Single point energy SP (Hartree)

Internal energy U (Hartree)

Enthalpy H (Hartree)

Gibbs free energy G (Hartree)

Note: some thiol adducts (**1, 2** and **5-7, 29, 30**) have two diastereomers: anti- and syn-, which refer to the relative positions of R1 group and sulfur atom (see below).

A picture containing text, clock

Description automatically generated

**MeS-**

S 0.20339887433186 2.24571966588315 -0.06724173811584

C -1.47956982376521 2.43113425953195 -0.77422472091630

H -1.47084675638465 3.05715095992724 -1.67330506946286

H -1.90694217538470 1.46210855376308 -1.05433077245951

H -2.16678311879730 2.89681256089458 -0.05937569904551

0 imaginary frequency

SP = -438.275660824718

U = -438.23558941

H = -438.23464520

G = -438.26222655

**MeSH**

S 0.25930103646637 1.84153926673218 -0.14274754485422

C -1.34722722044689 2.41383031156875 -0.77540619773663

H -1.22692403640588 2.95154424151231 -1.71620838249375

H -1.95079676008716 1.52198968506079 -0.95187572076964

H -1.85301486244200 3.04433108275544 -0.04356357918334

H 0.83269184291557 3.04996541237053 -0.01159857496243

0 imaginary frequencies

SP = -438.760535465403

U = -438.71008930

H = -438.70914509

G = -438.73756155

**Olefin 1**

C 2.33942435123110 -0.56602735420847 0.09870557284990

O 2.52106696239204 -1.75839658992164 0.24407389642266

C 0.99279796957114 0.07507082293113 0.06785267236255

C -0.10183383062944 -0.71305423213786 0.12063941873413

O 3.31777503144306 0.32223471305417 -0.06302369425612

C 4.66365119552303 -0.20625303716991 -0.07665665839723

H 4.77650578884973 -0.90775249725614 -0.90469664235728

H 5.30931557898416 0.65843369700055 -0.21629868991245

H 4.87883841610186 -0.69764368254252 0.87333515165311

C -1.52166521460121 -0.37235802590794 0.06504560330675

C -2.40977381924730 -1.42192661801666 -0.22008348127096

C -2.03810711039294 0.90827154550742 0.31730489058693

C -3.77724292403468 -1.18990639366827 -0.30311808705705

H -2.01450585775008 -2.41959467823017 -0.38840962919588

C -3.40791127671624 1.13146619060715 0.25447763848265

H -1.38408946359883 1.72658102043709 0.59095850139395

C -4.27785726732415 0.08886378791165 -0.06597065412998

H -4.45188363798752 -2.00648374619542 -0.53971596103691

H -3.79971322982741 2.12232515333162 0.46145456716254

H -5.34687709234316 0.27216848079120 -0.11777416004042

H 0.11021686148550 -1.77815221643702 0.17859154603587

C 0.95803848826050 1.49818614680903 -0.08590218378234

N 0.95712008061081 2.64599751331101 -0.21729961755444

0 imaginary frequencies

SP = -630.181545049113

U = -629.99165771

H = -629.99071350

G = -630.04325620

**1 TS**

C 4.39093426684985 -0.54107216645386 0.09187684276181

C 3.52078243381209 -0.79191100622000 -0.97025153071965

C 2.15386415907386 -0.58665017616145 -0.82129335687277

C 1.63652487068518 -0.12292773170810 0.39463658621530

C 2.51938567009451 0.14749432409201 1.44727726917782

C 3.88698106786005 -0.06926843214375 1.30204801326459

C 0.20215207538432 0.09157435814806 0.64824470681416

C -0.85416426521974 -0.62009279893329 0.14791696134787

C -0.73809557397165 -1.60852103225920 -0.87257510321131

N -0.65786082390629 -2.42384855954988 -1.68892672774120

C -2.19468880907474 -0.36081949383660 0.70930775116748

O -2.42445332041050 0.44537896525364 1.59032644791423

O -3.14355116982008 -1.12027503573995 0.14356663979226

C -4.48088768384799 -0.94628230562437 0.65144548058977

S 0.00497537225846 2.57089943145726 -0.59726247285508

C -1.51141469024285 2.11499514249625 -1.49812374390292

H -0.03050213184995 0.70223005915520 1.51061018363052

H -1.52804798096087 2.56086221662747 -2.49647293157258

H -2.41125328600567 2.43388928622314 -0.96384945272570

H -1.56529359328247 1.02578272691493 -1.62300681814972

H -4.51295565123107 -1.18968054315682 1.71509095188505

H -4.81198016404836 0.08170393953484 0.49381065499895

H -5.09812210079968 -1.63887788377174 0.08200357668460

H 2.12611682358858 0.52621852290947 2.38691791687829

H 4.55785860789920 0.13655060296951 2.13078255142902

H 5.45795048624260 -0.70410375494498 -0.02852153046456

H 3.91039524399149 -1.14242095130388 -1.92142739866339

H 1.49674216693173 -0.75751870397389 -1.66553946767284

1 imaginary frequency: -108.90 cm\*\*-1

SP = -1068.465910644519

U = -1068.23450852

H = -1068.23356431

G = -1068.29430598

**1 carbanion**

C -1.52647640066204 2.98696086012531 -0.01256195839942

S -0.11234687129981 2.15145633338522 0.74532527336821

C -0.03970015794793 0.62403968407089 -0.27523942820574

C 1.12555354593033 -0.21332509319442 0.18462832287373

C 1.00428908888550 -1.01071213949513 1.32865088570025

N 0.87963543880325 -1.67246676297099 2.28310540634864

C 2.36941234499597 -0.11209765761073 -0.46904300413285

O 2.62913140198007 0.59510094728103 -1.46147402680748

O 3.35300830826903 -0.90236474679795 0.08246409034517

C 4.63624915588584 -0.85359076247692 -0.55472080118593

C -1.35766294241727 -0.12916893935097 -0.29886258771419

H 0.17792809845386 0.94833030529415 -1.29423410633696

H -1.59562231183469 3.98470266487942 0.42677986731272

H -1.37967463438115 3.08581322821339 -1.09100163015233

H -2.45515809337621 2.44733633081653 0.18514682688705

H 5.27191255140389 -1.52900482573303 0.01840747828534

H 4.57183903691973 -1.19671651923624 -1.59013088224874

H 5.04949973666203 0.15738074071549 -0.52514698996262

C -1.83064497217747 -0.61270486789576 -1.52120257628021

C -3.01871752222570 -1.33861856950666 -1.58872935435255

C -3.75167445547186 -1.58691486178641 -0.43008025019941

C -3.28893008625665 -1.10248617913924 0.79293568888891

C -2.10188364206077 -0.37611335749450 0.85725288602617

H -1.26323215106884 -0.41587342945656 -2.42732772876799

H -3.37398764737378 -1.70462201540978 -2.54778478851560

H -4.67968657077916 -2.14907483462700 -0.47945957239545

H -3.85685447867187 -1.28659221613696 1.70056063345516

H -1.75743177018427 0.01566268353778 1.80926632616613

0 imaginary frequencies

SP = -1068.502109006414

U = -1068.26961052

H = -1068.26866632

G = -1068.32887900

**1 anti-adduct**

C -1.09095508465584 2.20899020103236 -0.38750524544623

H -2.05144216683021 1.73968773651013 -0.16688082588707

H -0.88899384927430 2.16684206787836 -1.45991024311933

S 0.23959078981881 1.40778877715816 0.53669054217310

C 2.66110237224833 -0.37657281464595 -0.18162946318092

O 2.99172584448792 -0.22491842639629 -1.33691837343386

C 1.35717830711285 -1.06240940644991 0.23023828553551

H 1.32959049153687 -1.18296803450729 1.31607895890241

C 0.14707831720231 -0.23086834522944 -0.26092290359973

H 0.26890152348394 -0.07622309104476 -1.33625397063905

O 3.35224700048620 0.03584933888334 0.86924349394132

C 4.56879332894431 0.76849751996456 0.57976970031712

H 4.32694694540081 1.66762608065913 0.01087455343102

H 4.98459640728484 1.02740337531064 1.55116261752623

H 5.25714779866909 0.13314976782344 0.02091264841106

C -1.16506084523601 -0.94043170922858 -0.01061244716157

C -1.97327516380797 -1.28764830990925 -1.09168260508210

C -1.57466656692388 -1.26494650088231 1.28482991046631

C -3.17726204027377 -1.96145258427710 -0.88389129675174

H -1.65765439455670 -1.03260513403945 -2.09966834071188

C -2.77352973218990 -1.93795556768812 1.49324427513406

H -0.95506584326088 -0.98773622791917 2.13321701618980

C -3.57829959192811 -2.28881591630183 0.40798052078008

H -3.79942807355877 -2.22834379521725 -1.73292366664388

H -3.08292736000658 -2.18830260990017 2.50366294724829

H -4.51476440726386 -2.81352492981893 0.57243028235738

C 1.30747629167984 -2.39840515187932 -0.37000571043780

N 1.25970679051231 -3.44820487287218 -0.84308597297965

H -1.12129708910162 3.25292856298718 -0.06951468733887

0 imaginary frequencies

SP = -1068.976258107704

U = -1068.72995008

H = -1068.72900587

G = -1068.78923505

**1 sync-adduct**

C -1.05011341370267 2.29565745207288 -0.07276337592870

H -2.02681031134941 1.85239524712467 0.12984363977072

H -0.92282660169439 2.45315964512239 -1.14571398614859

S 0.27348486473060 1.24793775114119 0.57081547635171

C 2.54142805791084 -0.44690807440362 -0.75086125986947

O 2.67223163861887 0.03181886571348 -1.85537883125810

C 1.24854963226271 -1.14110031090656 -0.32937902087026

C 0.04089298342356 -0.19060877340039 -0.51896248898825

H 0.10665447566484 0.16533393926655 -1.54925694634792

O 3.46827521169394 -0.43794653940444 0.19379551434302

C 4.72058978104492 0.20675196550117 -0.14604629885351

H 4.53933138550197 1.25676726450831 -0.37997504222611

H 5.34115407495806 0.11063492614461 0.74225028068213

H 5.17776402472582 -0.30369613362752 -0.99466090464296

C -1.27014584942570 -0.93622764812324 -0.34588203456724

C -1.78228616146000 -1.62649528727237 -1.44732765034679

C -1.95055035150306 -0.99347826419828 0.86986895772108

C -2.95410919039431 -2.36983379112670 -1.33524690647535

H -1.25662525588319 -1.57978762224771 -2.39793707529827

C -3.12596452338382 -1.73402061189289 0.98261338619260

