767000	-4.964651000	3.079498000
2186	H	6.266529000	-4.620878000	1.141773000
2187	H	6.268857000	-4.627718000	-1.078887000
2188	H	4.862485000	-4.989145000	-3.015611000
2189	H	2.820020000	-5.504689000	-3.704937000
2190	H	0.574145000	-6.077129000	-2.992163000
2191	H	-0.035916000	5.819886000	-3.757540000
2192	H	-2.288360000	5.264542000	-3.049981000
2193	H	-3.561576000	4.980662000	-1.234701000
2194	H	-3.583116000	4.953948000	1.193989000
2195	H	-2.267880000	5.278522000	2.917545000
2196	H	-0.040981000	5.850826000	3.664455000
2197	H	2.013894000	6.367954000	3.036341000
2198	H	3.417885000	6.715278000	1.096188000
2199	H	3.411806000	6.704174000	-1.123782000
2200	H	2.004090000	6.341011000	-3.059127000
2201	C	-3.804899000	-1.138128000	-1.193589000
2202	O	-4.441272000	-1.457368000	-2.092510000
2203	C	-7.279339000	0.042258000	0.922000000
2204	C	-6.083739000	0.441182000	0.043479000
2205	C	-8.470330000	-0.555644000	0.091711000
2206	O	-4.942172000	-0.268282000	0.265405000
2207	N	-7.581781000	1.233384000	1.717228000
2208	S	-7.835673000	-1.889095000	-1.053476000
2209	O	-6.090883000	1.371253000	-0.727926000
2210	C	-9.136090000	0.487865000	-0.817795000
2211	C	-9.501445000	-1.158811000	1.058383000
2212	H	-6.951012000	-0.740535000	1.613506000
2213	H	-5.052830000	-1.196587000	0.758995000
2214	H	-8.361057000	1.059784000	2.344545000
2215	H	-7.828684000	2.004136000	1.102508000
2216	H	-7.071507000	-2.558258000	-0.152062000
2217	H	-9.929038000	0.021535000	-1.410239000
2218	H	-8.413890000	0.949673000	-1.493102000
2219	H	-9.598020000	1.275737000	-0.212715000
2220	H	-10.330968000	-1.599890000	0.500264000
2221	H	-9.917939000	-0.388870000	1.721452000
2222	H	-9.055173000	-1.941875000	1.678662000
2223	Cl	-4.905724000	-2.936680000	1.106917000
2224	E=-4814,895086000,H=-4814,83412100 ,G=-4814,97994000 a.u.			

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2226	NTCOO/HCLP			
2227	C	-4.475496000	-4.523599000	2.271327000
2228	C	-5.287203000	-4.333766000	1.180063000
2229	C	-5.300617000	-3.077681000	0.493778000
2230	C	-5.301317000	-2.991992000	-0.954227000
2231	C	-4.853152000	-1.783194000	-1.549829000
2232	C	-3.996702000	-1.846015000	-2.700323000
2233	C	-3.227188000	-0.680964000	-3.031154000
2234	C	-1.876060000	-0.862136000	-3.433445000
2235	C	-0.986011000	0.243337000	-3.361635000
2236	C	0.347485000	0.011132000	-2.881345000
2237	C	1.093792000	1.108153000	-2.380396000
2238	C	1.951497000	0.905084000	-1.264000000
2239	C	2.432744000	2.074537000	-0.557286000
2240	C	2.470485000	1.995263000	0.887548000
2241	C	2.410787000	3.203805000	1.629561000
2242	C	1.534712000	3.254568000	2.772830000
2243	C	1.110173000	4.493944000	3.360196000
2244	C	-0.190810000	4.661582000	3.756535000
2245	C	-5.287088000	-4.157348000	-1.782329000
2246	C	-4.465498000	-4.216318000	-2.883882000
2247	C	-3.622214000	-3.113338000	-3.218776000
2248	C	-2.238924000	-3.298497000	-3.632659000
2249	C	-1.353095000	-2.196858000	-3.495030000
2250	C	-0.012808000	-2.425176000	-3.040562000
2251	C	0.728322000	-1.308303000	-2.528461000
2252	C	1.590702000	-1.502218000	-1.412209000
2253	C	2.056542000	-0.380676000	-0.704393000
2254	C	2.436100000	-0.537176000	0.779835000
