

Supporting Information: Efficient Evaluation of Electrostatic Potential with Computerized Optimized Code

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1 Redundancies of a VRR path for $(f|d)$

The following graph is a possible VRR path for the evaluation of $(f|d)$. The node like $(2, 1, 0|0, 0, 0)^2$ stands for $(f_{x^2y}|s)^2$ and its incoming lines indicate that it is calculated by

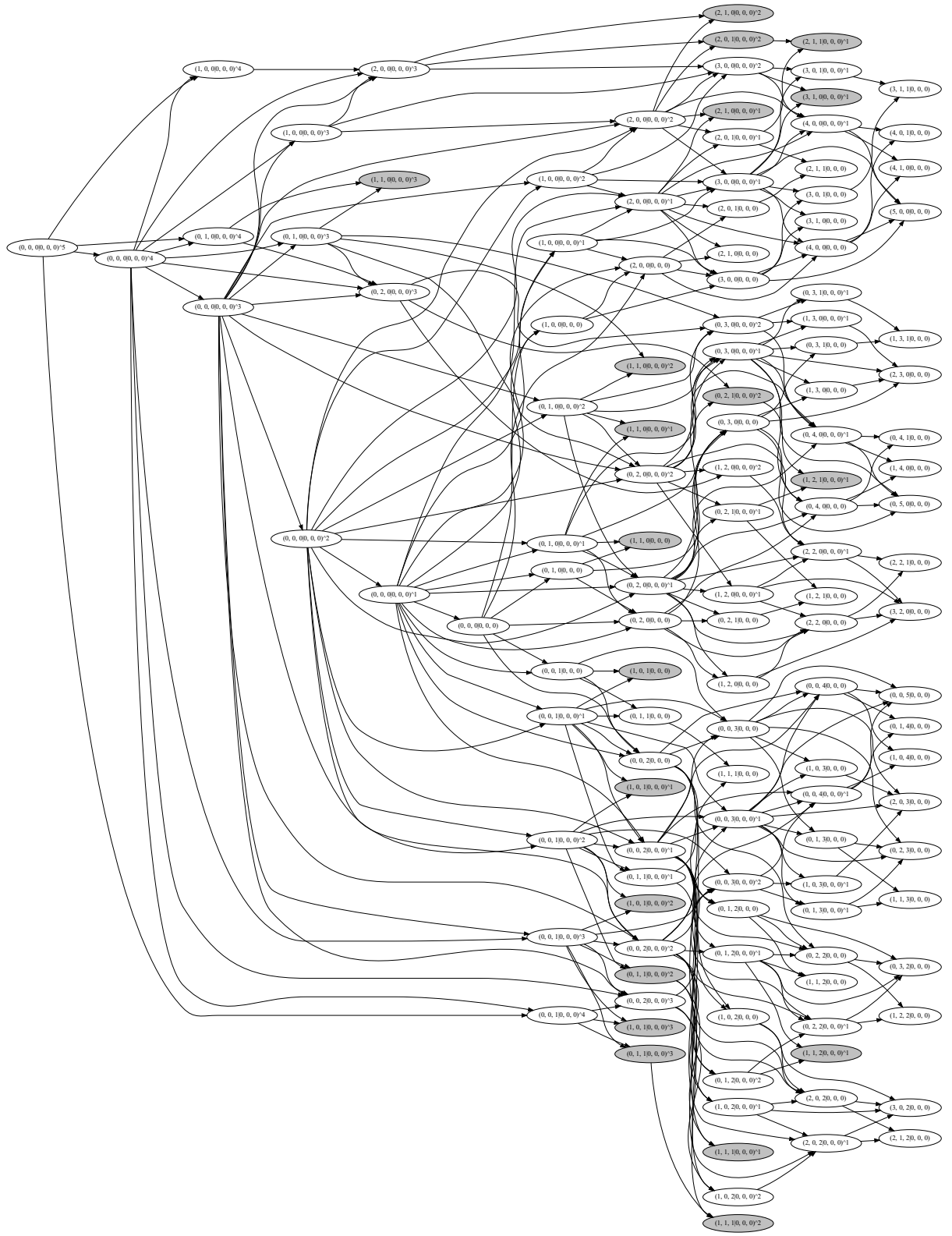
$$(f_{x^2y}|s)^2 = Y_{PA}(f_{x^2}|s)^2 - Y_{PC}(f_{x^2}|s)^3 \quad (1)$$

