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Supporting Information

Determination of Gluconate Binding Properties on Magnetite Surface and Investigation of Carboxymethylation and Hydrazination Mechanisms of the Gluconated Magnetite Surface: A Computational Study

RC(chloroacetate)(in water)

-1 1 (Charge and multiplicity)			
C	0.17019300	-0.80428500	0.00004800
C	-1.09149100	0.09251600	-0.00012400
O	-0.98447500	1.34163700	-0.00023800
O	-2.14903100	-0.60067400	0.00001100
Cl	1.77933800	0.07159000	0.00012300
H	0.17346500	-1.43700200	0.88769600
H	0.17362200	-1.43712300	-0.88751400

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies=	-688.205900
Sum of electronic and thermal Energies=	-688.200826
Sum of electronic and thermal Enthalpies=	-688.199882
Sum of electronic and thermal Free Energies=	-688.235473

RC(Gluconate) (in water)

-2 1				
C	0	2.90430500	-0.98287100	-0.45770500
H	0	3.86027200	-1.21043200	0.07803100
H	0	2.23192700	-1.83698600	-0.17940300
O	0	3.05308600	-0.81758600	-1.81126100
C	0	2.34850200	0.26262600	0.28797100
H	0	3.04751200	1.09233200	0.11165800
C	0	0.99022400	0.72621500	-0.25198700
H	0	1.11351400	0.76744100	-1.34300200
C	0	-0.16604400	-0.25274700	0.01524500
H	0	0.14728100	-1.23142000	-0.36622100
C	0	-1.46814200	0.10029700	-0.72921700
H	0	-1.34610700	-0.23526800	-1.77059200
O	-1	-3.75519900	0.07391100	-0.06517900
O	-1	-2.49030400	-1.86327600	0.20495900
O	0	2.33688200	0.04584900	1.71500900
H	0	1.43969300	-0.25207200	1.94965600
O	0	0.71729700	2.03977500	0.26345000
H	0	-0.20397700	2.23681000	0.01075100
O	0	-1.74301100	1.50834800	-0.73849500
H	0	-2.69057700	1.54360100	-0.48172100
O	0	-0.37539000	-0.36168100	1.43976300
H	0	-0.99855000	-1.10023900	1.55342900
C	0	-2.70016000	-0.64960000	-0.13573200

B3LYP/6-31+G(d,p)
 Sum of electronic and zero-point Energies= -761.369752
 Sum of electronic and thermal Energies= -761.355806
 Sum of electronic and thermal Enthalpies= -761.354861
 Sum of electronic and thermal Free Energies= -761.413174

TS (in water)

-3 1

C	0	-2.77103000	-0.39845700	-0.61745900
C	0	-3.03764300	-0.26409800	-2.14342400
O	0	-3.68887300	-1.19923500	-2.67291800
O	0	-2.59685200	0.78411000	-2.67881800
Cl	0	-7.16887600	0.57437600	2.55242900
H	0	-3.11677700	-1.37293800	-0.26790300
H	0	-3.33095600	0.38812100	-0.08736100
C	0	-0.76090900	0.92207800	-0.38169800
H	0	-1.49423400	1.73801700	-0.35794500
H	0	-0.24404200	1.00154400	-1.34883800
O	0	-1.39336700	-0.33020700	-0.24340300
C	0	0.20832800	1.11207700	0.78917600
H	0	-0.38117700	1.07132100	1.71566700
C	0	1.24545700	-0.00781100	0.92280800
H	0	0.69572300	-0.95062300	0.78280800
C	0	2.36083200	0.02794600	-0.13331100
H	0	1.88533600	0.12170900	-1.11972200
C	0	3.19630500	-1.26053700	-0.17336400
H	0	2.62385800	-1.99795000	-0.75920700
O	-1	5.50304600	-1.77237200	-0.39118500
O	-1	4.56088000	-0.21234600	-1.84047700
O	0	0.79320700	2.40796100	0.69921400
H	0	1.73956100	2.29384200	0.52324800
O	0	1.78538800	0.06573300	2.23717300
H	0	2.52472600	-0.56063300	2.24991000
O	0	3.44571500	-1.80338000	1.12009300
H	0	4.38844300	-2.05742900	1.04466800
O	0	3.18742300	1.17035300	0.09891000
H	0	3.81274800	1.16011600	-0.64705000
C	0	4.57238600	-1.05449700	-0.88934500

B3LYP/6-31+G(d,p)
 Sum of electronic and zero-point Energies= -1449.556057
 Sum of electronic and thermal Energies= -1449.536556
 Sum of electronic and thermal Enthalpies= -1449.535612
 Sum of electronic and thermal Free Energies= -1449.607449

CP1 (in water)

-1 1

Cl	0.00000000	0.00000000	0.00000000

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -460.384689

Sum of electronic and thermal Energies= -460.383272

Sum of electronic and thermal Enthalpies= -460.382328

Sum of electronic and thermal Free Energies= -460.399711

P1 (in water)

-2 1

C	0	3.48411900	0.10203600	-0.90697100
C	0	4.72467200	-0.59579700	-0.28878400
O	0	4.57069100	-1.66703400	0.35497100
O	0	5.81536500	0.00487200	-0.52462200
H	0	3.59482300	0.07326900	-1.99619800
H	0	3.49745000	1.15910100	-0.60858600
C	0	1.68647500	-0.17532300	0.66103700
H	0	2.48787000	0.02026000	1.38272000
H	0	1.13879500	-1.05673200	1.01335200
O	0	2.22202600	-0.49408300	-0.62155500
C	0	0.76213900	1.05520100	0.62082800
H	0	1.32917500	1.89758500	0.20506000
C	0	-0.46104200	0.87741700	-0.29557500
H	0	-0.07626000	0.48508500	-1.24849400
C	0	-1.49736900	-0.14353000	0.21014100
H	0	-0.97477400	-1.09302400	0.37755300
C	0	-2.61468000	-0.44794700	-0.80923700
H	0	-2.21016300	-1.17926100	-1.52525100
O	-1	-4.97400100	-0.65721500	-0.58575100
O	-1	-3.60552500	-1.94444800	0.78978900
O	0	0.41783500	1.41695400	1.96432500
H	0	-0.46893800	1.05051500	2.14452100
O	0	-1.03329400	2.17350200	-0.49433700
H	0	-1.87903000	2.02043300	-0.95822000
O	0	-3.03644900	0.71222800	-1.53875100
H	0	-4.01610100	0.65619500	-1.48063400
O	0	-2.02550800	0.31857700	1.46895700
H	0	-2.56955500	-0.41554700	1.80644900
C	0	-3.86138100	-1.09283700	-0.12751700