2255	C	2.089001000	0.768234000	1.501562000
2256	C	1.159066000	0.819451000	2.544760000
2257	C	0.747248000	2.107971000	3.044010000
2258	C	-0.612923000	2.284869000	3.466828000
2259	C	-1.140259000	3.599311000	3.601561000
2260	C	-2.498786000	3.834067000	3.167748000
2261	C	-2.985373000	5.142611000	2.845986000
2262	C	-3.799071000	5.332952000	1.756232000
2263	C	-1.642959000	-4.586614000	-3.750161000
2264	C	-0.346837000	-4.803152000	-3.329095000
2265	C	0.422550000	-3.745759000	-2.766695000
2266	C	1.304485000	-3.950692000	-1.619863000
2267	C	1.689401000	-2.836894000	-0.855021000
2268	C	1.708368000	-2.943648000	0.588317000
2269	C	1.691948000	-1.739325000	1.346255000
2270	C	0.774849000	-1.636197000	2.391002000
2271	C	0.377356000	-0.341721000	2.885082000
2272	C	-0.963124000	-0.159004000	3.279502000
2273	C	-1.498794000	1.169144000	3.371396000
2274	C	-2.835673000	1.396992000	2.965602000

2275	C	-3.235942000	2.736198000	2.649716000
2276	C	-4.092308000	2.936111000	1.514151000
2277	C	-4.177239000	4.227380000	0.929365000
2278	C	-4.180962000	4.314970000	-0.518343000
2279	C	-3.806220000	5.511224000	-1.205928000
2280	C	-2.987672000	5.450241000	-2.309322000
2281	C	1.401095000	-5.241345000	-0.989745000
2282	C	1.372675000	-5.341365000	0.374507000
2283	C	1.276798000	-4.158413000	1.182344000
2284	C	0.402503000	-4.080350000	2.326086000
2285	C	-0.010525000	-2.792103000	2.745910000
2286	C	-1.366498000	-2.601363000	3.174446000
2287	C	-1.874351000	-1.267312000	3.225654000
2288	C	-3.210529000	-1.035576000	2.821193000
2289	C	-3.613631000	0.295464000	2.496073000
2290	C	-4.462469000	0.493052000	1.371036000
2291	C	-4.500853000	1.784802000	0.764907000
2292	C	-4.510594000	1.869551000	-0.652428000
2293	C	-4.104863000	3.105387000	-1.258678000
2294	C	-3.250241000	3.043166000	-2.410597000
2295	C	-2.506927000	4.192675000	-2.785979000
2296	C	-1.124326000	4.004557000	-3.200148000
2297	C	-0.170554000	5.061936000	-3.174401000
2298	C	1.121835000	4.833172000	-2.748299000
2299	C	-0.384573000	-5.196283000	2.769887000
2300	C	-1.681223000	-5.012136000	3.172963000
2301	C	-2.265607000	-3.703339000	3.166162000
2302	C	-3.625075000	-3.467681000	2.734521000
2303	C	-3.989450000	-2.147031000	2.360567000
2304	C	-4.844363000	-1.948075000	1.223464000
2305	C	-4.874957000	-0.648615000	0.619925000
2306	C	-4.883160000	-0.561640000	-0.797272000
2307	C	-4.489326000	0.663054000	-1.411406000
2308	C	-3.633238000	0.600209000	-2.559046000
2309	C	-2.856454000	1.748194000	-2.887560000
2310	C	-1.505838000	1.564212000	-3.290042000
2311	C	-0.608877000	2.681160000	-3.205917000
2312	C	0.728566000	2.446786000	-2.746970000
2313	C	1.530035000	3.536729000	-2.325586000
2314	C	2.410421000	3.333745000	-1.177389000
2315	C	2.879697000	4.452945000	-0.402294000
2316	C	2.864831000	4.393064000	0.964013000
2317	H	1.283998000	-6.321160000	0.831663000
2318	H	1.342773000	-6.144512000	-1.587068000
2319	H	0.021418000	-5.822655000	-3.294998000
2320	H	-2.248469000	-5.443290000	-4.025677000
2321	H	-4.351947000	-5.164265000	-3.399027000
2322	H	-5.795772000	-5.059871000	-1.460986000
2323	H	-5.803128000	-5.189168000	0.757095000
2324	H	-4.374739000	-5.522646000	2.681504000