H -1.56647062079993 -0.45156772361289 1.72814174636546

C -3.63008170393898 -2.42471883313903 -0.11705877628851

H -3.34186858274420 -2.90031120559554 -2.19985366434228

H -3.64939360245116 -1.76825116850049 1.93354376914769

H -4.54715560743205 -2.99930992304658 -0.02695090362538

C 1.30120005802667 -1.68388375029148 1.03128755757368

N 1.30510378857093 -2.12863786924001 2.09416800113772

H 1.11845303995376 -1.98783409384942 -1.01160282544670

H -0.97962124092459 3.25621056728391 0.44104966223859

0 imaginary frequencies

SP = -1068.976311765819

U = -1068.73014561

H = -1068.72920140

G = -1068.78935629

**2**

C 2.75998750332620 -0.66474041082891 0.12003258989921

O 2.83504052154611 -1.87221136272165 0.36998450687627

C 1.42147534753252 0.02056588018758 0.03895065620203

C 0.30443670890867 -0.72453391886984 0.16031080113057

C -1.10724443004383 -0.34780105943614 0.08397338676370

C -2.02630361766145 -1.39011721710342 -0.11518872857676

C -1.58780448589428 0.96123892019353 0.24163208148918

C -3.38798687872813 -1.12758417066851 -0.20564420057746

H -1.66010663990396 -2.40842457229459 -0.21014034293854

C -2.95198185630179 1.21720315651544 0.17296216987048

H -0.91045412274948 1.78014311058237 0.44870307128174

C -3.85278089409118 0.17812272518661 -0.06083958678421

H -4.08625709327973 -1.94133474398599 -0.37379031080382

H -3.31458517638689 2.23130823199850 0.30842593706952

H -4.91714763922944 0.38572464143565 -0.11668128096985

N 3.84446941260356 0.09397686622714 -0.10129049127966

H 4.75417558674374 -0.34337304335608 -0.05734008661443

H 3.79182259508719 1.08156093631037 -0.30297477274823

H 0.48713667323728 -1.78654375857413 0.30596558727637

C 1.40881506584666 1.42565727222991 -0.23453375218407

N 1.45531241943822 2.55611151697221 -0.47138523438202

0 imaginary frequencies

SP = -570.990570943936

U = -570.81792143

H = -570.81697722

G = -570.86591224

**2 TS**

C 4.40721686023953 -0.52965845251720 0.08264306117324

C 3.53177132797962 -0.76866153745238 -0.97727885981467

C 2.16482060209579 -0.57384489079644 -0.81570676274479

C 1.65348166630718 -0.13423388972947 0.41198089988112

C 2.54196926556851 0.12761624308675 1.46189704948183

C 3.90926698261324 -0.07853654741856 1.30311825701840

C 0.22016472918845 0.06361590531828 0.67503445790039

C -0.82399766940549 -0.64780210195937 0.16919864194161

C -0.67506444381581 -1.65424190055101 -0.82850558310042

N -0.61050763210343 -2.49415702816658 -1.62361986180815

C -2.19659140154192 -0.37684527780553 0.68277738042230

O -2.38651009691613 0.41964183467736 1.61346999024729

N -3.21411283820645 -1.04081512139831 0.10183950499191

S -0.04834520191319 2.66931663467874 -0.60319805891681

C -1.51861799458262 2.06488971952154 -1.49312314350397

H -0.01854745806006 0.71125533175432 1.50762680714856

H -1.61913105441559 2.54124972747071 -2.47400954217140

H -2.44262144305789 2.25363212996635 -0.93599886463443

H -1.45292835509617 0.98322713789334 -1.66835642817185

H 2.15256032713892 0.49098227639935 2.40883909723197

H 4.58517839545368 0.12024932273810 2.12922802102680

H 5.47417391658992 -0.68421839371619 -0.04776305820476

H 3.91708998490706 -1.10017078465103 -1.93677700420869

H 1.50360354718242 -0.73095105039109 -1.65965758501610

H -3.07970000861954 -1.65994464362617 -0.68313967136242

H -4.15320200753004 -0.86343464332552 0.42743125519305

1 imaginary frequency: -125.29 cm\*\*-1

SP = -1009.273091542553

U = -1009.05925290

H = -1009.05830870

G = -1009.11650183

**2 carbanion**

C 2.26912843422667 -1.06315046314295 -0.05376095380345

H 2.57534872582996 -0.04567707257693 0.19915897798725

H 2.27323448972646 -1.19056959213470 -1.13911874871817

S 0.63555490590634 -1.43933398846040 0.62754830914404

C -2.71738414152772 -1.29814012868529 -0.71915793237109

O -2.36794779113309 -1.86930771965662 -1.79388198137765

C -1.85354941379121 -0.47595854943391 0.04902197750435

C -0.41511536655266 -0.29255470199646 -0.35750436339954

H -0.33262332183219 -0.61899572258036 -1.39472328184498

C 0.07768889657520 1.14007257188799 -0.27834067577846

C 0.27453564753104 1.85760665371160 -1.46005445871878

C 0.34123520620838 1.76928281042823 0.94134047600992

C 0.71235236804794 3.18123794889747 -1.42853205175785

H 0.08504520097515 1.37284193614370 -2.41452644390321

C 0.77763670425486 3.09156493017736 0.97667551936112

H 0.22252562936436 1.21567349750644 1.86730239141989

C 0.96288843819708 3.80381885992437 -0.20828644806071

H 0.86282842063525 3.72195857650942 -2.35864171675964

H 0.97821740239305 3.56675192867259 1.93283315030991

H 1.30666740367991 4.83365367110835 -0.17933047040226

C -2.31236655440385 0.06793978964401 1.25226586917249

N -2.71232154120519 0.52455619158735 2.25222459944007

N -4.00707415438557 -1.52928640219316 -0.25637141976158

H -4.65015484423189 -1.82678195283218 -0.97725004876494

H -4.39440693492188 -0.86093916065639 0.39556732612753

H 2.98009619043362 -1.76610391184957 0.38653239894574

0 imaginary frequencies

SP = -1009.306036415135

U = -1009.09057380

H = -1009.08962959

G = -1009.14671959

**2 anti-adduct**

C 2.26147113409861 -1.07888232551280 -0.35362227565547

H 2.63995941010924 -0.07117342216569 -0.17308099057958

H 2.06901865445201 -1.22324617561721 -1.41877659281844

S 0.76177549645106 -1.38246765011824 0.60758402534217

C -2.28977925623604 -1.74916666064246 0.00532485082019

O -2.34879305754399 -2.10141442046925 -1.17280477874048

C -1.74762530438685 -0.35537705435304 0.37094963806499

H -1.74840805528309 -0.21115888692322 1.45511238467948

C -0.32503735469166 -0.15694971005165 -0.19921178191747

H -0.35760366628833 -0.39785133544219 -1.26417738499225

C 0.16722321482244 1.26246934712220 -0.02614679911158

C 0.55345227038880 1.99483138394680 -1.14755821939145

C 0.24146620147057 1.85424639630947 1.23781257464885

C 1.00724969971107 3.30706848152644 -1.01244547622493

H 0.49856444158486 1.53578020710175 -2.13094528399950

C 0.68910459537488 3.16411020828778 1.37344855815826

H -0.04620633102643 1.28835802773205 2.11963542087184

C 1.07425473776669 3.89419162893646 0.24768193109855

H 1.30753647900723 3.86737186261225 -1.89289981815666

H 0.74090652727106 3.61698461848885 2.35915084357612

H 1.42631978027967 4.91579794509169 0.35576059133321

C -2.64727793640183 0.64998369789179 -0.20090906043384

N -3.35084134443190 1.44167835672977 -0.65621133505689

N -2.67677702333292 -2.50437523784958 1.03577831433412

H -3.03148463994171 -3.43519714333248 0.86107190521384

H -2.61163286555767 -2.17059963258506 1.98638808890578

H 3.00616619233423 -1.80544450671445 -0.02274132996888

0 imaginary frequencies

SP = -1009.787755193776

U = -1009.55824709

H = -1009.55730288

G = -1009.61397432

**2 sync-adduct**

C -1.20414676034452 2.11220788877367 -0.10672251053712

H -2.07401492426607 1.48271260628928 0.09048593274192

H -1.08870290404711 2.26717239967080 -1.18166022819751

S 0.29150299296096 1.37084645543555 0.58467286754252

C 2.87346303755370 0.08565913161022 -0.76171572356830

O 2.79694848563635 0.55840710109450 -1.89639507092544

C 1.72413912161099 -0.80874082364630 -0.26729738380543

C 0.36018305370064 -0.10962216584740 -0.47173143340753

H 0.36298986369286 0.23222010372554 -1.50801745568741

C -0.79076257086831 -1.08042697615510 -0.29009580532590

C -1.30200925979802 -1.71735215888282 -1.42141762805678

C -1.32312913822358 -1.39171276400464 0.96261477289970

C -2.32199274654198 -2.65927658215043 -1.30565405664900

H -0.89504264725943 -1.47564287944374 -2.39989407583338

C -2.34435120568998 -2.33122879722770 1.08110819673144

H -0.94842090777155 -0.88704743149450 1.84754935587684

C -2.84504942357621 -2.97002989480697 -0.05188150591143

H -2.71001814016129 -3.14715746869846 -2.19478800890326

H -2.75107625415726 -2.56100637530702 2.06156929711699

H -3.64255336620004 -3.70121262053092 0.04180146379860

N 3.91286598711639 0.28816082891904 0.05284271786172

H 4.68638896758209 0.84781030355424 -0.28018021449435

H 3.96953151151931 -0.11511892301867 0.97636546087644

C 1.88771378164835 -1.28753630200944 1.10803271898231

N 2.02286638411484 -1.66848780373204 2.18772571201175

H 1.74097887045505 -1.69353249167341 -0.91333422962464

H -1.34356180868617 3.07834563955674 0.38179683448726

0 imaginary frequencies

SP = -1009.786597840873

U = -1009.55761419

H = -1009.55666998

G = -1009.61391006

**3**

C 2.29844522299987 -0.17675945637763 -0.00001948628463

C 0.98367695164404 -0.40719409330041 0.00001969817195

C 0.47201067430729 -1.75130716662293 0.00001187178260

N 0.07246257055844 -2.83420889293966 0.00000500109199

C 0.00350739771185 0.72274543713236 0.00007651143731

H 2.66782191940084 0.84344113551982 -0.00001343789465

H 3.01288203125427 -0.99269404791980 -0.00005529433380

O -1.25148496551748 0.28832263675794 0.00003395124032

O 0.32909720732469 1.89084623647912 0.00001327256776