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -989.259194

Sum of electronic and thermal Energies= -989.240194

Sum of electronic and thermal Enthalpies= -989.239250

Sum of electronic and thermal Free Energies= -989.314425

P1 (in gas)

-1 1

C	0	2.45105200	-0.54789800	-0.75749000
C	0	3.68809600	-0.78025500	0.10019700
O	0	4.34738200	0.05762700	0.67529800
O	0	3.98632400	-2.10833300	0.16382000
H	0	2.59905100	-1.07490100	-1.70685500
H	0	1.59558000	-1.03124400	-0.25863400
H	0	4.75268100	-2.19372400	0.75502200
C	0	1.59278900	1.58424100	-0.02802700
H	0	2.18840200	2.49049800	0.11529500
H	0	1.58775500	1.04377800	0.92539300
O	0	2.23165100	0.80386700	-1.05220700
C	0	0.17150000	1.99726200	-0.43611000
H	0	0.22617500	2.46123900	-1.43136300
C	0	-0.81185200	0.82457000	-0.55253300
H	0	-0.30505200	0.01354500	-1.09472500
C	0	-1.22913500	0.27420400	0.83916000
H	0	-0.35229300	0.30116700	1.49557900
C	0	-1.72363100	-1.18400500	0.82027900
H	0	-2.06391800	-1.41138900	1.84371000
O	0	-2.92134700	-2.47462500	-0.78013600
O	-1	-3.79178800	-0.46445800	-0.15716800
O	-1	-0.25183500	2.98052600	0.51340800
H	0	-1.12392900	2.71166000	0.85375300
O	0	-1.91631500	1.29890900	-1.31930800
H	0	-2.69661500	0.73640500	-1.13808600
O	0	-0.65995400	-2.06014500	0.45962800
H	0	-1.10849600	-2.67596700	-0.16089200
O	0	-2.20948000	1.11605600	1.45428600
H	0	-3.05311500	0.85243800	1.02085500
C	0	-2.93270800	-1.40460300	-0.13214600

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -989.622262
Sum of electronic and thermal Energies= -989.603493
Sum of electronic and thermal Enthalpies= -989.602549
Sum of electronic and thermal Free Energies= -989.676145

EDC (in gas)

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0 1

C	2.07439800	0.79635600	0.39525000
N	2.76501300	0.02922600	1.05823800
N	1.46137400	1.70742900	-0.15178200
C	3.61600100	-1.06085000	0.58549900
H	4.62199500	-0.87235900	0.97883800
H	3.26589600	-1.98002600	1.07015600
C	0.04998600	1.75399200	-0.52614300

H	-0.35629600	2.68710700	-0.11610000
H	0.00502600	1.85660500	-1.61815000
C	3.66922800	-1.24579000	-0.93092800
H	4.03763600	-0.34169000	-1.42672300
H	4.34184500	-2.07187000	-1.18580900
H	2.67896500	-1.47890400	-1.33734500
C	-0.80106600	0.56547200	-0.06942700
H	-0.72892300	0.47310200	1.02103700
H	-0.38851400	-0.35728500	-0.49646700
C	-2.27533300	0.73659300	-0.49673800
H	-2.66013500	1.67608900	-0.07767300
H	-2.32043200	0.84091900	-1.58933800
N	-3.21354100	-0.32134200	-0.12281400
C	-2.95797500	-1.60351100	-0.76334700
H	-2.05238700	-2.12056800	-0.39270900
H	-3.81078000	-2.26981400	-0.59386300
H	-2.85145800	-1.46177800	-1.84414500
C	-3.43265600	-0.44938100	1.31117100
H	-3.67112200	0.53089300	1.73705200
H	-4.28758900	-1.11079400	1.48886300
H	-2.56914800	-0.86410800	1.86486300

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -479.089384
Sum of electronic and thermal Energies= -479.075336
Sum of electronic and thermal Enthalpies= -479.074392
Sum of electronic and thermal Free Energies= -479.133265

TS1 (in gas)

-1 1

C	0	0.35952000	-2.68590200	-1.12588800
C	0	1.81640000	-2.20539300	-1.25056500
O	0	2.63822500	-2.61293000	-0.36335200
O	0	2.12854100	-1.43452300	-2.20535100
H	0	0.23013300	-3.54846300	-1.79014800
H	0	0.19960100	-3.01990600	-0.09010000
H	0	3.36582400	-0.87085100	-1.74030200
C	0	4.39792100	-1.45340600	-0.13598500
N	0	5.06037700	-1.99681800	0.71959000
N	0	4.19547900	-0.57620400	-1.05774300
C	0	4.68027700	-2.80389000	1.87254200
H	0	4.02473000	-3.59987200	1.50762800
H	0	5.59573300	-3.25628700	2.26370600
C	0	4.51511900	0.85359900	-0.85252600
H	0	5.39641400	0.92318500	-0.20540700
H	0	4.79595100	1.24721800	-1.83540600
C	0	-0.61189000	-0.58241400	-0.66457700
H	0	0.34341500	-0.04605400	-0.73170500
H	0	-0.75857900	-0.89687800	0.38140900
O	0	-0.59398700	-1.72831700	-1.51560300
C	0	-1.71339300	0.38001500	-1.11139600