There are 20 gray rendered nodes that have no outgoing lines, suggesting that they do not participate in the subsequent calculations of $(f|s)$, $(g|s)$, and $(h|s)$. They can be removed before generating the evaluation code using this graph.

These redundancies are:

- $(d_{xy}|s)^3$; $(d_{xz}|s)^3$; $(d_{yz}|s)^3$;

- $(d_{xy}|s)^2; (d_{xz}|s)^2; (d_{yz}|s)^2;$
- $(f_{x^2y}|s)^2; (f_{x^2z}|s)^2; (f_{xyz}|s)^2; (f_{y^2z}|s)^2;$
- $(d_{xy}|s)^1; (d_{xz}|s)^1;$
- $(f_{x^2y}|s)^1; (f_{xyz}|s)^1;$
- $(g_{x^3y}|s)^1; (g_{x^2yz}|s)^1; (g_{xy^2z}|s)^1; (g_{xyz^2}|s)^1;$
- $(d_{xy}|s); (d_{xz}|s).$



2 XYZ Coordinates for Test Molecules

2.1 Dopamine

22

Dopamine

O	-2.37174600	1.90861300	0.06193300
O	-3.47550500	-0.49048300	0.37909800
N	4.36507700	0.14895900	0.30224300
C	2.11669300	-0.08224000	-0.68623000
C	0.63101000	-0.21763400	-0.43463000
C	2.93181000	0.08197300	0.60782500
C	-0.18514000	0.91890400	-0.32146400
C	0.03631300	-1.46977900	-0.26788800
C	-1.54801700	0.82244800	-0.04976600
C	-1.33027100	-1.58006900	0.00534400
C	-2.13317500	-0.44758200	0.11794600
H	2.30809500	0.78370600	-1.33638200
H	2.49841500	-0.96162700	-1.21711000
H	2.54421300	0.95349200	1.16670200
H	2.76421700	-0.79469600	1.24529500
H	0.25146900	1.90906200	-0.45398700
H	0.63797600	-2.37079700	-0.35493500
H	-1.78288900	-2.56304600	0.12788500
H	4.89999500	0.19806600	1.16799900
H	4.56670300	1.01348400	-0.19982700
H	-1.84204100	2.70822200	-0.08056800
H	-3.73902700	-1.41975200	0.46415000

2.2 Remdesivir

77

Remdesivir

C	1.47121600	-3.35668100	2.51342700
C	1.09040800	-2.17353200	3.41102400
C	1.28928700	-0.76720000	2.81474800
C	0.90107400	0.33807600	3.81707600
C	-0.57179900	0.31202500	4.23334500
C	2.70865800	-0.51319100	2.31859900
O	2.90177100	-1.25697800	1.09213700
C	3.88251300	-0.84801200	0.28168300
O	4.68197500	0.02516600	0.54045800
C	3.91060000	-1.67456100	-1.00888900
C	4.89914500	-1.08384700	-2.01301800
N	2.56305400	-1.87173300	-1.57116000
P	1.43142000	-0.65772900	-1.77661300
O	0.95998200	-0.49806700	-3.17258000
O	2.08207100	0.59791200	-1.02565300
C	2.42303800	1.82957200	-1.69703700
C	1.52323100	2.94256800	-1.19495400
C	1.39240500	3.02070000	0.32998900
C	0.08858600	2.26235600	0.60795900
C	-0.75423500	2.59926800	-0.67053200
O	0.19718700	2.71995000	-1.71903400
C	-1.48041000	3.88514200	-0.48670000
N	-2.09202400	4.86324100	-0.36499900
C	-1.73397300	1.53197800	-1.07794100