C -2.28073895395940 1.30531503413325 -0.00001001615237

H -3.22218801372777 0.75986896558613 -0.00004108453722

H -2.19172518699901 1.92035851497958 0.89665908723047

H -2.19165985499761 1.92034769657221 -0.89668007431973

0 imaginary frequencies

SP = -398.951601568867

U = -398.84836953

H = -398.84742532

G = -398.88863552

**3 carbanion**

S -1.97735390351998 -0.66271227630333 -0.70689308397640

C -3.32681612448667 -1.46218373004919 0.19581389383342

H -4.03044033822966 -1.86595269848017 -0.53549948349243

H -2.95024828539833 -2.28217193388528 0.81235323753412

H -3.85039818473160 -0.73990106691031 0.82731658946671

C -0.97251672157735 -0.08192288080950 0.71409273535384

H -0.66493891306725 -0.95624355002747 1.28986319882501

H -1.62512960770828 0.52769684642175 1.34466915466417

C 0.21766806088192 0.71035445205584 0.26285936148972

C 0.06522015426859 2.08319920989294 0.02767640921576

N -0.08074216597020 3.22775792617866 -0.15825978251570

C 1.47615075962608 0.15395895550500 -0.03809711717401

O 2.48926277217617 0.76934054226540 -0.43256818739849

O 1.53481694242219 -1.20510159534495 0.15070684238364

C 2.79297256875711 -1.83079012052047 -0.13369279988514

H 2.64591436415832 -2.89060405258643 0.07555127299322

H 3.58274401615410 -1.43326175479814 0.50811071120427

H 3.06714660624485 -1.69583927260431 -1.18280895252170

0 imaginary frequencies

SP = -837.277652818271

U = -837.13061774

H = -837.12967353

G = -837.17856014

**3 TS**

O -0.97332523200921 0.89151403186225 -0.39449961659235

C -1.53206152627797 -0.27372862669349 -0.10777719000600

C -1.16089074619700 -0.76861372238431 1.24996400487744

C -0.10601001132695 -0.32010542567711 1.93591630394820

O -2.26585333296461 -0.89121623210126 -0.85617888263796

S 2.35324893210781 -1.05774350908829 -0.66378261756655

C 2.36580203438590 0.76041891227146 -0.89533757620696

C -1.95399813949615 -1.86015040820318 1.74566935165656

H 0.50423171121379 0.48336016815540 1.54309066369886

H 0.15945588061664 -0.75221139674755 2.89525762138249

H 1.84239439286533 1.05324692298371 -1.81169961055563

H 1.87989703680535 1.28016312311868 -0.06192718060684

H 3.38853102833576 1.14689496260245 -0.96576849167426

C -1.18030321630249 1.38786710683903 -1.73594610725558

N -2.59001554366460 -2.73467228614370 2.15043328333645

H -0.62944594842756 2.32483540936788 -1.78332457321633

H -2.24402359785032 1.55931069991028 -1.90845744343072

H -0.78653172181366 0.67208426992771 -2.45941193915077

1 imaginary frequency: -52.25cm\*\*-1

SP = -837.231470792289

U = -837.08662744

H = -837.08568323

G = -837.13796905

**3 adduct**

S -1.68211531261718 -0.36797199321755 -0.62031376620883

C -2.98793307826325 -1.47943404808678 -0.04708327535601

H -3.52559720463569 -1.83256547278928 -0.92922332026171

H -2.56043947346177 -2.33596395353418 0.47811824166750

H -3.68439223066210 -0.94963623692247 0.60594968262524

C -0.97549542739869 0.06333177080067 0.99540865240118

H -0.74778537694388 -0.85102987443496 1.54469417376762

H -1.68363655174411 0.65989869509700 1.57314658975382

C 0.32775803067444 0.85776840425105 0.81697619989112

H 0.75818690330711 1.03563886128968 1.80832477608455

C 0.08120033442918 2.16591316275745 0.20143788652515

N -0.13095734561941 3.19847315904030 -0.26390334401046

C 1.35972233080887 0.08855685178636 -0.00404106260628

O 1.83982280985171 0.47870487155572 -1.04554161377693

O 1.65824192758519 -1.05973531269931 0.58487540841684

C 2.60976084135715 -1.90474348275148 -0.10537059346071

H 2.71472260790330 -2.78790355918784 0.52126606940747

H 3.56368540722896 -1.38422319861899 -0.20080439227627

H 2.21786480820018 -2.17281064433537 -1.08762331258329

0 imaginary frequencies

SP = -837.753498403696

U = -837.59237248

H = -837.59142827

G = -837.64012960

**4**

C 2.76236424781593 -0.69817999541402 0.07741307023334

O 2.81690401943506 -1.93013207970382 0.08706822035216

C 1.42427699869907 -0.00246024170359 0.05548865312651

C 0.28901358427191 -0.70381233010389 0.03181635655821

H -0.67752829176285 -0.21225677910216 0.01593254137229

N 3.85030185881128 0.08373113947157 0.08474289912873

H 4.76082770336492 -0.35484086231262 0.09859430361921

H 3.79985471349675 1.09211660838540 0.07394219802034

H 0.32609680009199 -1.78803611985930 0.02807977427076

C 1.37702757799759 1.43487862112383 0.06063197116179

N 1.35526478777835 2.58951903921861 0.06260801215667

0 imaginary frequencies

SP = -339.761096928746

U = -339.67517184

H = -339.67422763

G = -339.71282125

**4 TS**

N -0.69696349073878 0.25305580822810 -1.29733586791469

C -1.64352944063925 -0.03944054675746 -0.38782935988982

C -1.10506644707314 -0.46117870640065 0.93093598172610

C 0.11638963506737 -0.06809937302539 1.37212650516956

O -2.86408786651442 0.01821978470013 -0.61774545503106

S 2.13032912943697 -1.12066534656086 -0.18645428379643

C 2.96314564524873 0.50190347184357 -0.06675608059012

C -1.87749536665115 -1.41292077628867 1.65892839848039

H 0.60964459284351 0.78066669114457 0.92104680118198

H 0.50642135672332 -0.42158368118569 2.31926086251568

H 2.34163330400156 1.30183004837889 -0.48706658784615

H 3.18289681723347 0.76105907963495 0.97433235311157

H 3.90912361050612 0.50180683510150 -0.61605249144961

H -0.99635716020891 0.47939379670051 -2.23599740282349

H 0.25402684087338 -0.10424725523940 -1.14285108709479

N -2.50846116010877 -2.18135983027411 2.25349771425087

1 imaginary frequency: -91.46 cm\*\*-1

SP = -778.045601455201

U = -777.91694027

H = -777.91599606

G = -777.96236877

**4 carbanion**

C 2.42797567931278 -0.65278108286795 -0.41723760094565

H 2.43165951924392 0.40402529101426 -0.69638517826427

H 2.45389239004577 -1.26934931157968 -1.31925321201466

S 0.97585933654031 -1.04294520887896 0.58969829816020

C -2.45369209357165 -1.92740061727133 -0.14368531698938

O -2.04578365680103 -2.92775095179069 -0.80609637744559

C -1.70589477878713 -0.73366583304863 0.00730867705380

C -0.34417606222586 -0.57819905882133 -0.59793442216981

H -0.24451780005914 -1.21526655732344 -1.47892639328397

H -0.15876733153674 0.45628207654845 -0.89986944506869

C -2.20702175217941 0.30940454068608 0.79166920812681

N -2.62266565916170 1.18804190555544 1.44357601332760

N -3.72684521685051 -1.99829213813162 0.41062511147532

H -4.05733645657026 -2.94349073092259 0.54851448186405

H -3.93755061029166 -1.37138955686079 1.17521636861434

H 3.31955949289228 -0.86216876630718 0.17794178755991

0 imaginary frequencies

SP = -778.082095720422

U = -777.95216660

H = -777.95122239

G = -777.99764602

**4 adduct**

C 2.16242257244988 -1.12416332165991 -0.43644941339173

H 2.50230190409032 -0.08767172473086 -0.38487372997272

H 1.93978434839392 -1.39379489905574 -1.47079493007907

S 0.71071957896273 -1.37074198456459 0.61340181797263

C -2.38784622567104 -1.69547951436230 -0.04413416087144

O -2.44315542650831 -2.01463936371709 -1.23218365436091

C -1.81441507603983 -0.32727151349074 0.36522177725316

H -1.83278472954114 -0.21097057675382 1.45290570932355

C -0.38450572400592 -0.15374169267035 -0.16965482960933

H -0.37982851149066 -0.30801927363474 -1.25075388905907

H -0.03623347824651 0.85738386289977 0.05051574427371

C -2.67376614222252 0.71829641910497 -0.19542087623559

N -3.34393326973951 1.54506739616092 -0.63913389604178

N -2.80089240324013 -2.47194192890604 0.96033053298038

H -3.16831107306798 -3.39169292699837 0.75582996843117

H -2.73007808651750 -2.17078907399343 1.92131806799661

H 2.95243074239420 -1.77574488362766 -0.05805723860957

0 imaginary frequencies

SP = -778.563079828020

U = -778.41876069

H = -778.41781648

G = -778.46385626

**5**

C 0.48881888787335 0.28032253683399 -0.05583600275588

C -0.47247050788650 -0.65663324248725 0.04494242226804

C -1.92926883053543 -0.45469022147840 0.03428629705549

C -2.72565149861134 -1.42269969222403 -0.59362651432666

C -2.54427562903009 0.64024788074366 0.65345792197643

C -4.10726926457284 -1.27579700573743 -0.63930912827704

H -2.25231054825629 -2.28499706830620 -1.05466414315809

C -3.92913386187923 0.77294383801752 0.62377184233904

H -1.94753207529848 1.37071185337052 1.18883230789764

C -4.71181009961204 -0.17649922535400 -0.03052014135673

H -4.71353018305615 -2.02289507103076 -1.14231735300128

H -4.39817552865324 1.61766569065168 1.11880298535965

H -5.79184248809833 -0.06711122527254 -0.05508413546563

C 1.94302335940652 -0.02590372609722 0.00593278709059

C 2.42064002103516 -1.17715037892449 0.63753594769118

C 2.88413428777895 0.82849728766715 -0.57182878812838

C 3.78632304560402 -1.42169437283575 0.64273902628039

H 1.75346021373882 -1.87193089252366 1.13467406501785

C 4.23025878042566 0.49373126806527 -0.50582609871140

H 2.58440229647362 1.74240679335501 -1.07368018053982

N 4.69703732867247 -0.61196955777952 0.08586129437588

H 4.16980622726216 -2.31439012391014 1.12920192292979

H 4.97066576021682 1.15094207185406 -0.95358593777392