H	0	-1.67613800	0.44279100	-2.20718000
C	0	-3.13640200	-0.08535800	-0.74690700
H	0	-3.18179900	-1.17158800	-0.91475100
C	0	-3.46818000	0.16781700	0.74519000
H	0	-2.60079300	-0.15046400	1.33540300
C	0	-4.68533900	-0.59956000	1.30178400
H	0	-4.81140900	-0.24057000	2.33770500
O	-1	-6.78644200	-1.28267900	0.42429200
O	-1	-6.14774200	0.94376100	0.19342300
O	0	-1.38163300	1.66212500	-0.56059700
H	0	-2.16739700	1.98906200	-0.07973000
O	0	-4.01977200	0.58626400	-1.64476300
H	0	-4.87950700	0.74729200	-1.20787200
O	0	-4.43966200	-1.99725400	1.30527600
H	0	-5.29773000	-2.35672100	0.99377300
O	0	-3.64231100	1.57127000	1.00237800
H	0	-4.57690700	1.74162300	0.73102200
C	0	-6.02009800	-0.28817700	0.55999800
C	0	3.97599600	-1.98970900	2.95895500
H	0	3.03389500	-1.58027200	2.58372300
H	0	3.75079100	-2.63498900	3.81483200
H	0	4.60670700	-1.16571900	3.30835300
C	0	3.33738100	1.64477300	-0.27440100
H	0	3.07854300	1.23082300	0.70750500
H	0	2.46222100	1.50698900	-0.91814600
C	0	3.67569100	3.14784700	-0.14993800
H	0	4.56451600	3.26249400	0.48777400
H	0	3.95055300	3.53068700	-1.14286700
N	0	2.63898900	4.02675400	0.38275700
C	0	2.29844500	3.76596100	1.77589900
H	0	1.66724900	4.57933800	2.14991000
H	0	1.74730000	2.82204800	1.93754400
H	0	3.21251600	3.74196200	2.38088500
C	0	1.44849700	4.13101300	-0.46490000
H	0	0.83246800	4.96446500	-0.10982500
H	0	1.75387800	4.35619100	-1.49270800
H	0	0.81250100	3.23130300	-0.47657200

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies=	-1468.696498
Sum of electronic and thermal Energies=	-1468.663933
Sum of electronic and thermal Enthalpies=	-1468.662989
Sum of electronic and thermal Free Energies=	-1468.772121

INT (in gas)

-1 1

C	0	1.13920900	-0.73581000	-1.86667100
C	0	-0.34304900	-0.97354000	-1.60933000

O	0	-1.01543900	0.20345800	-1.80613700
O	0	-0.85555900	-2.01808600	-1.27035000
H	0	1.23465600	-0.26785900	-2.85311200
H	0	1.48983200	0.00515500	-1.13030800
H	0	-2.73976300	-1.54141900	-1.51103600
C	0	-2.38259000	0.43910700	-1.54413200
N	0	-2.78224500	1.62044800	-1.30818900
N	0	-3.20192100	-0.65235000	-1.66882400
C	0	-1.83553600	2.73389000	-1.30824300
H	0	-1.02388500	2.55626100	-0.59014100
H	0	-1.35655500	2.83026500	-2.29381100
C	0	-4.61392800	-0.54585000	-1.31877600
H	0	-4.99542400	0.37666900	-1.76611000
H	0	-5.12663900	-1.38773800	-1.80029700
C	0	2.26069700	-2.45344300	-0.59920400
H	0	2.08176100	-3.53160400	-0.63915400
H	0	1.61986100	-2.04662200	0.19113800
O	0	1.89090700	-1.91790300	-1.88135700
C	0	3.74573600	-2.22695000	-0.27610600
H	0	4.33892400	-2.60017700	-1.12324100
C	0	4.13544600	-0.75606000	-0.08001200
H	0	3.69543000	-0.17808200	-0.90488800
C	0	3.58377000	-0.17896500	1.25417000
H	0	2.59077300	-0.60725400	1.42917100
C	0	3.40886700	1.35065600	1.25068000
H	0	3.11342100	1.63593500	2.27316400
O	-1	4.56218800	3.11171700	0.14938200
O	-1	5.77800600	1.61281300	1.44990600
O	0	4.02667000	-3.02662100	0.87686900
H	0	4.45834300	-2.45723500	1.53841800
O	0	5.55737900	-0.70342500	-0.16450100
H	0	5.87155900	0.11850500	0.26348600
O	0	2.38381000	1.72132600	0.33153400
H	0	2.79074200	2.50023100	-0.11088800
O	0	4.38789400	-0.58681500	2.36399600
H	0	5.15345000	0.03012100	2.34310800
C	0	4.72161300	2.11617700	0.91240200
C	0	-2.55576300	4.03551600	-0.96091100
H	0	-3.01702600	3.96862500	0.03035100
H	0	-1.85246500	4.87582400	-0.95788300
H	0	-3.34858100	4.24673900	-1.68708400
C	0	-4.89680500	-0.54849000	0.19200200
H	0	-4.34425900	0.28061100	0.64528900
H	0	-4.50957600	-1.47896400	0.62661200
C	0	-6.40578800	-0.41244700	0.47795100
H	0	-6.76806600	0.52372600	0.03219000
H	0	-6.94401700	-1.22719900	-0.02724600
N	0	-6.83559500	-0.41885200	1.87999800
C	0	-6.59968100	-1.68055300	2.56753600
H	0	-7.00551000	-2.50620000	1.97279900
H	0	-5.53289000	-1.89417200	2.76752500
H	0	-7.12103400	-1.67100700	3.53162400
C	0	-6.36116200	0.72354000	2.65029500
H	0	-6.59084700	1.65026700	2.11427500
H	0	-6.88190300	0.75135300	3.61434200
H	0	-5.27504100	0.70814000	2.85616500