C	-1.93794000	0.94651800	-2.32698200
C	-2.98970600	0.02064800	-2.21697000
C	-3.42599800	0.04434700	-0.89376900
N	-2.63479100	0.98374800	-0.21527900
N	-2.76329000	1.27387600	1.11462500
C	-3.70232300	0.57922000	1.71741000
N	-4.50876600	-0.37489900	1.20754600
C	-4.36396600	-0.65029200	-0.08825700
N	-5.16120300	-1.60692800	-0.63213300
O	-0.45914300	2.71796600	1.81706900
O	1.26343800	4.37578600	0.70360200
O	0.25305000	-0.92890900	-0.67871200
C	-0.65593700	-1.97173500	-0.72402600
C	-0.90208000	-2.72668700	-1.87129200
C	-1.85983800	-3.74166700	-1.81971600
C	-2.57136500	-3.99579200	-0.64636300
C	-2.32287100	-3.21949800	0.48835800
C	-1.36831200	-2.20664200	0.45282500
H	0.96463800	-3.30205700	1.54511900
H	2.54606700	-3.39100900	2.31669900
H	1.18605100	-4.29979700	2.99378700
H	0.03512500	-2.27776500	3.69046600
H	1.65680800	-2.23197000	4.35265300
H	0.64375200	-0.66316400	1.93396100
H	1.54020000	0.26273300	4.70868000
H	1.10371400	1.31414300	3.36278900
H	2.87390600	0.54516600	2.10226300

H	3.46756800	-0.83265700	3.04251500
H	-1.21994200	0.33952200	3.34982300
H	-0.82675000	-0.58073000	4.81344300
H	-0.81309600	1.18650900	4.84680200
H	4.25660000	-2.67154800	-0.70361000
H	4.95622800	-1.72039800	-2.90203400
H	4.58195700	-0.08440700	-2.32296400
H	5.89514000	-1.00114400	-1.57125400
H	2.56257200	-2.51440600	-2.35567600
H	3.46739000	2.03380200	-1.44605700
H	2.30905600	1.70928600	-2.77711800
H	1.89492400	3.90027100	-1.57537100
H	2.24562800	2.54635900	0.83555200
H	0.26492800	1.18424600	0.60758700
H	0.63188100	4.39091700	1.44660800
H	-1.36805400	2.34368300	1.86123400
H	-1.34033400	1.15765500	-3.19963500
H	-3.37934000	-0.60712600	-3.00521400
H	-3.81997600	0.80290300	2.77356000
H	-5.66503600	-2.17047800	0.04034500
H	-4.81853300	-2.09649400	-1.44695800
H	-0.38822100	-2.49626700	-2.79689000
H	-1.17842600	-1.58630600	1.32020800
H	-2.04992700	-4.33268700	-2.71135500
H	-3.30858700	-4.79285000	-0.61427500
H	-2.87918200	-3.39022900	1.40502200

2.3 MOF-5

400

MOF-5

Zn	7.58818388	7.58818388	5.34473612
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Zn	7.58818388	5.34473612	18.27765612

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0	5.66353259	18.59645259	16.38994125

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0	5.66353259	5.66353259	3.45702125
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0	20.20230741	5.66353259	22.40881875
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0	3.45702125	5.66353259	5.66353259
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0	3.45702125	20.20230741	20.20230741
0	22.40881875	5.66353259	5.66353259
0	22.40881875	7.26938741	7.26938741
0	3.45702125	18.59645259	18.59645259
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0	22.40881875	7.26938741	18.59645259

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O	3.45702125	7.26938741	18.59645259
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C	15.81393486	6.46646000	19.39938000
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C	10.05190514	19.39938000	19.39938000
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C	15.81393486	19.39938000	6.46646000