H -0.14906098359033 -1.69237340688855 0.10696747376321

C 0.14521436653599 1.65698479372252 -0.30046332334881

N -0.08659307594320 2.76758119656860 -0.51877454720155

0 imaginary frequencies

SP = -649.439246115871

U = -649.22247365

H = -649.22152944

G = -649.27401524

**5 TS**

C -0.35008357812512 1.70550151658841 -1.72375321280427

H -1.08234898168992 2.51373546150681 -1.82386093016751

H -0.90954156589387 0.75888014021209 -1.72279701360206

S 0.62702706850471 1.85881142092694 -0.20319338268867

C -1.33348837130801 -0.85018246939788 -0.04426784998016

C -0.21270422342509 -0.56011724134578 0.69183409157850

H -0.35278769514270 -0.00110234751201 1.60650434633318

C 1.07352650520252 -1.27857719314438 0.58940061704285

C 1.70961940335712 -1.63719070127585 1.78446422880572

C 1.67459558121489 -1.61496870852258 -0.62855785668400

C 2.90798707386017 -2.34698098992511 1.76564613815386

H 1.25614311937696 -1.35946398313398 2.73219465432684

C 2.87602042779286 -2.31538434331885 -0.64528912076933

H 1.22253577781917 -1.29546057870969 -1.56117203563579

C 3.49321134403280 -2.69026486040519 0.54938332978579

H 3.38630266594832 -2.62393900568690 2.70052986339559

H 3.34085115636560 -2.56112496165930 -1.59561525611152

H 4.43185179836475 -3.23608030961472 0.52975414313421

C -1.29931575010826 -1.83252282795788 -1.07651040514988

N -1.32332738726076 -2.64409244547672 -1.90466400709166

C -2.62762806411605 -0.18557191778983 0.19570046218352

C -3.81727769478597 -0.66923640010835 -0.36697127302493

C -2.72452184158409 0.97818157898469 0.97044029106406

C -5.00671576296341 0.00068436885306 -0.12851875471440

H -3.82349254586528 -1.55975467550668 -0.98710200068117

C -3.96610066079478 1.57208893732657 1.14505413528536

H -1.84388443670303 1.44099453629125 1.39849983418746

N -5.10887067849877 1.11075741194110 0.61716311025631

H -5.93057874697366 -0.37533193647505 -0.56080651969130

H -4.04627236095899 2.47873169813577 1.73955872009257

H 0.28430842435808 1.70879082620014 -2.61602834682921

1 imaginary frequency: -172.47 cm\*\*-1

SP = -1087.720804629751

U = -1087.46277782

H = -1087.46183361

G = -1087.52221219

**5 carbanion**

C 1.99191210070029 2.00019612812891 -0.04410306554214

H 2.84175135521873 1.31375914019747 -0.04600435031988

H 1.71914351848405 2.24421417020248 0.98610832006394

S 0.57604524724642 1.28777353734087 -0.91672553139242

C -1.13841221092616 -0.72964843415277 -0.18683526497194

C 0.15781087485551 -0.08450933369883 0.23877829829399

H 0.01167769166708 0.39127269325418 1.21332635931839

C 1.29504852843663 -1.07930947322886 0.39222613980715

C 1.54290451209013 -1.63695388779896 1.64880024616793

C 2.07834791898647 -1.48606600675833 -0.68947002482194

C 2.55091973527217 -2.58394200672351 1.82344183251110

H 0.93910573131176 -1.32531906590065 2.49761810567148

C 3.08949088586478 -2.42891246633334 -0.51859809006392

H 1.90216932268684 -1.05001718840061 -1.66775739296893

C 3.33000043934476 -2.98200178591048 0.73827334800158

H 2.73104683316867 -3.00557635912647 2.80817179102756

H 3.69245765155633 -2.73100866771948 -1.37033472250645

H 4.12036408734091 -3.71507465367946 0.87075281800116

C -1.09993877173075 -1.91248877366730 -0.92503287447933

N -1.08746765122462 -2.90881693863065 -1.54277025154079

C -2.40077222663337 -0.12444219874845 0.07848376272388

C -3.63889733870295 -0.71605310063627 -0.30055991174814

C -2.53469254178154 1.12550581311567 0.74118731360109

C -4.83260089006860 -0.08766892697425 -0.01612209307601

H -3.65583177958484 -1.67068976981074 -0.81783270779699

C -3.78672963211276 1.66124052503080 0.97575159758725

H -1.66313345323850 1.68454323543830 1.06125926414164

N -4.95475147531510 1.09610744528800 0.61857982517148

H -5.76476226551472 -0.56286011515059 -0.31599138544576

H -3.86138094634391 2.61966467581671 1.48659218587250

H 2.27719474894633 2.92014178923666 -0.55941354128750

0 imaginary frequencies

SP = -1087.745626796115

U = -1087.48633884

H = -1087.48539463

G = -1087.54576856

**5 anti-adduct**

C -1.40605095487375 2.22332864368384 -0.39358413016733

H -2.37975318749163 1.79427082898608 -0.15068532381563

H -1.20609322718317 2.11770814837797 -1.46229193086818

S -0.09267856411898 1.44352998214682 0.57298095018138

C 0.90997917345428 -1.10186898093561 0.49317323664479

H 0.73497844822796 -1.16847790389050 1.57119475542535

C -0.19526576972376 -0.22724564202543 -0.15341853041168

H 0.02891371255231 -0.13378613834078 -1.21944297328882

C -1.56389476711117 -0.85317874034660 0.00659949004283

C -2.28335707405437 -1.23300744784269 -1.12564736355334

C -2.11034918696768 -1.07875599253484 1.27279975470980

C -3.53024863830351 -1.84569082940606 -0.99760004938974

H -1.86232777305964 -1.05441293468143 -2.11146354469270

C -3.35190309883789 -1.69253654715525 1.40212606342540

H -1.56190070387746 -0.77394399835940 2.15982068121471

C -4.06545753148165 -2.07812902644887 0.26611298478061

H -4.08088605786876 -2.13958433870547 -1.88630328799143

H -3.76647308641073 -1.86831927694498 2.39044331651752

H -5.03538942154192 -2.55567993702349 0.36880464253002

C 0.79788038952425 -2.46693245534765 -0.03845623720047

N 0.71897472020580 -3.53392366866425 -0.46895664252392

C 2.30608917468670 -0.55549389768946 0.24461525346769

C 2.86177048641235 -0.54912224214181 -1.03231051186391

C 3.04918163916855 -0.01785888094850 1.28855160043205

C 4.12396616265732 0.00150861106058 -1.20611872279754

H 2.32661035637129 -0.96183659182211 -1.88220152035878

C 4.30638397640325 0.50787007663392 1.01132859113269

H 2.66053828662231 -0.00294440933210 2.30160868133147

N 4.85065960579294 0.52833357606483 -0.21066673847726

H 4.57591523621010 0.01986137528302 -2.19404405867827

H 4.90394403234395 0.93320001126840 1.81303420455705

H -1.40733635772731 3.28427862708188 -0.13564264031432

0 imaginary frequencies

SP = -1088.236869811167

U = -1087.96372180

H = -1087.96277759

G = -1088.02333023

**5 sync-adduct**

C -1.35977061291379 2.24468292957729 -0.12188721190328

H -2.35483107785662 1.82604497492042 0.03830319127496

H -1.15870301997281 2.33491208720275 -1.19160068516872

S -0.09082966475499 1.23319122467225 0.67339158198676

C 0.88766611906377 -1.26098219525118 0.04115229245175

C -0.21885872281789 -0.25203535875091 -0.37141070473210

H 0.01734297774656 0.04653312050560 -1.39540327977226

C -1.58243334615534 -0.92024585040722 -0.37194894533688

C -1.97742912682213 -1.61176058608216 -1.52062864677558

C -2.42430001668711 -0.91109774385192 0.74016948325337

C -3.19454806139574 -2.28779186081232 -1.55643950769774

H -1.32452005677347 -1.62010257444923 -2.38996378914123

C -3.64426497131957 -1.58376627303647 0.70414773979108

H -2.12993391730806 -0.36857417506029 1.63300902537287

C -4.03269303826442 -2.27396058087887 -0.44227184123797

H -3.49045605102105 -2.82005840220901 -2.45563770081225

H -4.29396004560873 -1.56450905060309 1.57423579330049

H -4.98527107811302 -2.79471109284590 -0.46950038401129

C 2.28491965919609 -0.70091991230983 -0.16704293593879

C 2.74829427106692 -0.54065378941997 -1.47183284497930

C 3.12030618975208 -0.31550287569249 0.87454151279714

C 4.00947634368972 0.00038800392326 -1.67344468284072

H 2.13884405104575 -0.83340113353484 -2.32113126498288

C 4.36908269041289 0.21546820958556 0.56736353972012

H 2.82056036309934 -0.41761635032866 1.91230166350517

N 4.82431228957492 0.38104179894453 -0.67926492911498

H 4.38694300545933 0.13300995674758 -2.68362453161820

H 5.03457665248281 0.52383659729688 1.36901524047996

C 0.67602777706640 -1.73975205084250 1.41273001089020

N 0.50692607467576 -2.12524679250256 2.48617882726548

H 0.76931802027059 -2.13474525169308 -0.60766688551011

H -1.31067367681813 3.23563499718637 0.33385086948490

0 imaginary frequencies

SP = -1088.235892384227

U = -1087.96275984

H = -1087.96181563

G = -1088.02217515

**6**

C 0.80375424223845 0.23134927606515 -0.10165954081093

C -0.16506503259187 -0.68354898246790 0.03550604202061

C -1.61473500715398 -0.44615400676817 0.03539084243573

C -2.44200134406331 -1.45494820412853 -0.47825782975581

C -2.19341786285018 0.71846646235706 0.55483457435386

C -3.82069302028432 -1.28220489683213 -0.51357372220009

H -1.99507295418278 -2.36971790174103 -0.85672226352840

C -3.57482816190775 0.88142740818983 0.52848688307941

H -1.57363241241577 1.48407197593147 1.00851753568009

C -4.38919539541933 -0.11180519152552 -0.01246796267684

H -4.45253604002768 -2.06368557832385 -0.92409154300535

H -4.01657138198043 1.78306400075183 0.94118894907674

H -5.46683580098732 0.01982449810717 -0.03029228111812

N 2.17632790620625 -0.12553718037205 0.01582189789971

C 2.75459245912347 -0.91665848409058 0.93878701907147

C 4.20873775726860 -0.24798046184153 -0.42101560594483

H 2.20416743184869 -1.36629597585526 1.75254636307711

H 5.16211148895784 -0.09933514427556 -0.90751147862873