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -1468.729748
Sum of electronic and thermal Energies= -1468.696329
Sum of electronic and thermal Enthalpies= -1468.695385
Sum of electronic and thermal Free Energies= -1468.808449

H_2NNH_2 (in gas)

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0 1

N	-0.70913800	-0.07146200	-0.09687800
H	-1.14798700	-0.33524000	0.77898100
H	-1.07105200	0.83547200	-0.38593800
N	0.70913800	-0.07146100	0.09687800
H	1.14798700	-0.33524300	-0.77898000
H	1.07105200	0.83547300	0.38593600

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -111.828092
Sum of electronic and thermal Energies= -111.824834
Sum of electronic and thermal Enthalpies= -111.823890
Sum of electronic and thermal Free Energies= -111.850685

TS2 (in gas)

-1 1

C	0	1.32014900	-2.18593400	-1.40267800
O	0	2.73634800	-1.05458400	-1.61069600
O	0	1.64302200	-3.36067100	-1.57419100
H	0	4.81523000	-0.80641200	-2.41126800
C	0	3.74918500	-1.10253200	-0.78212600
N	0	3.58292900	-1.36877000	0.48326600
N	0	4.98768900	-0.85765400	-1.41245800
C	0	4.67262200	-1.71379900	1.37875500
H	0	4.43877900	-2.69401200	1.81998600
H	0	5.62440300	-1.84139300	0.84471500
N	0	1.01417500	-1.80997600	0.08322800
H	0	0.40977300	-0.97150900	0.15947900
H	0	1.99489700	-1.61837500	0.51209600
N	0	0.38883800	-2.87720000	0.82186700

H	0	-0.60031800	-2.87615400	0.57250700
H	0	0.79783800	-3.72947200	0.43016500
H	0	0.93535000	-1.43203200	-3.35465800
C	0	5.24879300	1.64437000	-1.12606800
H	0	4.30934800	1.69412200	-0.56361700
H	0	4.99169600	1.79908100	-2.18179700
C	0	6.22474600	2.73829600	-0.64723800
H	0	6.49175900	2.54404400	0.40069900
H	0	7.15777500	2.66407900	-1.22405800
N	0	5.77949200	4.13273100	-0.72526300
C	0	4.82962900	-0.70617300	2.52557400
H	0	3.88694500	-0.60587800	3.07341500
H	0	5.60461400	-1.03407100	3.22950000
H	0	5.10133400	0.28825900	2.15356400
C	0	0.40288700	-1.47030600	-2.39836100
H	0	-0.48490900	-2.10577400	-2.52069200
O	0	0.04448100	-0.16983400	-1.97165200
C	0	-1.34361200	0.14279500	-1.87287200
H	0	-1.94665600	-0.77487600	-1.89330200
H	0	-1.64082400	0.77048300	-2.72619700
C	0	-1.56482600	0.88901100	-0.55682500
H	0	-0.91176200	1.77134600	-0.55405100
C	0	-3.00749200	1.39911000	-0.39614200
O	0	-1.13822200	0.04796500	0.52373900
H	0	-3.29382400	1.85447700	-1.36072100
C	0	-4.04841600	0.29551200	-0.10433900
O	0	-2.98525700	2.40192900	0.61788300
H	0	-1.94108000	-0.21388600	1.02478100
H	0	-4.04449200	-0.44650500	-0.90872000
C	0	-5.47183200	0.85472400	0.00051600
O	0	-3.71101900	-0.39619000	1.11482300
H	0	-3.87305500	2.45637800	1.01623800
H	0	-5.65558900	1.52013000	-0.85545000
O	0	-5.58530800	1.58365100	1.22807200
C	0	-6.58258500	-0.25683000	-0.00672300
H	0	-4.19196700	0.07320000	1.81946600
H	0	-6.41914900	1.15091200	1.58589100
O	-1	-7.34134000	-0.15932100	1.02174000
O	-1	-6.57472800	-1.02918800	-0.99630900
C	0	5.85220600	0.23958800	-0.95951900
H	0	6.78665800	0.16500100	-1.53082000
H	0	6.11880300	0.07642500	0.08731000
C	0	4.66568800	4.45033000	0.16062700
H	0	3.70424800	3.99862300	-0.14337600
H	0	4.89442200	4.11058100	1.17613000
H	0	4.52709500	5.53697700	0.19138900
C	0	5.55304300	4.60791600	-2.08306500
H	0	5.41747400	5.69538100	-2.06831400
H	0	6.42920800	4.38561700	-2.70235200
H	0	4.66454000	4.16784100	-2.57341600

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -1580.540746

Sum of electronic and thermal Energies= -1580.505216

Sum of electronic and thermal Enthalpies= -1580.504272

Sum of electronic and thermal Free Energies= -1580.620579

P2 (in gas)

-1 1				
C	0	4.12395200	0.59307200	0.08762700
O	0	5.18986300	0.85362300	0.65643000
N	0	3.82635000	-0.62975700	-0.41078400
H	0	2.88566700	-0.86145500	-0.72958800
N	0	4.70418000	-1.72012500	-0.23093900
H	0	5.55186600	-1.52284700	-0.76156000
H	0	4.99047000	-1.73042600	0.74853900
H	0	2.66322300	1.92001900	0.90675500
C	0	3.06022300	1.67980000	-0.08937400
H	0	3.58852900	2.56998200	-0.45236000
O	0	2.03556200	1.34801300	-1.00559800
C	0	0.70913200	1.21130400	-0.48254500
H	0	0.06434200	1.22353700	-1.36441900
H	0	0.45118000	2.08100900	0.13925000
C	0	0.51194600	-0.08086000	0.31926300
H	0	1.17308900	-0.05797700	1.19569700
C	0	-0.92114100	-0.22497000	0.87269300
O	0	0.93899800	-1.21376700	-0.45266400
H	0	-1.21242300	0.71497600	1.35178500
C	0	-1.96675100	-0.51751400	-0.21431900
O	0	-0.95538100	-1.23605800	1.88061900
H	0	0.16050600	-1.63538300	-0.85900200
H	0	-1.81267900	0.15411800	-1.06946000
C	0	-3.42471700	-0.36992200	0.26599400
O	0	-1.73800600	-1.87540600	-0.65930400
H	0	-1.03944400	-2.08143200	1.41266900
H	0	-3.49981000	-0.67667500	1.31611400
O	0	-4.24493300	-1.22314400	-0.53629000
C	0	-3.90739700	1.11035000	0.10045200
H	0	-2.61002400	-2.16010300	-0.99639100
H	0	-4.85063700	-0.54438000	-0.93884400
O	-1	-4.92167800	1.20549200	-0.67290600
O	-1	-3.22055600	1.97232800	0.71897800