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C	6.46646000	6.46646000	11.54113088
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C	6.46646000	19.39938000	14.32470912
C	19.39938000	6.46646000	11.54113088
C	19.39938000	19.39938000	11.54113088
C	6.46646000	6.46646000	14.32470912
C	19.39938000	6.46646000	14.32470912
C	6.46646000	19.39938000	11.54113088
C	11.54113088	6.46646000	6.46646000
C	14.32470912	19.39938000	19.39938000
C	14.32470912	6.46646000	19.39938000
C	11.54113088	19.39938000	6.46646000
C	11.54113088	19.39938000	19.39938000
C	14.32470912	6.46646000	6.46646000
C	14.32470912	19.39938000	6.46646000
C	11.54113088	6.46646000	19.39938000
C	7.32435232	12.23917231	5.60856768
C	18.54148768	13.62666769	20.25727232
C	18.54148768	13.62666769	5.60856768
C	7.32435232	12.23917231	20.25727232
C	18.54148768	12.23917231	20.25727232

C	7.32435232	13.62666769	5.60856768
C	7.32435232	13.62666769	20.25727232
C	18.54148768	12.23917231	5.60856768
C	5.60856768	7.32435232	12.23917231
C	20.25727232	18.54148768	13.62666769
C	5.60856768	18.54148768	13.62666769
C	20.25727232	7.32435232	12.23917231
C	20.25727232	18.54148768	12.23917231
C	5.60856768	7.32435232	13.62666769
C	20.25727232	7.32435232	13.62666769
C	5.60856768	18.54148768	12.23917231
C	12.23917231	5.60856768	7.32435232
C	13.62666769	20.25727232	18.54148768
C	13.62666769	5.60856768	18.54148768
C	12.23917231	20.25727232	7.32435232
C	12.23917231	20.25727232	18.54148768
C	13.62666769	5.60856768	7.32435232
C	13.62666769	20.25727232	7.32435232
C	12.23917231	5.60856768	18.54148768
C	12.23917231	7.32435232	20.25727232
C	13.62666769	18.54148768	5.60856768
C	13.62666769	18.54148768	20.25727232
C	12.23917231	7.32435232	5.60856768
C	12.23917231	18.54148768	5.60856768
C	13.62666769	7.32435232	20.25727232
C	13.62666769	7.32435232	5.60856768
C	12.23917231	18.54148768	20.25727232

C	7.32435232	5.60856768	13.62666769
C	18.54148768	20.25727232	12.23917231
C	18.54148768	5.60856768	12.23917231
C	7.32435232	20.25727232	13.62666769
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C	7.32435232	5.60856768	12.23917231
C	7.32435232	20.25727232	12.23917231
C	18.54148768	5.60856768	13.62666769
C	5.60856768	12.23917231	18.54148768
C	20.25727232	13.62666769	7.32435232
C	5.60856768	13.62666769	7.32435232
C	20.25727232	12.23917231	18.54148768
C	20.25727232	12.23917231	7.32435232
C	5.60856768	13.62666769	18.54148768
C	20.25727232	13.62666769	18.54148768
C	5.60856768	12.23917231	7.32435232
H	7.98452615	11.67040835	4.94839385
H	17.88131385	14.19543165	20.91744615
H	17.88131385	14.19543165	4.94839385
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H	20.91744615	17.88131385	14.19543165
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H	20.91744615	7.98452615	11.67040835
H	20.91744615	17.88131385	11.67040835
H	4.94839385	7.98452615	14.19543165
H	20.91744615	7.98452615	14.19543165
H	4.94839385	17.88131385	11.67040835
H	11.67040835	4.94839385	7.98452615
H	14.19543165	20.91744615	17.88131385
H	14.19543165	4.94839385	17.88131385
H	11.67040835	20.91744615	7.98452615
H	11.67040835	20.91744615	17.88131385
H	14.19543165	4.94839385	7.98452615
H	14.19543165	20.91744615	7.98452615
H	11.67040835	4.94839385	17.88131385
H	11.67040835	7.98452615	20.91744615
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H	14.19543165	17.88131385	20.91744615
H	11.67040835	7.98452615	4.94839385
H	11.67040835	17.88131385	4.94839385
H	14.19543165	7.98452615	20.91744615
H	14.19543165	7.98452615	4.94839385
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H	17.88131385	20.91744615	11.67040835
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H	7.98452615	20.91744615	14.19543165
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H	17.88131385	4.94839385	14.19543165
H	4.94839385	11.67040835	17.88131385
H	20.91744615	14.19543165	7.98452615
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H	4.94839385	11.67040835	7.98452615
C	6.46646000	6.46646000	24.52482514
H	6.72761628	5.49204401	24.88149149
H	7.17975067	7.17983615	24.88149149
H	5.49201300	6.72749985	24.88149200
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H	5.54781232	19.81624352	24.88149200
C	19.39938000	6.46646000	24.52482514
H	20.01888108	7.26264310	24.88149149
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H	19.77914430	5.53186499	24.88149200
C	19.39938000	19.39938000	24.52482514
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C	6.46646000	6.46646000	1.34101486