N 3.10886584756897 0.31763080674165 -0.86751558571094

N 4.04707575921852 -1.02394501459487 0.69065679593099

H 0.15497546730322 -1.71786967472524 0.13705452308367

C 0.58009393110944 1.61893005829903 -0.39163544985626

N 0.42721212302127 2.73470221109905 -0.64484816247315

0 imaginary frequencies

SP = -643.374132673238

U = -643.18768179

H = -643.18673758

G = -643.23773346

**6 TS**

C 0.08668708481131 1.86171650865738 1.55339228855486

H 0.48750437950732 2.81999095400607 1.89794690353523

H 0.86549221281165 1.10571117111897 1.72298110751355

S -0.34651635299832 1.92286739255024 -0.20587617265500

C 1.65398627625240 -0.62465665385906 0.15012053086204

C 0.53676777547725 -0.44611761989565 -0.62998412024735

H 0.71047200677310 -0.08011123415457 -1.63276982740409

C -0.72271954405490 -1.19969069923137 -0.43759125719973

C -1.36720321208806 -1.70828041758680 -1.56976841839408

C -1.28784016097396 -1.42349096732938 0.82364359631258

C -2.54277198649804 -2.44490838228301 -1.44684602106106

H -0.94141134696768 -1.52388259601547 -2.55235308399914

C -2.46439432060179 -2.15504215813643 0.94436027760667

H -0.82978871039683 -0.99891838119709 1.70969445559185

C -3.09385098881668 -2.67299609453898 -0.18810406474986

H -3.02916569994374 -2.83638753611563 -2.33538836724950

H -2.89792929648676 -2.31450022208288 1.92736944816179

H -4.01275166474050 -3.24303920864581 -0.08846464115776

C 1.71004728972769 -1.34510744650038 1.36572016512025

N 1.79319666334585 -1.94817162329071 2.35517728068220

N 2.89670305440373 -0.04710828310627 -0.26078814358526

C 3.53398266002360 -0.21257409118417 -1.43002142971505

C 4.61841600493245 1.13644002071647 -0.24563855940242

H 3.17039699098930 -0.87187574679391 -2.20503890107520

H 5.38653533310305 1.82174551559148 0.08417029858050

N 3.58952137989678 0.82748766744408 0.51642951193036

N 4.63151639582737 0.52843052022314 -1.46554177972520

H -0.77456222331561 1.60706961163978 2.17902892316884

1 imaginary frequency: -192.74 cm\*\*-1

SP = -1081.653851811863

U = -1081.42739889

H = -1081.42645468

G = -1081.48411877

**6 carbanion**

C 0.36535204761587 1.71450462805995 1.78604977969389

H 0.41354106367200 2.76045608573812 2.09845518844620

H 1.34851203726589 1.26365085258161 1.92501021157180

S -0.07142014286023 1.71787871449043 0.03289056301952

C 1.56133877721978 -0.62995952704960 0.07574480232162

C 0.32955254366584 -0.02830315139019 -0.52023521410697

H 0.51449376926157 0.13601007253844 -1.58525434613675

C -0.86270068794158 -0.96049969621196 -0.40917988858170

C -1.20776545692862 -1.75212840538115 -1.50735585705221

C -1.60122087165007 -1.09302667277683 0.76885236860898

C -2.26559308418061 -2.65703374187456 -1.43275797537605

H -0.64034037676438 -1.65733221295812 -2.42998367215518

C -2.65887298056893 -1.99608327226756 0.84821226450106

H -1.35601160998531 -0.48876244286684 1.63472147845171

C -2.99552211301702 -2.78275236637110 -0.25248495529292

H -2.52109980836803 -3.26026443316256 -2.29931952417878

H -3.22093548755017 -2.08549606623540 1.77345339569255

H -3.82116692853256 -3.48574176456720 -0.19176127795361

C 1.55682495531461 -1.31043992778405 1.27857717881521

N 1.55122675659421 -1.92849240979707 2.28104741692211

N 2.81946624184982 -0.07477563031715 -0.33204026852758

C 3.44522930305297 -0.27912324117356 -1.49906628671801

C 4.55832663119227 1.10253086632858 -0.38702173431382

H 3.06619941904808 -0.96136837036852 -2.24650178347362

H 5.34026112149768 1.78842794993071 -0.09060080912395

N 3.53539236500281 0.83087394590150 0.39759569754152

N 4.54941610879308 0.45239770001011 -1.58486885337443

H -0.37216359269899 1.19945251697402 2.40368210077943

0 imaginary frequencies

SP = -1081.670905679180

U = -1081.44178501

H = -1081.44084080

G = -1081.49895071

**6 anti-adduct**

C -1.22517266309632 2.22445374179382 -0.36351717400846

H -2.18557357547733 1.76255536208403 -0.12830869811823

H -1.02603726099037 2.15453605240242 -1.43510441422660

S 0.11086347441527 1.45147426783080 0.57747649376093

C 1.17365773311579 -1.05758749216451 0.39094749447155

H 1.06270958736345 -1.15647414237006 1.47340936477155

C 0.03268266558502 -0.19943403414086 -0.19444207332339

H 0.21828121332878 -0.07293710936417 -1.26470607687757

C -1.30168247240318 -0.88856331057174 -0.00756653677767

C -2.04079670348137 -1.26832586823495 -1.12723545669131

C -1.79455134895990 -1.16912456362599 1.26892003485004

C -3.25652058525527 -1.93468123716531 -0.97532514251732

H -1.66026262691642 -1.04651123713365 -2.12050700679066

C -3.00519773112931 -1.83689537743921 1.42121507944590

H -1.23053151487950 -0.86467136651885 2.14622524796619

C -3.73893580991529 -2.22220638071105 0.29853922869656

H -3.82461032459140 -2.22750490173425 -1.85317157969718

H -3.37872827213781 -2.05533195669419 2.41720503083452

H -4.68455893517834 -2.74227471999856 0.41934928345841

C 1.11999322743512 -2.41508412585174 -0.18293651292334

N 1.07488706162071 -3.47255486186085 -0.63719926026970

N 2.48644146788019 -0.47194110892434 0.16070554883090

C 3.05625094973821 -0.12674806548956 -1.00559891935697

C 4.30702134952146 0.44619474582205 0.58032790919619

H 2.60031011353337 -0.32134000552278 -1.96658935263036

H 5.14697711768041 0.85289766160721 1.12486439631530

N 3.28176752796660 -0.10248074701942 1.19546164135606

N 4.22101417048405 0.45606961955998 -0.78188649247893

H -1.25213083525663 3.27668816143574 -0.07369305726640

0 imaginary frequencies

SP = -1082.174236284816

U = -1081.93136152

H = -1081.93041731

G = -1081.98923714

**6 sync-adduct**

C -1.30564005593802 2.15898155224828 -0.19219411455512

H -2.24848564079426 1.65558267129288 0.02797978721590

H -1.16288248012543 2.23421408425834 -1.27230245223797

S 0.08803074577009 1.29576142715471 0.56872655809531

C 1.21239253718689 -1.15258130818117 -0.04916373811903

C 0.03347580338832 -0.22623637864773 -0.42761230137178

H 0.20915315322154 0.05249312063672 -1.46991015735780

C -1.26905292219643 -1.00270967374773 -0.34570431845090

C -1.68971617248870 -1.71655315980534 -1.47003103305951

C -2.02763900065206 -1.06378543226167 0.82387714548480

C -2.85053069431660 -2.48508993371843 -1.42659430412793

H -1.10275107349866 -1.66826275202475 -2.38376644448164

C -3.19039832437719 -1.82949200146038 0.86768312874379

H -1.71482929185977 -0.50283877839096 1.69885017280396

C -3.60449570210297 -2.54251839106943 -0.25587849476451

H -3.16787266275003 -3.03358021727449 -2.30841971398205

H -3.77518016808765 -1.86585786241865 1.78198003918048

H -4.51271633129734 -3.13676476807195 -0.22044552112636

N 2.51651985440121 -0.53979823473425 -0.26895052313724

C 3.14501577144423 -0.39516604387335 -1.44640988066002

C 4.25208868614505 0.55993714735817 0.06055795019571

H 2.76562546587431 -0.80668018740604 -2.37093945159989

H 5.03332689461230 1.11316856505149 0.56193625180143

N 3.21532478609722 0.07907959233110 0.71302364481319

N 4.25886011522741 0.29787545191173 -1.27829950475952

C 1.12025453370685 -1.63386686524668 1.33753926220212

N 1.01082674795010 -2.03948951528137 2.40946375164946

H 1.15693011880346 -2.03313769308575 -0.69492679284588

H -1.32783469334384 3.16364558445672 0.23466105445101

0 imaginary frequencies

SP = -1082.172688433853

U = -1081.92960490

H = -1081.92866069

G = -1081.98748220

**7**

C 0.80084650603370 0.21760957507920 -0.07032708863923

C -0.17024809387027 -0.69913562353663 0.03543288244362

C -1.61981262340259 -0.45366539868638 0.04474031667206

C -2.45138810653631 -1.41877298164684 -0.54110382348772

C -2.19461560059481 0.67989395884877 0.63129482096556

C -3.82853238942405 -1.23360842833716 -0.57464716041377

H -2.00890253931920 -2.30984963364306 -0.97709719753887

C -3.57497984349775 0.85546171205627 0.60567911219850

H -1.57153594540901 1.41038357315200 1.13596332534307

C -4.39326501695031 -0.09414351629401 -0.00278745931086

H -4.46224409094782 -1.98149627180576 -1.04131961993504

H -4.01255837243734 1.73292347280305 1.07170694016827

H -5.46976191077186 0.04654300029203 -0.01996618250365

N 2.17359141570233 -0.12663480508746 0.03285292414309

C 2.72574671648918 -1.07874311786794 0.83380739362555

C 4.24157189930715 -0.10363524521049 -0.44342743212284

C 4.07127711494186 -1.09617000984345 0.54934416481769

H 2.12614468746750 -1.63925255539829 1.53598194571078

H 5.15282355413058 0.20861122286315 -0.93590250906567

H 4.82701765614880 -1.72065533410148 1.00211016045848

N 3.09218046615774 0.48042571160946 -0.75515339057773

H 0.14446818527444 -1.73735217316567 0.10341791841367

C 0.55941641526279 1.61163283873022 -0.32192720941709

N 0.38048991624524 2.72889002919044 -0.55019283194786

0 imaginary frequencies

SP = -627.318894661869

U = -627.12108347

H = -627.12013927

G = -627.17125519

**7 TS**

C 0.10664900962977 1.85433190032469 1.56558585029400

H 0.54642253826272 2.80346851291013 1.88642892926584