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies=	-1025.051044
Sum of electronic and thermal Energies=	-1025.030869
Sum of electronic and thermal Enthalpies=	-1025.029924
Sum of electronic and thermal Free Energies=	-1025.105768

CP2 (in gas)

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0 1

O	-2.55482900	2.39900100	0.39153700
H	-0.59974400	1.91910400	-0.88037200
C	-2.19143200	1.26136700	0.08839100
N	-2.91160700	0.13315300	0.48435100
N	-1.04290600	1.04033800	-0.64384500
C	-3.27158800	-0.94673200	-0.44844600
H	-3.94489800	-0.57143100	-1.23445300
H	-2.36998100	-1.30303500	-0.94961400
H	-3.70486200	0.45134600	1.03155900
C	1.29308100	0.32067000	-0.21932700
H	1.30465700	0.89019600	0.71759200
H	1.63625900	0.99871100	-1.01250000
C	2.24096300	-0.89533300	-0.12495100
H	1.87970500	-1.56590000	0.66650000
H	2.18635000	-1.46233100	-1.06418100
N	3.65334700	-0.63008900	0.14093400
C	-3.93661200	-2.09986800	0.29985900
H	-4.85061500	-1.76909000	0.80672500
H	-4.21505700	-2.89619100	-0.39784900
H	-3.26284700	-2.51696900	1.05500500
C	-0.14665900	-0.11243400	-0.51825800
H	-0.16317900	-0.71161900	-1.44046100
H	-0.51649800	-0.74779000	0.29260600
C	3.92160800	-0.05951400	1.45371500
H	4.99911800	-0.09022000	1.64818100
H	3.59249600	0.99083900	1.56591400
H	3.42340500	-0.65669600	2.22462400
C	4.34430800	0.07782500	-0.92727100
H	5.42338600	0.04971700	-0.74136100
H	4.15484300	-0.42078900	-1.88378600
H	4.05224800	1.14044800	-1.02877700

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -555.546403

Sum of electronic and thermal Energies= -555.531426

Sum of electronic and thermal Enthalpies= -555.530482

Sum of electronic and thermal Free Energies= -555.590326

P1 (in water)

-1 1

C	0	3.12243700	-1.14293400	-0.08806500
C	0	4.49383700	-0.47571500	-0.11085300
O	0	4.74544700	0.62293700	-0.56334600
O	0	5.42328800	-1.28711400	0.43182900
H	0	3.17835200	-2.02994900	-0.72805700
H	0	2.91801300	-1.48808400	0.93560500

H	0	6.29117900	-0.84824900	0.38123600
C	0	1.62933900	0.66966000	0.33154100
H	0	2.41600100	1.40534300	0.53453900
H	0	1.34574400	0.19645300	1.28266100
O	0	2.09424400	-0.32563000	-0.58575100
C	0	0.44311300	1.39757700	-0.30517700
H	0	0.74916400	1.71359700	-1.31158600
C	0	-0.80315800	0.51299900	-0.48700700
H	0	-0.45764400	-0.46109000	-0.85791900
C	0	-1.56412700	0.26386100	0.83639600
H	0	-0.82312800	0.04636800	1.61211000
C	0	-2.54053300	-0.93320400	0.82642400
H	0	-3.05274300	-0.91131600	1.80162500
O	0	-3.95306900	-1.91659300	-0.82701300
O	-1	-4.14623000	0.31101300	-0.45978000
O	-1	0.19505400	2.57424800	0.47838300
H	0	-0.72705300	2.53987800	0.79396600
O	0	-1.61537800	1.15016700	-1.48387700
H	0	-2.55504000	0.93328100	-1.33085800
O	0	-1.81727500	-2.14882900	0.69101300
H	0	-2.35925400	-2.67350800	0.06871600
O	0	-2.25589900	1.44781700	1.26570800
H	0	-3.08879300	1.46246800	0.74868000
C	0	-3.64695000	-0.84379800	-0.25459800

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -989.710157

Sum of electronic and thermal Energies= -989.690983

Sum of electronic and thermal Enthalpies= -989.690039

Sum of electronic and thermal Free Energies= -989.763641

EDC (in water)

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0 1

C	2.05296100	0.77600100	0.43242700
N	2.72465100	-0.01966700	1.08333900
N	1.45789800	1.71156200	-0.09595400
C	3.55669600	-1.11620200	0.56665100
H	4.52687300	-1.03808000	1.06861300
H	3.10425100	-2.05326100	0.91053500
C	0.04985300	1.75127400	-0.51341600
H	-0.36463000	2.69234800	-0.13404700
H	0.03946900	1.82707400	-1.60756700
C	3.74156300	-1.13655500	-0.94876400
H	4.21552800	-0.21471300	-1.30185300
H	4.38223800	-1.97798200	-1.23190000
H	2.78244900	-1.25225000	-1.46469200
C	-0.80710900	0.57028800	-0.05259400
H	-0.77125500	0.50814900	1.04163100
H	-0.37870800	-0.35945100	-0.44584000
C	-2.26655500	0.72805800	-0.53152900