H	6.20536810	7.44089324	0.98434851
H	7.44088982	6.20535535	0.98434851
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C	19.39938000	6.46646000	1.34101486
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C	6.46646000	19.39938000	1.34101486
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H	19.44086808	24.88149149	5.45850769
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C	19.39938000	24.52482514	19.39938000
H	19.46528689	24.88149149	20.40603058
H	20.23821139	24.88149149	18.83897745
H	18.49464168	24.88149200	18.95313195
C	6.46646000	1.34101486	6.46646000
H	6.42517599	0.98434851	5.45849931
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C	6.46646000	1.34101486	19.39938000
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H	5.62791432	0.98434851	18.83855002
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H	5.70897804	24.88149149	18.73311414
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H	20.15708751	0.98434851	18.73337066
H	19.59730700	0.98434851	20.38857867
H	18.44374545	0.98434800	19.07619066
C	19.39938000	1.34101486	6.46646000
H	19.65600755	0.98434851	5.49084152
H	20.11597643	0.98434851	7.17651540
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C	1.34101486	19.39938000	6.46646000
H	0.98434851	20.37391854	6.72715859
H	0.98434851	19.13788208	5.49213564
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C	1.34101486	19.39938000	19.39938000
H	0.98434851	19.05251046	20.34667649
H	0.98434851	20.39319755	19.22612933

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H	0.98434851	6.65016361	5.47452144
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H	0.98434851	6.72792051	20.37371440
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2.4 ATP

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ATP

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O	0.85433321	-1.99818418	-0.28384837
O	3.30416915	-1.37752592	-0.67760000
O	2.34372480	-3.45521858	-1.76546539
O	1.59564532	-1.09946542	-2.64067560
O	2.41057817	0.22117798	1.07450037
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O	4.99594492	0.14737726	0.63918921
O	1.57988407	2.61042658	0.98666775
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N	-0.82717948	2.83327765	-2.16444364
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C	-2.67394794	-3.08309712	0.46244964
C	-2.84492327	-0.78321950	0.92142279

C	-1.27599147	-2.51249775	0.67976216
C	-0.41580515	-2.55533335	-0.57545473
C	-2.11401564	1.18060361	-0.49742913
C	-3.95785272	1.46908613	0.66813304
C	-2.64733121	2.44305340	-0.70191936
C	-1.95977601	3.28293359	-1.57231445
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H	-3.29278355	-1.64784258	-1.02364463
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H	-3.28957158	-0.75977034	1.92412121
H	-0.75329022	-3.00374210	1.50828306
H	-0.86453520	-1.98353447	-1.39275422
H	-0.28136853	-3.58986763	-0.90724500
H	-4.99938780	-2.09677647	1.21424925
H	-4.05262206	-3.94455018	1.54182891
H	-4.76959966	1.23698579	1.34405871
H	0.48827120	1.25594912	-2.35831795
H	-3.27363183	4.91913402	-1.39671163
H	-1.91150286	5.17257194	-2.47345688
H	1.75548072	-3.96413562	-2.36314332
H	3.96483995	1.27153416	-1.83370963
H	1.36695076	3.50546906	1.32700048
H	0.14635697	1.54177115	3.33794304