H 0.85972474982818 1.07267041972878 1.73574174525199

S -0.33932701076019 1.89800017431265 -0.18890319120309

C 1.64477739800861 -0.60526648723568 0.12075617306074

C 0.51114528152971 -0.39179362625396 -0.64063890252609

H 0.68144389298123 -0.04861774135853 -1.65266168820854

C -0.73519182795953 -1.17360063010994 -0.44492111672320

C -1.35527849959731 -1.73312079703261 -1.56568700017820

C -1.30665201787255 -1.37623594265846 0.81713424260897

C -2.51342220340813 -2.49643667230879 -1.43092617037627

H -0.92529382734718 -1.56833745192150 -2.55003735229849

C -2.46416784477022 -2.13502803939138 0.95053237986773

H -0.86508897926086 -0.91412094729328 1.69294594297446

C -3.07019736411065 -2.70253924193138 -0.17133104716710

H -2.98077555662802 -2.92651021905470 -2.31191900064352

H -2.90148995341697 -2.27788006121843 1.93451029612176

H -3.97465237478910 -3.29370172557595 -0.06270775039543

C 1.69543133630151 -1.35465166832877 1.31523740598497

N 1.77385750938753 -1.98599094626153 2.28972501405188

N 2.89174942061422 -0.03678107982598 -0.29110947408548

C 3.49315287654825 -0.19814582406682 -1.49588062397412

C 4.65584432732586 1.15046731377544 -0.19494936090172

H 3.06196952553589 -0.83980341397840 -2.25082943129568

H 5.39191754140900 1.81628449432681 0.23651791387125

N 3.59120982570427 0.79100993269395 0.51793179860235

C 4.64303495335035 0.56495573168787 -1.47859359055163

H -0.75645696518853 1.64198094116771 2.20391051647958

H 5.37127423869211 0.67321309487810 -2.26909250790697

1 imaginary frequency: -264.46 cm\*\*-1

SP = -1065.596148789852

U = -1065.35698708

H = -1065.35604288

G = -1065.41493649

**7 carbanion**

C -1.80929154975447 1.89551371976723 -0.00996895121483

H -2.62431119475881 1.18157321967629 0.12904390963634

H -1.62898952430033 2.04175114995229 -1.07836243207331

S -0.29936136765048 1.33446428824340 0.81626125533445

C 1.41876402792455 -0.76239018310161 0.18782272752185

C 0.12784369053387 -0.12865077058117 -0.23965938614686

H 0.26978366572281 0.27645549684818 -1.24556472508529

C -1.01348320798005 -1.12710409159822 -0.30293089930875

C -1.35331680002413 -1.69344353399907 -1.53353844778884

C -1.72192770201798 -1.51977663301066 0.83460481278078

C -2.37790523296350 -2.63328423199959 -1.63039076979432

H -0.81086079950330 -1.39051597816525 -2.42588741235458

C -2.74687409605991 -2.45937916823151 0.74297963234664

H -1.48026257488629 -1.07183525650033 1.79350517573173

C -3.07988744068218 -3.01947149617801 -0.48960998021428

H -2.63121003605866 -3.05821579705512 -2.59749580845071

H -3.28998137434796 -2.75164783962001 1.63732301616401

H -3.88259775264437 -3.74767936850524 -0.56061051208850

C 1.49218931259821 -1.58485055912339 1.29487213662049

N 1.55043665900008 -2.31552238222643 2.21826389060620

N 2.63211031034062 -0.09979907896335 -0.19873141074519

C 3.21742516781354 -0.17794314734859 -1.41874823612106

C 4.31213659521315 1.22023823388990 -0.11673911069825

C 4.30892718682273 0.66845937200568 -1.41538412728958

H 2.81263140714250 -0.82823101465285 -2.18103591964746

H 5.01175105263616 1.92491256212944 0.31502764246971

H 5.00519979360357 0.85179645942963 -2.22108143951016

N 3.29402028468549 0.76570321824321 0.60999766952792

H -2.09741850040486 2.85293281067515 0.43047769979185

0 imaginary frequencies

SP = -1065.612338326724

U = -1065.37194084

H = -1065.37099663

G = -1065.43039421

**7 anti-adduct**

C -1.26303546071385 2.21152706539160 -0.39021303425007

H -2.22030966195149 1.74481929614465 -0.15147076247127

H -1.06172666259370 2.12930223941563 -1.46063528611495

S 0.07853493258791 1.46310718931249 0.56281862125611

C 1.16209160218998 -1.03917465032911 0.41829170916348

H 1.04078094579650 -1.12009156145596 1.50107951811168

C 0.01991843570153 -0.19760483733244 -0.18910998266143

H 0.21571794811574 -0.08284053477324 -1.25870162985762

C -1.31321591157784 -0.89076006457366 -0.00763250291937

C -2.03849098525187 -1.28932302558265 -1.12991954179355

C -1.81878122890172 -1.15810229077625 1.26677993104237

C -3.25263090394063 -1.95980707198903 -0.98289620964556

H -1.64812858648278 -1.07851990940948 -2.12182647147534

C -3.02775897578046 -1.83005185413594 1.41463767348309

H -1.26552417841959 -0.83969561945150 2.14597111305026

C -3.74761434534825 -2.23338041540059 0.28924155716710

H -3.80953959954025 -2.26686437431982 -1.86308942090202

H -3.41106579507153 -2.03785363016877 2.40922387843123

H -4.69195311568462 -2.75662913400340 0.40645740744691

C 1.10947837902775 -2.40749937580932 -0.13309526290928

N 1.07603949237339 -3.47000505635929 -0.57733357261598

N 2.47380711085476 -0.46181668272255 0.18693408926435

C 3.03943689415091 -0.16596671508740 -1.01054347071098

C 4.31291154209044 0.47327904928997 0.67583302904791

C 4.24405000686382 0.44182893013178 -0.73547001634459

H 2.54770372126069 -0.41372939362214 -1.94124418212906

H 5.09902149414674 0.86933803650476 1.30473142492749

H 4.97013159398834 0.80727893314461 -1.44658477855898

N 3.23727085349023 -0.07364623423768 1.23092872658062

H -1.30060954138013 3.26751169220476 -0.11536255361254

0 imaginary frequencies

SP = -1066.119220897813

U = -1065.86473789

H = -1065.86379368

G = -1065.92288341

**7 syn-adduct**

C -1.22008467960809 2.19294693482494 -0.14209362331203

H -2.18298255511305 1.73256674772368 0.08543792080794

H -1.09307734064561 2.28166912354084 -1.22323548626252

S 0.14396347903337 1.25055685881458 0.57694068351610

C 1.15896590424084 -1.22170028363077 -0.10175460433713

C 0.00836417311220 -0.24602640906654 -0.44774500672874

H 0.17780177438257 0.04826215454021 -1.48659853796028

C -1.32202087091449 -0.97341990155616 -0.36403437432016

C -1.75705694772454 -1.68769010670237 -1.48296897171477

C -2.09299088708857 -0.99332670269067 0.79843363030400

C -2.94337282725412 -2.41604958165074 -1.44093614261591

H -1.16032748995205 -1.67162884699615 -2.39163819230136

C -3.28239470622224 -1.71760754413663 0.84047863709973

H -1.76804620738036 -0.43387874517106 1.66990914731460

C -3.71027993198034 -2.43154234690418 -0.27714222973586

H -3.27097250824539 -2.96544345407077 -2.31849349836255

H -3.87688098966921 -1.72085562439402 1.74926645100110

H -4.63898525032618 -2.99333028426908 -0.24293735138842

N 2.47924771283924 -0.64062740958804 -0.29530358392789

C 3.03899073430088 -0.35890992395989 -1.49829302261667

C 4.26749547256583 0.39772040043352 0.17286005920949

C 4.21206497431117 0.31528827142605 -1.23606771638827

H 2.56578663761181 -0.66197620896793 -2.42173827530584

H 5.03312995497157 0.84267499358439 0.79451684888177

H 4.92983634249458 0.68396600571846 -1.95396822325139

N 3.20938947267915 -0.17391057595955 0.73823658200846

C 1.03921637999134 -1.74196826023119 1.26890568658175

N 0.89642131335635 -2.18193791028426 2.32343684054965

H 1.06911709528470 -2.08073770829353 -0.77264913744570

H -1.18708822905139 3.18994633791688 0.30182549070089

0 imaginary frequencies

SP = -1066.117146475762

U = -1065.86263549

H = -1065.86169128

G = -1065.92043754

**8**

C -0.60783845919810 -1.91220865428826 -0.00000507936244

C 0.33770449249400 -0.97378458332132 0.00000853378040

C 0.00462055639346 0.47971713173005 0.00001622286658

O -1.15619250744539 0.87649812460576 0.00000805856660

C 1.16750010501980 1.42753379466472 -0.00000159248825

H 1.39288471387450 -1.23351875754451 0.00001316669428

H -0.35378111871453 -2.96799319718185 -0.00001044518182

H -1.66201873074968 -1.64724191409642 -0.00001109104855

H 0.82685244018112 2.46336370543119 -0.00000854582432

H 1.78928496144134 1.23337357121144 0.88058893892876

H 1.78927154670347 1.23335777878921 -0.88059816693125

0 imaginary frequencies

SP = -231.397677515062

U = -231.30123360

H = -231.30028939

G = -231.33438998

**8 TS**

C -3.29172916130897 -0.46692725112944 -0.23215822098356

C -1.93603361432066 0.15316780134815 0.01990396373782

C -1.00415212277090 -0.58894091446032 0.82553124022749

C 0.25889486967077 -0.12144765472035 1.07625315655940

O -1.66613472809607 1.25724849966592 -0.50467027261604

S 2.08604085425214 -0.64542230508170 -0.66021144450594

C 3.20051161355799 0.52305105581523 0.18757521974493

H -1.30758054470074 -1.57402827727037 1.16827204267875

H -4.03596879820855 0.30921729789706 -0.42362184700925

H -3.21931157755511 -1.10062371708560 -1.12425923532895

H -3.61103757036177 -1.09755932286429 0.60083902931339

H 0.50611481695180 0.91138925170494 0.86243586692626

H 0.90618759064259 -0.63564576931083 1.77573007101926

H 3.06572929758661 1.54722583471211 -0.17523121902054

H 3.01076947633762 0.52440986035101 1.26829252859927

H 4.25016859832327 0.25118261042847 0.04033512065769

1 imaginary frequency: -220.85 cm\*\*-1

SP = -669.669397808018

U = -669.53213614

H = -669.53119193

G = -669.57607917

**8 carbanion**

C -3.18115641685496 -0.57774424261015 -0.24085639094345

C -1.84053621960769 0.11522412817585 -0.06458676822009