H	-2.66582600	1.67538000	-0.14645600
H	-2.27401400	0.80228500	-1.62681800
N	-3.21517400	-0.32798300	-0.15948300
C	-2.90870200	-1.62922700	-0.74789700
H	-2.00526500	-2.10667500	-0.32695200
H	-3.75047400	-2.30972100	-0.58109500
H	-2.76546800	-1.52202900	-1.82804400
C	-3.45757000	-0.42309800	1.27762600
H	-3.71318900	0.56429800	1.67553500
H	-4.30432200	-1.09378600	1.45839600
H	-2.59610600	-0.81220400	1.85022100

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -479.097510
Sum of electronic and thermal Energies= -479.083559
Sum of electronic and thermal Enthalpies= -479.082615
Sum of electronic and thermal Free Energies= -479.140547

TS1 (in water)

-1 1

C	0	0.26193100	-1.37636600	-1.02828800
C	0	-1.09334700	-0.66815700	-1.20083900
O	0	-1.31201200	0.38546400	-0.51310500
O	0	-1.90351800	-1.20409100	-2.00223700
H	0	0.06365600	-2.32969700	-0.52710600
H	0	0.65309300	-1.60339900	-2.03025200
H	0	-3.29747600	-0.25612000	-1.69916500
C	0	-3.11333400	1.34328100	-0.54272000
N	0	-3.00157200	2.40618700	0.01023600
N	0	-3.83204800	0.50703300	-1.23256000
C	0	-2.29750100	2.95569900	1.15869700
H	0	-2.93675000	2.81292900	2.03710300
H	0	-1.38361600	2.37316500	1.30765100
C	0	-5.30906400	0.49056100	-1.16072800
H	0	-5.64734800	1.50673400	-0.94105100
H	0	-5.66016700	0.23347800	-2.16453300
C	0	1.85698400	0.38898700	-0.91868500
H	0	1.12068400	1.14999500	-1.20416300
H	0	2.34954600	0.02930400	-1.83490400
O	0	1.22408900	-0.69745000	-0.24520200
C	0	2.87573500	1.03070800	0.02682600
H	0	2.33641000	1.45132900	0.88287000
C	0	3.94302500	0.06978100	0.59055800
H	0	3.44184800	-0.69775100	1.18451800
C	0	4.75398900	-0.64794200	-0.50462800
H	0	4.04922600	-1.27171500	-1.06727400
C	0	5.86330800	-1.58716600	0.02439400
H	0	6.25079400	-2.12531000	-0.85500000

O	-1	7.48216900	-1.32557700	1.75747200
O	-1	7.56775000	0.09778300	-0.08230200
O	0	3.49784100	2.14445600	-0.63069500
H	0	4.18478700	1.76160300	-1.21437400
O	0	4.77580600	0.79168400	1.50549400
H	0	5.03991600	1.61607900	1.06913600
O	0	5.32440300	-2.52208100	0.94835600
H	0	5.95817800	-2.48010000	1.69482000
O	0	5.32876900	0.28332700	-1.44050700
H	0	6.25642800	0.43376600	-1.10990400
C	0	7.08586700	-0.85298500	0.64234200
C	0	-1.98421900	4.43579000	0.96357900
H	0	-2.90085500	5.01526400	0.81797000
H	0	-1.47105000	4.81915600	1.85060700
H	0	-1.33435800	4.58805300	0.09663300
C	0	-5.84094800	-0.50516400	-0.12628600
H	0	-5.45853800	-1.50416400	-0.36482900
C	0	-7.38562900	-0.51063700	-0.11288400
H	0	-7.74260600	0.50206100	0.11539900
H	0	-7.74909400	-0.75615000	-1.11919600
N	0	-8.04210800	-1.42758500	0.82462900
C	0	-7.80800900	-2.83922400	0.53167000
H	0	-8.03380200	-3.04084000	-0.52041900
H	0	-6.77258300	-3.17025400	0.73124700
H	0	-8.47497100	-3.45189500	1.14743100
C	0	-7.79429200	-1.11301200	2.22920100
H	0	-8.01003400	-0.05587700	2.41490800
H	0	-8.46121200	-1.71297900	2.85738300
H	0	-6.75782500	-1.31549700	2.55527400
H	0	-5.45152700	-0.23365500	0.86163300

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -1468.796317
Sum of electronic and thermal Energies= -1468.762274
Sum of electronic and thermal Enthalpies= -1468.761329
Sum of electronic and thermal Free Energies= -1468.876151

INT (in water)

-1 1

C	0	0.51165400	1.21081000	-0.69439000
C	0	-0.88588700	0.60566300	-0.79402200
O	0	-1.80396100	1.58008700	-0.57066600
O	0	-1.13669000	-0.55503600	-1.04156300
H	0	0.60854800	1.94708700	-1.49946500
H	0	0.59223500	1.75125700	0.25910800
H	0	-3.04598400	-0.26374200	-1.67265600
C	0	-3.21707200	1.41809800	-0.57778800
N	0	-3.92818800	2.19727000	0.12970900
N	0	-3.68710800	0.49162800	-1.46170800
C	0	-3.30375600	3.24958200	0.93253300
H	0	-2.57367100	2.81947100	1.63210600
H	0	-2.74461200	3.94234500	0.28725000