2325	H	-2.299906000	-5.881659000	3.367707000
2326	H	-0.005119000	-6.205972000	2.655315000
2327	H	-0.524001000	5.647191000	4.063673000
2328	H	1.777903000	5.348731000	3.362118000
2329	H	3.067215000	5.292311000	1.535997000
2330	H	3.103607000	5.396252000	-0.887972000
2331	H	1.775005000	5.685950000	-2.598698000
2332	H	-0.489230000	6.085841000	-3.337446000
2333	H	-2.588062000	6.374277000	-2.713463000
2334	H	-4.027117000	6.480405000	-0.771778000
2335	H	-4.028262000	6.346833000	1.445955000
2336	H	-2.596617000	6.010620000	3.367442000
2337	C	3.956849000	-0.766084000	1.001385000
2338	O	4.415825000	-1.510032000	1.835788000
2339	C	6.631971000	1.007210000	-0.868940000
2340	C	6.029354000	0.346478000	0.369441000
2341	C	7.777130000	0.140710000	-1.503582000
2342	O	4.702976000	-0.017396000	0.129325000
2343	N	6.989706000	2.363849000	-0.456676000
2344	S	7.125752000	-1.593385000	-1.792176000
2345	O	6.563796000	0.236439000	1.439482000
2346	C	8.991295000	-0.025269000	-0.577695000
2347	C	8.205523000	0.764215000	-2.838725000
2348	H	5.836738000	1.090139000	-1.614423000
2349	H	6.070891000	-2.120955000	2.373454000
2350	H	7.281813000	2.915343000	-1.257786000
2351	H	7.757934000	2.348163000	0.208960000
2352	H	6.154139000	-1.269712000	-2.669716000
2353	H	9.760348000	-0.625646000	-1.070972000
2354	H	8.728917000	-0.500524000	0.369371000
2355	H	9.428993000	0.953848000	-0.360275000
2356	H	8.969405000	0.147712000	-3.318233000
2357	H	8.633569000	1.759191000	-2.674139000
2358	H	7.361089000	0.865541000	-3.527323000
2359	Cl	7.052216000	-2.825961000	2.881619000
2360	E=-4814,87366700,H=-4814,93526900 ,G=-4815,02203300 a.u.			
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2362	NTCOCl/PCA3R			
2363	C	3.127987000	5.025360000	3.013777000
2364	C	4.146800000	5.086079000	2.095049000
2365	C	4.554899000	3.912808000	1.383864000
2366	C	4.837145000	3.935098000	-0.038859000
2367	C	4.775950000	2.706929000	-0.749220000
2368	C	4.152032000	2.676883000	-2.041871000
2369	C	3.725828000	1.406463000	-2.554670000
2370	C	2.465994000	1.335924000	-3.208947000
2371	C	1.837043000	0.069248000	-3.349060000
2372	C	0.419918000	-0.012246000	-3.130997000
2373	C	-0.151901000	-1.272922000	-2.821608000
2374	C	-1.219234000	-1.331958000	-1.884452000

2375	C	-1.557925000	-2.622485000	-1.323345000
2376	C	-1.875622000	-2.658001000	0.087915000
2377	C	-1.697017000	-3.879922000	0.788661000
2378	C	-1.054820000	-3.833653000	2.078319000
2379	C	-0.489115000	-4.999711000	2.696096000
2380	C	0.721319000	-4.926101000	3.334186000
2381	C	4.723257000	5.130284000	-0.815097000
2382	C	4.124493000	5.100025000	-2.053013000
2383	C	3.615786000	3.875007000	-2.582452000
2384	C	2.326612000	3.802516000	-3.254433000
2385	C	1.688528000	2.535771000	-3.329681000
2386	C	0.269963000	2.451054000	-3.139448000
2387	C	-0.295099000	1.171749000	-2.817959000
2388	C	-1.366689000	1.102716000	-1.883355000
2389	C	-1.703575000	-0.139417000	-1.314807000