C -0.86525543300860 -0.49329137223215 0.67700674880602

C 0.48929286964529 0.10445051412978 0.88917147644295

O -1.72597112685798 1.28209461057046 -0.65364780512678

S 1.69227517664345 -0.52054041569933 -0.35221621176607

C 3.18929941238091 0.32897647133227 0.20724293539276

H -1.06078246226121 -1.47459537006609 1.10163547320916

H -3.98352778134913 0.06117207764978 0.14619527308822

H -3.37766660483451 -0.73449658039547 -1.30779183661690

H -3.22460078090591 -1.54377498159238 0.26974366502246

H 0.46242461161545 1.19371494390029 0.79576056936395

H 0.89414553092998 -0.14644833883672 1.87455454191128

H 3.06801600811908 1.41364395243945 0.14800855971128

H 3.43589165939929 0.04568677240974 1.23398099662975

H 4.01291555694653 0.03123083082469 -0.44576522690454

0 imaginary frequencies

SP = -669.700847520365

U = -669.56039951

H = -669.55945530

G = -669.60135735

**8 adduct**

H -2.28458472139823 3.53395325734485 0.03259900231455

C -1.33368168640936 2.99703230831147 0.03426138254223

S -1.70241678138700 1.22757431645415 -0.00059964476133

C -0.00431694359485 0.58653202989683 0.01329497502752

C -0.03127697616476 -0.93330537171115 -0.00904500431934

C 1.34400479924480 -1.55899211608493 0.01603729232973

O 2.36225623755276 -0.88043695438889 0.02165644686278

C 1.39078872600293 -3.06081899756203 0.03319581795747

H 2.42191211388108 -3.41510680547920 0.00490973923791

H -0.78117762133684 3.25901795991109 0.93966284748395

H -0.75926381019848 3.29070284554186 -0.84743805545281

H 0.50132772008190 0.94821749846149 0.91201172752538

H 0.52457138504775 0.97371154585504 -0.86100363278018

H -0.58715685942911 -1.33597057373036 0.84601065217431

H -0.54034373544084 -1.30955552985087 -0.90449623954397

H 0.89547150523523 -3.42509540159356 0.93919963232128

H 0.83262364831301 -3.45485701137579 -0.82187493891948

0 imaginary frequencies

SP = -670.202431432085

U = -670.04908987

H = -670.04814566

G = -670.09258187

**9**

C 0.00530569983665 0.11367825472020 0.09572884347351

C 1.46116997306816 -0.14298625974711 -0.02320428224180

C 2.34031684869340 0.84887051313863 0.09313896141801

H 1.76277036551378 -1.16896021349739 -0.20720667147309

H 3.40639070319011 0.66268532553284 0.00647892233947

H 2.01756717123345 1.86999875513381 0.27699187919701

O -0.70490785241513 -1.01152764980264 -0.05519362955452

O -0.50748438637052 1.19920683317943 0.30404046515939

C -2.13895808021017 -0.88061962232147 0.03947237561821

H -2.53155074205234 -1.88511090174318 -0.10848901638483

H -2.41613440734447 -0.50393371270888 1.02561975587319

H -2.50568829314291 -0.20940832188426 -0.73915860342454

0 imaginary frequencies

SP = -306.661485261095

U = -306.55917939

H = -306.55823518

G = -306.59587082

9 TS

C 3.18847078209398 -1.89265511680161 0.37237209381313

S 2.32298791596492 -0.39740308076120 0.95137923612158

C 0.55406446184655 -0.78129217192964 -0.73839058744448

C -0.35423831820939 0.22785207119183 -0.96387769579451

C -1.52147173526645 0.35283454083122 -0.14514443804650

H 3.91294085229389 -2.24367610583844 1.11295202692063

H 2.47662215037288 -2.70799527160482 0.19548138157175

H 3.72773366488590 -1.70956851361207 -0.56303756772098

H 0.26876120361102 -1.63887447984633 -0.14089573407365

H 1.34989514698928 -0.94860804987810 -1.45423779073620

H -0.16310048076119 1.00829115751758 -1.69247986081667

O -2.31179137826629 1.40888486778079 -0.50992363748511

O -1.84657938485625 -0.37161367421313 0.80379461707296

C -3.49961904675491 1.61547720001462 0.26905155494237

H -3.98629537435066 2.48899273942692 -0.16441640584741

H -4.16253519578115 0.74957524681904 0.20393128085405

H -3.24676126381213 1.81062064090332 1.31394852666905

1 imaginary frequency: -254.09 cm\*\*-1

SP = -744.931435361980

U = -744.78799104

H = -744.78704683

G = -744.83397870

**9 carbanion**

C 3.05307452496660 -1.87615853692798 0.42274346665405

S 2.01362908765125 -0.39950966546290 0.55289416074148

C 0.71630180037542 -0.82273310458335 -0.68715852432041

C -0.26831932606342 0.28189434078548 -0.86358118380903

C -1.42527684761499 0.34454355611898 -0.12687556343318

H 3.89710406112653 -1.76256527699948 1.10675588953829

H 2.49318559339526 -2.77285610076811 0.70084505570595

H 3.43906260600258 -1.98911675791564 -0.59401359818379

H 0.23386957572878 -1.74215047947309 -0.34274093804886

H 1.24457202683046 -1.04754695936986 -1.61892678609359

H -0.03084969591798 1.09805984614050 -1.53865132366123

O -2.21283636041584 1.47863560535181 -0.40675342338607

O -1.86480849666427 -0.47515329669992 0.74272560231340

C -3.43843400609479 1.59503514419730 0.31294569119828

H -3.90798379127014 2.51361911010565 -0.04412056542991

H -4.10464411211235 0.74976775482797 0.11648472960035

H -3.26585663992310 1.67445182067263 1.39070531061427

0 imaginary frequencies

SP = -744.954617247090

U = -744.80851123

H = -744.80756702

G = -744.85263322

**9 adduct**

C 3.16106720144552 -2.01407024992220 0.00000355295294

S 2.55371564591999 -0.31119211259373 -0.00001626829308

C 0.77126336897334 -0.65481223785438 -0.00000643323537

C 0.00114499290256 0.65748060782148 0.00000019079885

C -1.48848819977975 0.44137742934022 0.00000367012039

H 4.25221032925516 -1.97592097456399 -0.00000109261301

H 2.82416934013351 -2.54387492540712 0.89389704132197

H 2.82416245782921 -2.54389934029484 -0.89387286916982

H 0.52550326096063 -1.24289664916539 0.88741457242706

H 0.52549318738055 -1.24289418971235 -0.88742627497578

H 0.24478341085978 1.26303362991304 0.87893522338308

H 0.24477820072678 1.26303966465683 -0.87893222511178

O -2.15385393383746 1.60291891527307 0.00000968634049

O -2.04468841955625 -0.64048258345557 -0.00001093102814

C -3.59518568139947 1.51665510911727 0.00000200555111

H -3.94689275795698 2.54689094286999 0.00000836861474

H -3.93999791756893 0.99685730644722 -0.89563692144755

H -3.94000748628818 0.99684265753044 0.89562870436391

0 imaginary frequencies

SP = -745.465985620872

U = -745.30567418

H = -745.30472997

G = -745.35009412

**10**

C -0.58200123427116 -0.52467932511720 -0.00000004669615

C -0.00181051000884 0.78888543534317 -0.00000014009234

C 1.31987834362566 0.95886576603552 0.00000004156209

H -0.70296288744206 1.61730503587404 0.00000006760877

H 1.74095888262042 1.95904615855504 0.00000001600850

H 2.00414365052160 0.11587970939034 0.00000000088108

N -1.06291524504562 -1.57587978008091 0.00000006072805

0 imaginary frequencies

SP = -170.946621901273

U = -170.89073393

H = -170.88978972

G = -170.92038758

**10 TS**

C -2.71560934486485 0.43612702160686 -0.36194451812332

S -1.50891348337008 -0.92787740357620 -0.32921837858782

C 0.17384280399661 0.49434675482555 0.66948835828351

C 1.47140890694425 0.01554915374443 0.70589648232353

C 2.31509914279635 0.16349025252663 -0.41043742172234

N 3.01238651791899 0.29267532940556 -1.33775086879771

H -3.73648751744698 0.05806007873895 -0.46820937764648

H -2.67192083364405 1.01234310456559 0.57009299237489

H -2.52310511878453 1.12393562585210 -1.19182285687579

H -0.40305127789941 0.50219653356335 1.58642503502097

H -0.08927427283484 1.25838087454125 -0.05330716145446

H 1.82366247718856 -0.62958932579413 1.50348471520502

1 imaginary frequency: -250.69 cm\*\*-1

SP = -609.216757582980

U = -609.12019228

H = -609.11924807

G = -609.16007884

**10 carbanion**

C -2.65717982992953 0.39586567347544 -0.26086519227110

S -1.13239038716366 -0.57983571758341 -0.32145924710075

C 0.03452013991692 0.59467766216616 0.50963484583330

C 1.40930382272682 0.02774371223895 0.67584139857568

C 2.25727794585794 -0.00196477813918 -0.41416609303164

N 2.99561961290899 0.01655195491736 -1.33856856369430

H -3.45859012774437 -0.19069760036207 -0.71580344357727

H -2.93206246159781 0.62179693505731 0.77292021874044

H -2.54497356218435 1.32909175716509 -0.81903135974188

H -0.41665006846298 0.83832176461834 1.47589056008361

H 0.04244205558162 1.50566533834161 -0.09652805852693

H 1.55072086009040 -0.75757870189560 1.41483193471085

0 imaginary frequencies

SP = -609.233845366129

U = -609.13563443

H = -609.13469022

G = -609.17462160

**10 adduct**

C -2.73929990859299 0.50620693226591 -0.00000041220375

S -1.45528745899467 -0.76589626115027 -0.00000046126378

C -0.00296862274756 0.32100100297947 0.00000069350805

C 1.26585713500618 -0.53734565917173 0.00000047349506

C 2.45968495059557 0.30589730435951 -0.00000097070417

N 3.39371656797323 0.98412657171794 -0.00000224433739

H -3.70531224114756 -0.00269013371894 -0.00000164885131

H -2.66543487458653 1.12918667646515 0.89414217650068

H -2.66543399579342 1.12918821922817 -0.89414183324555

H -0.02816610008413 0.95528079625961 0.88906259300284

H -0.02816554494702 0.95528224353105 -0.88906015123695

H 1.31013364613119 -1.17787771665417 0.88532982046753

H 1.31013244718773 -1.17787897611170 -0.88532803513125

0 imaginary frequencies

SP = -609.752393616221