C	0	-5.11634700	0.18585900	-1.54224600
H	0	-5.66013300	1.13365600	-1.51108600
H	0	-5.28627300	-0.26097700	-2.52760100
C	0	1.80414900	-0.52344300	0.30895600
H	0	0.92401700	-1.11447900	0.58783200
H	0	2.05989600	0.13327600	1.15282700
O	0	1.53652500	0.26463600	-0.85638000
C	0	2.95339200	-1.48442300	-0.00617800
H	0	2.63313300	-2.15253800	-0.81328800
C	0	4.26457700	-0.81010400	-0.46404400
H	0	4.07554300	-0.27349900	-1.39658500
C	0	4.80819800	0.20844600	0.55490300
H	0	4.06372200	1.00977300	0.63323900
C	0	6.14496200	0.87538100	0.15251900
H	0	6.32423600	1.66867600	0.89508900
O	-1	8.15350700	-0.01296400	-0.77915200
O	-1	7.48415300	-0.72806300	1.33206800
O	0	3.18925800	-2.32444000	1.13174200
H	0	3.72682700	-1.79066200	1.75300100
O	0	5.21745000	-1.82938900	-0.78494700
H	0	5.23185100	-2.45736300	-0.04652000
O	0	6.04213700	1.45560000	-1.14002000
H	0	6.85411600	1.13715500	-1.58711700
O	0	4.94234500	-0.36810800	1.86721300
H	0	5.89692300	-0.64939500	1.92334000
C	0	7.38010700	-0.06475300	0.23180600
C	0	-4.36397000	4.02336500	1.71338600
H	0	-4.91393800	3.35839800	2.38811000
H	0	-3.89776400	4.81201100	2.31378700
H	0	-5.08569100	4.49035600	1.03443300
C	0	-5.62352600	-0.75786100	-0.44196800
H	0	-5.41144900	-0.31005000	0.53460100
H	0	-5.06638700	-1.70068400	-0.49879700
C	0	-7.13593400	-1.02146200	-0.59636500
H	0	-7.66989400	-0.06401600	-0.53415000
H	0	-7.32697100	-1.42479300	-1.59986400
N	0	-7.76556300	-1.93545300	0.36519900
C	0	-7.28599400	-3.31164100	0.26988100
H	0	-7.34240500	-3.65157600	-0.76931900
H	0	-6.24627300	-3.44710800	0.61964300
H	0	-7.92562000	-3.96148700	0.87675600
C	0	-7.74494400	-1.44709400	1.74140100
H	0	-8.13550800	-0.42491600	1.77691400
H	0	-8.38923400	-2.08031600	2.36084600
H	0	-6.73867300	-1.44710400	2.19851600

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies= -1468.818070

Sum of electronic and thermal Energies= -1468.785218

Sum of electronic and thermal Enthalpies= -1468.784274

Sum of electronic and thermal Free Energies= -1468.893689

H_2NNH_2 (in water)

```
 0 1
 N                 -0.71432500    0.09852300   -0.08016200
 H                 -1.14509700   -0.80136200   -0.27169000
 H                 -1.04948400    0.40495900    0.83282500
 N                  0.71432500   -0.09852200   -0.08016200
 H                  1.14509700    0.80136300   -0.27168900
 H                  1.04948400   -0.40496000    0.83282400
```

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -111.836955
Sum of electronic and thermal Energies= -111.833673
Sum of electronic and thermal Enthalpies= -111.832729
Sum of electronic and thermal Free Energies= -111.859590

TS2 (in water)

```
-1 1
 C                 0    1.19818500   -1.57358300   -2.16073400
 O                 0    2.50608700   -0.37880500   -2.10813700
 O                 0    1.60672700   -2.67733900   -2.56759900
 H                 0    4.63431500    0.09471300   -2.77846700
 C                 0    3.52329800   -0.59857400   -1.29040200
 N                 0    3.30202700   -1.11484200   -0.10714500
 N                 0    4.73879400   -0.23717900   -1.82760300
 C                 0    4.32224600   -1.69978400    0.75655900
 H                 0    4.04788200   -2.75126900    0.92097300
 H                 0    5.30803300   -1.71527600    0.27963100
 N                 0    0.84785600   -1.53130400   -0.66149000
 H                 0    0.25065400   -0.72137700   -0.42891100
 H                 0    1.89409900   -1.40238900   -0.16964500
 N                 0    0.20789400   -2.71824200   -0.16004200
 H                 0   -0.70713700   -2.79920200   -0.60513800
 H                 0    0.76553700   -3.49587400   -0.51490600
 H                 0    0.73256700   -0.53616100   -3.97043400
 C                 0    6.44044600    1.55617600   -1.84852300
 H                 0    5.65472600    2.30577100   -2.00079000
 H                 0    6.76397900    1.21697400   -2.84082100
 C                 0    7.63334800    2.17464400   -1.08805900
 H                 0    7.28824000    2.50974600   -0.10133300
 H                 0    8.38514500    1.39423300   -0.91292400
 N                 0    8.31943500    3.30730900   -1.71887900
 C                 0    4.40496000   -1.00436500    2.11918500
 H                 0    3.42783400   -1.01080200    2.61411400
 H                 0    5.12064300   -1.51998000    2.76916400
 H                 0    4.72340000    0.03874300    2.01685500
 C                 0    0.22684600   -0.76315700   -3.02642900
 H                 0   -0.62865300   -1.41444700   -3.24380300
 O                 0   -0.19270300    0.43864000   -2.39563000
 C                 0   -1.59120200    0.60763700   -2.15730700
```

H	0	-2.09573200	-0.36656000	-2.15708400
H	0	-2.03242800	1.22753500	-2.94992500
C	0	-1.74208300	1.28706000	-0.79498200
H	0	-1.13243300	2.19863600	-0.80743700
C	0	-3.18713000	1.72085900	-0.49801400
O	0	-1.18680600	0.44422600	0.22849200
H	0	-3.54445300	2.27225900	-1.38127200
C	0	-4.16401200	0.54572800	-0.26365500
O	0	-3.13582700	2.59574200	0.63354400
H	0	-1.93186100	-0.01241600	0.66756100
H	0	-4.10691800	-0.14559500	-1.10781700
C	0	-5.62463400	0.99999500	-0.14545300
O	0	-3.77358900	-0.21477100	0.89667600
H	0	-4.04344200	2.69766400	0.97270800
H	0	-5.88443300	1.56738200	-1.04940900
O	0	-5.77122000	1.84064900	1.00435500
C	0	-6.61292500	-0.20133100	-0.03567900
H	0	-4.02531500	0.30254400	1.67909800
H	0	-6.48767000	1.38416200	1.50583100
O	-1	-7.34134000	-0.15932100	1.02174000
O	-1	-6.57472800	-1.02918800	-0.99630900
C	0	5.85368700	0.36700300	-1.08231400
H	0	6.64092200	-0.37622700	-0.90323100
H	0	5.48975100	0.70034800	-0.10502300
C	0	7.48520600	4.49757800	-1.86134400
H	0	6.68647000	4.39368600	-2.61803400
H	0	7.01628600	4.73759000	-0.90160400
H	0	8.11151000	5.34612900	-2.15676300
C	0	9.00019100	2.96647300	-2.96515900
H	0	9.64167200	3.80115500	-3.26750200
H	0	9.63404000	2.08709500	-2.81194300
H	0	8.31346900	2.75395000	-3.80458600