2390	C	-2.357802000	-0.174485000	0.068554000
2391	C	-1.880567000	-1.426988000	0.803328000
2392	C	-1.173770000	-1.363157000	2.008180000
2393	C	-0.595317000	-2.573345000	2.536203000
2394	C	0.668795000	-2.498642000	3.212343000
2395	C	1.431983000	-3.683455000	3.404616000
2396	C	2.865517000	-3.603057000	3.236315000
2397	C	3.671365000	-4.757523000	2.971105000
2398	C	4.691805000	-4.696654000	2.054203000
2399	C	1.499818000	4.946496000	-3.446192000
2400	C	0.132709000	4.861968000	-3.279943000
2401	C	-0.481404000	3.631069000	-2.912372000
2402	C	-1.578931000	3.566655000	-1.950839000
2403	C	-1.848182000	2.343938000	-1.312698000
2404	C	-2.151187000	2.338584000	0.102397000
2405	C	-2.009870000	1.111622000	0.809115000
2406	C	-1.304558000	1.121656000	2.012199000
2407	C	-0.737930000	-0.095457000	2.534315000
2408	C	0.514635000	-0.028063000	3.177661000
2409	C	1.296652000	-1.221367000	3.329597000
2410	C	2.702850000	-1.140508000	3.185206000
2411	C	3.432445000	-2.342557000	2.908879000
2412	C	4.503688000	-2.279072000	1.954091000
2413	C	4.968838000	-3.479220000	1.354203000
2414	C	5.254896000	-3.458020000	-0.067652000
2415	C	5.278863000	-4.651913000	-0.853956000
2416	C	4.683239000	-4.679209000	-2.093220000
2417	C	-2.064734000	4.759640000	-1.308775000
2418	C	-2.308564000	4.762794000	0.037777000
2419	C	-2.108697000	3.569015000	0.809471000
2420	C	-1.462991000	3.588308000	2.098493000
2421	C	-0.866600000	2.385133000	2.550029000
2422	C	0.395167000	2.445683000	3.230741000
2423	C	1.159869000	1.244136000	3.338900000
2424	C	2.565881000	1.321185000	3.195712000

2425	C	3.298493000	0.128422000	2.912338000
2426	C	4.359598000	0.191849000	1.965582000
2427	C	4.784330000	-1.016836000	1.336197000
2428	C	5.069466000	-0.993976000	-0.054765000
2429	C	5.056539000	-2.238764000	-0.768547000
2430	C	4.434681000	-2.268906000	-2.062146000
2431	C	4.038900000	-3.515680000	-2.613338000
2432	C	2.749523000	-3.585260000	-3.284730000
2433	C	2.057807000	-4.814947000	-3.481337000
2434	C	0.690873000	-4.887616000	-3.308471000
2435	C	-1.031398000	4.806113000	2.724953000
2436	C	0.177063000	4.862804000	3.368748000
2437	C	1.021258000	3.706189000	3.434110000
2438	C	2.455233000	3.786431000	3.268803000
2439	C	3.157881000	2.599418000	2.930904000
2440	C	4.227933000	2.663577000	1.974614000
2441	C	4.646320000	1.445561000	1.346041000
2442	C	4.930386000	1.465914000	-0.045143000
2443	C	4.927526000	0.234770000	-0.763585000
2444	C	4.303034000	0.204587000	-2.053080000
2445	C	3.866443000	-1.051024000	-2.564936000
2446	C	2.606602000	-1.118734000	-3.219154000
2447	C	1.971382000	-2.398875000	-3.349203000
2448	C	0.553802000	-2.477646000	-3.153322000
2449	C	-0.057190000	-3.736649000	-2.930962000
2450	C	-1.153108000	-3.802650000	-1.967794000
2451	C	-1.505380000	-5.046858000	-1.335222000
2452	C	-1.755833000	-5.084790000	0.009176000
2453	H	-2.519315000	5.703609000	0.534903000
2454	H	-2.094275000	5.697156000	-1.852880000
2455	H	-0.446199000	5.779033000	-3.287049000