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -1580.640849
Sum of electronic and thermal Energies= -1580.605354
Sum of electronic and thermal Enthalpies= -1580.604410
Sum of electronic and thermal Free Energies= -1580.717994

P2 (in water)

-1 1

C	0	4.11617600	0.67770000	0.06878400
O	0	5.11479900	1.12646600	0.64965200
N	0	3.87418600	-0.63979900	-0.09135900
H	0	2.97740900	-0.96006200	-0.45041000
N	0	4.70219100	-1.63385300	0.47170900
H	0	5.57055100	-1.66991900	-0.06106300
H	0	4.95528400	-1.34091100	1.41510200
H	0	2.60248900	2.16740300	0.32077800
C	0	3.07516800	1.63426300	-0.51375500
H	0	3.62447800	2.37336800	-1.10743100
O	0	2.11651100	1.00514600	-1.35213900

C	0	0.76296400	0.97314800	-0.88987600
H	0	0.17481100	0.73436000	-1.77958300
H	0	0.45804800	1.96491100	-0.52832500
C	0	0.53598800	-0.07625900	0.20382500
H	0	1.17346500	0.15807500	1.06350700
C	0	-0.91405900	-0.12351400	0.73630400
O	0	0.97306600	-1.37578900	-0.22909500
H	0	-1.15171100	0.83357000	1.20712900
C	0	-1.96594800	-0.36239000	-0.35731100
O	0	-0.99352400	-1.10235600	1.77527100
H	0	0.31965400	-1.70409500	-0.87402000
H	0	-1.91425700	0.46563600	-1.08027600
C	0	-3.42063200	-0.45092200	0.16187100
O	0	-1.63068200	-1.58593000	-1.03358900
H	0	-0.60170000	-1.91963700	1.43042000
H	0	-3.44211400	-1.05650300	1.07322400
O	0	-4.20332300	-1.10381200	-0.84363700
C	0	-4.01567900	0.95755500	0.44964900
H	0	-2.43110200	-1.84934300	-1.52019500
H	0	-4.80482500	-0.38177900	-1.13627700
O	-1	-4.95785200	1.28629500	-0.36183300
O	-1	-3.49261900	1.59035700	1.42137400

B3LYP/6-31+G(d,p)
Sum of electronic and zero-point Energies= -1025.139931
Sum of electronic and thermal Energies= -1025.118554
Sum of electronic and thermal Enthalpies= -1025.117610
Sum of electronic and thermal Free Energies= -1025.198608

CP2 (in water)

---

0 1

O	-2.62833400	2.40417600	0.41489600
H	-0.60574900	1.97127800	-0.78234200
C	-2.23389000	1.26367800	0.09768700
N	-2.96483500	0.13855700	0.43541000
N	-1.05132100	1.08782600	-0.56896700
C	-3.23491800	-0.98756600	-0.47837300
H	-3.99307000	-0.69151700	-1.21719500
H	-2.32820100	-1.22727200	-1.03284700
H	-3.78945600	0.42337300	0.95305200
C	1.27906200	0.34268900	-0.19031300
H	1.29759700	0.86139700	0.77520600
H	1.61713900	1.05774500	-0.95102700
C	2.22102600	-0.88032600	-0.16379100
H	1.86199400	-1.58791000	0.59485500
H	2.16071300	-1.39493400	-1.13151200
N	3.64033600	-0.62975000	0.10992800
C	-3.71289100	-2.21181000	0.29802200
H	-4.62153400	-1.98805600	0.86823400
H	-3.94466600	-3.02749700	-0.39406200
H	-2.94509600	-2.55681200	0.99789900
C	-0.16086600	-0.07818800	-0.50214700

H	-0.18516300	-0.63000300	-1.45118300
H	-0.52847300	-0.74836100	0.28030200
C	3.89977800	-0.10436600	1.44786800
H	4.97739400	-0.12476900	1.64228600
H	3.55457400	0.93538200	1.59323900
H	3.40638500	-0.73476300	2.19474600
C	4.31171000	0.15433400	-0.92330200
H	5.39211300	0.13909300	-0.74456100
H	4.12215400	-0.28947300	-1.90604800
H	3.99468400	1.21259300	-0.95671200

B3LYP/6-31+G(d,p)

Sum of electronic and zero-point Energies=	-555.561438
Sum of electronic and thermal Energies=	-555.546389
Sum of electronic and thermal Enthalpies=	-555.545445
Sum of electronic and thermal Free Energies=	-555.606017

Table S.1. Electronic energies of all species involved in carboxymethylation and hydrazination reactions.

Species	Electronic energy (E_e)
RC (Chloroacetate)	-688.2460432
RC (Gluconate)	-761.5382608
TS	-1449.770383
CP1	-460.3846886
P1	-989.4721362

Species (in gas phase)	Electronic energy (E_e)
P1	-989.8495605
EDC	-479.089384
TS1	-1468.696498
INT	-1468.729748
H_2NNH_2	-111.8814855
TS2	-1580.540746
CP2	-555.546403
P2	-1025.306709

Species (in water)	Electronic energy (E_e)
P1	-989.9362188
EDC	-479.097510
TS1	-1468.796317
INT	-1468.818070
H_2NNH_2	-111.8903881
TS2	-1580.640849
CP2	-555.561438
P2	-1025.394971