2456	H	1.947357000	5.926460000	-3.571793000
2457	H	3.905458000	6.039856000	-2.548584000
2458	H	4.957883000	6.091861000	-0.371435000
2459	H	4.534786000	6.057696000	1.808376000
2460	H	2.741301000	5.949661000	3.429203000
2461	H	0.545535000	5.824159000	3.710454000
2462	H	-1.591928000	5.722064000	2.572098000
2463	H	1.196699000	-5.842547000	3.667147000
2464	H	-0.945222000	-5.971044000	2.538558000
2465	H	-1.862255000	-6.046017000	0.500573000
2466	H	-1.427435000	-5.978238000	-1.885025000
2467	H	0.219954000	-5.864550000	-3.317975000
2468	H	2.613566000	-5.737002000	-3.613448000
2469	H	4.573993000	-5.633188000	-2.597911000
2470	H	5.620956000	-5.584349000	-0.418009000
2471	H	5.185087000	-5.616799000	1.759855000
2472	H	3.388880000	-5.722843000	3.377102000
2473	C	-3.925761000	-0.263303000	0.070485000
2474	O	-4.634378000	0.016477000	0.983348000

2475	C	-8.378183000	0.670925000	0.404561000
2476	C	-9.000319000	1.160452000	-0.902400000
2477	C	-8.904457000	-0.746148000	0.832591000
2478	O	-8.109335000	1.225238000	-1.907923000
2479	N	-8.588236000	1.751187000	1.371150000
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2482	C	-10.405830000	-0.759533000	1.155801000
2483	C	-8.093443000	-1.245537000	2.037463000
2484	H	-7.299991000	0.577666000	0.246189000
2485	H	-8.580680000	1.558568000	-2.692661000
2486	H	-8.144437000	1.530226000	2.257734000
2487	H	-9.581960000	1.878546000	1.544630000
2488	H	-7.355449000	-1.805242000	-0.738293000
2489	H	-10.722803000	-1.766301000	1.442304000
2490	H	-11.008576000	-0.423560000	0.310427000
2491	H	-10.608092000	-0.098312000	2.004130000
2492	H	-8.407790000	-2.253916000	2.317303000
2493	H	-8.255563000	-0.594454000	2.904110000
2494	H	-7.021383000	-1.261886000	1.820283000
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2503	C	4.901726000	-1.185288000	1.845490000
2504	C	3.965621000	-1.415945000	2.908410000
2505	C	3.000328000	-0.392963000	3.190924000
2506	C	1.662647000	-0.788996000	3.463154000
2507	C	0.623391000	0.171231000	3.333641000
2508	C	-0.611396000	-0.241651000	2.726567000
2509	C	-1.471529000	0.747926000	2.184864000
2510	C	-2.173042000	0.464182000	0.981947000
2511	C	-2.731977000	1.574060000	0.254872000
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2515	C	-1.447121000	4.302614000	-3.464451000
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2520	C	2.375128000	-3.146455000	3.645152000
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2524	C	-1.456402000	-1.868928000	1.105795000

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2552	C	1.893604000	5.650653000	2.581209000
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2653	C	-5.025454000	-4.538848000	-1.416142000
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2692	C	0.888462000	-3.900329000	2.312812000
2693	C	0.405270000	-2.632428000	2.721028000
2694	C	-0.932357000	-2.528721000	3.231648000
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