U = -609.63926671

H = -609.63832250

G = -609.67793957

**11**

C 2.46229656238406 0.19548843248980 -0.00947271878271

O 2.79841744465538 1.36892573157196 -0.01785658591406

C 1.07651317516863 -0.30845354492370 -0.00349206429775

C 0.04765383136614 0.54765744964360 -0.00708931140708

O 3.35070795485123 -0.81105569510045 -0.00490179262047

C 4.74291724624805 -0.43432995754800 -0.01132224539691

H 4.97828571507619 0.15013435240918 0.88002053204493

H 5.29642216558038 -1.37177302857127 -0.00755631331002

H 4.97281828008070 0.13971344801362 -0.91082475948347

C -1.38217359454754 0.20040580902497 -0.00475000509111

C -2.31786485120592 1.24249393651450 -0.01409156916162

C -1.84269027899173 -1.12400103826584 0.00494129895375

C -3.68385518304604 0.97171964762298 -0.01436029828507

H -1.96670007044901 2.27075724606541 -0.02155055291085

C -3.20566693024565 -1.39342409435337 0.00522367962984

H -1.13695081497797 -1.94846615204728 0.01244472603560

C -4.13027977512812 -0.34712188421449 -0.00474771673802

H -4.39755660483095 1.78992125816392 -0.02191127263835

H -3.55095706230297 -2.42282529403022 0.01290879414913

H -5.19458598066612 -0.56267156811206 -0.00480364490354

H 0.26936944992362 1.61319453304787 -0.01350046813198

H 0.95322932105766 -1.38568958740113 0.00258228825975

0 imaginary frequencies

SP = -537.891743324345

U = -537.70261922

H = -537.70167501

G = -537.75086721

**11 TS**

C 3.31681804188638 -1.11031090771368 -1.21731793341337

C 1.96308078570360 -0.87009456066952 -1.00080773544837

C 1.51683561061646 -0.34314382477911 0.21700258176842

C 2.46103776701729 -0.07241477752193 1.21424692334413

C 3.81561245808568 -0.31639903708930 1.00118049785163

C 4.25006189349847 -0.83408720535645 -0.21791558294015

C 0.07914423438675 -0.08809427182487 0.49662816161193

C -0.94604494652488 -0.69647703060573 -0.21651167348746

C -2.27842248673360 -0.67419626106706 0.28395834499612

O -2.67343087205061 -0.17566281451158 1.34920857630088

O -3.17193612347410 -1.29518633335211 -0.55581007873740

C -4.54145707084394 -1.30399525814074 -0.13072546415346

S 0.11604370272727 2.29809958795392 0.04770004852683

C -1.51359948169857 2.39392997851175 -0.72532313061200

H -0.12712320512920 0.14285906228253 1.53470812732930

H -0.79047725308784 -1.12221397994971 -1.20066572378621

H -1.49211036032604 3.02444172066281 -1.61887548516585

H -1.81607760451864 1.38411223640332 -1.04293486154055

H -2.27729957267480 2.78080009594737 -0.04399906072794

H -5.08980885099889 -1.82358628849123 -0.91656795420676

H -4.65315416835794 -1.83958250287148 0.81518177687293

H -4.92164645028738 -0.28494431201439 -0.02495978837077

H 2.12570499612787 0.33512072741483 2.16449104742124

H 4.53284478381104 -0.10246188387120 1.78845025407439

H 5.30598864573163 -1.02292917161240 -0.38790108214813

H 3.64483537504049 -1.51583755702333 -2.17027455516382

H 1.25337815207350 -1.08695143071070 -1.79276023019556

1 imaginary frequency: -310.52 cm\*\*-1

SP = -976.163685209415

U = -975.93375631

H = -975.93281210

G = -975.98893792

**11 carbanion**

C 1.35630744286679 2.84770356784815 0.28383575685960

S 0.03547473959824 2.06799278971849 -0.67798157731633

C -0.07819866153279 0.42662742733152 0.17313516922386

C -1.20699055658173 -0.36949439331524 -0.39727551041918

C -2.47105636823250 -0.29518451949669 0.13175231533435

O -2.87588548048591 0.36658368113296 1.14027768947514

O -3.41747250591167 -1.07640163814510 -0.55748907463392

C -4.71313372813936 -1.17279313579171 0.03253066479265

C 1.25616536772122 -0.28798728298456 0.11008323061820

H -0.28964470526944 0.66399056266828 1.21946338862265

H -1.03730693420812 -0.96654107646386 -1.28668121268362

H 1.43543286260869 3.88969266362757 -0.03494269666504

H 1.11442765402715 2.82606444012492 1.35003345934258

H 2.31565591810454 2.35275420138853 0.11659509004500

H -5.29231208314733 -1.82222094021157 -0.62664069907922

H -4.66587148480897 -1.62018049501127 1.03029475470038

H -5.20147639099983 -0.19630496812249 0.09723808801205

C 2.00013317371923 -0.49305483545460 1.27215152087233

C 3.22565376641084 -1.16238983177382 1.22766951256132

C 3.72405216006613 -1.62803382058034 0.01468378833791

C 2.98965933021811 -1.41931445587671 -1.15472689594583

C 1.76916727796750 -0.75429207997410 -1.10557061586828

H 1.61641688270165 -0.12945843573411 2.22201682882896

H 3.78965273406764 -1.31663089337775 2.14324896989707

H 4.67763019023317 -2.14646726497217 -0.02472289980018

H 3.37236939301016 -1.77335639063797 -2.10797321242620

H 1.21009900599657 -0.58504587591636 -2.02163683268623

0 imaginary frequencies

SP = -976.179310835303

U = -975.94843985

H = -975.94749564

G = -976.00458472

**11 adduct**

C 1.08041658120619 2.06198597018255 0.29338384962113

H 2.02925025505933 1.56767323398385 0.07507846358511

H 0.90943363203220 2.08144676603032 1.37200927410937

S -0.28389828803711 1.23139509364869 -0.55122035232429

C -2.73619333077932 -0.66290059506519 0.26289188832550

O -2.95468794195197 -0.20909310025344 1.37014117416150

C -1.40815576671006 -1.21983217528349 -0.18767219417648

H -1.39609644139389 -1.32577912612611 -1.27395685595965

C -0.23033044660093 -0.37944482152484 0.31225592125749

H -0.37007728663145 -0.17824210298185 1.37695457530778

O -3.67468257913688 -0.75696553283549 -0.68424217670325

C -4.99692833535410 -0.30278934499171 -0.32026036351042

H -4.96810380848508 0.75571292177777 -0.05638914633063

H -5.60988652947514 -0.45794513891069 -1.20627083424066

H -5.37731566311894 -0.89229215454530 0.51575653253350

C 1.09290551259698 -1.08753321322604 0.12156951288220

C 1.88302654797964 -1.38679692994271 1.23106698196584

C 1.54084911702815 -1.45532914843821 -1.15023580203219

C 3.09715206120703 -2.05786437079388 1.07750537235402

H 1.54500876721662 -1.09479683290084 2.22191093953484

C 2.75021551826922 -2.12495572277563 -1.30607767323523

H 0.94123679695090 -1.21213983816025 -2.02289161073120

C 3.53232780053132 -2.43066852011501 -0.19076845589987

H 3.70151995464397 -2.28559046970698 1.95077448661883

H 3.08557810851196 -2.40880999572527 -2.29942372925542

H 4.47664745443595 -2.95287549619027 -0.31340572957000

H -1.33473558634775 -2.22384437015115 0.24458537590026

H 1.11925389635319 3.08745501502122 -0.07983942418804

0 imaginary frequencies

SP = -976.690322747026

U = -976.44465010

H = -976.44370589

G = -976.50061415

12

C 2.05172515899590 0.48559198247364 0.00115695320603

C 1.08244278654138 -0.44183638768242 -0.00533678191671

C -0.36456911803636 -0.18250090524630 -0.00091753873889

C -1.22984227601388 -1.28331017655387 -0.00563712796337

C -0.90771500250255 1.11009321127333 0.00803902629787

C -2.61005727006141 -1.10145295121288 -0.00160938610375

H -0.81218691899724 -2.28629411922861 -0.01267805237298

C -2.28515524671525 1.29061654563132 0.01224999853346

H -0.25814516778462 1.97947360145614 0.01174969889032

C -3.13981688389108 0.18622832912177 0.00742046216503

H -3.26943709728968 -1.96389552838992 -0.00541089268165

H -2.69634783953357 2.29540523752359 0.01934939545166

H -4.21580891356361 0.33259666609503 0.01072827601716

C 3.42500329983941 0.09085618441446 -0.00349331465566

N 4.54195677184335 -0.21203067135658 -0.00677814533777

H 1.36949838937986 -1.49091261878636 -0.01439259280647

H 1.86621532778935 1.55429160046762 0.01051002201568

0 imaginary frequencies

SP = -402.176835701162

U = -402.03473860

H = -402.03379439

G = -402.07646735

12 TS

C 3.65980133617000 -0.12676410719751 -0.19635904925404

C 2.80066530588117 -0.44530040753185 -1.24945668427064

C 1.42893254535251 -0.53302272661695 -1.03665527666743

C 0.88997770847618 -0.31004343063659 0.23544904992557

C 1.75797604481412 0.00464479012993 1.28567740787532

C 3.13249797798541 0.09897290540228 1.07317978982358

C -0.56999505686891 -0.41045022409257 0.51250470465093

C -1.40067963793443 -1.23734358429176 -0.25165402827476

C -2.66791089133351 -1.59197292943986 0.22955968876028

N -3.72366113346632 -1.88716865516397 0.63738567952764

S -1.06402781254479 1.86668548565397 0.19687828892552

C -2.65533770389900 1.63709696226241 -0.62621790905245

H -0.81303299939258 -0.33574224661037 1.56607882737830

H -1.16176808784279 -1.53213902720737 -1.26659452720746

H -2.78087761998438 2.35387475909159 -1.44239003763798

H -2.68486609892678 0.62732404072083 -1.06089850921536

H -3.50083382420115 1.73731492839384 0.06111287222502

H 1.34888992237121 0.18245516568611 2.27700951714408

H 3.79069651270452 0.34665134931994 1.90106822553089

H 4.73014440047519 -0.05649824919571 -0.36629682801804

H 3.20211703394846 -0.62252053474571 -2.24328575851148

H 0.77552107821591 -0.76980126393069 -1.87062544365751

1 imaginary frequency: -291.47 cm\*\*-1

SP = -840.447151849971

U = -840.26414941

H = -840.26320520

G = -840.31378288

12 carbanion

C 2.91088458466246 -0.09930535885118 -1.22501491030962

C 1.52268582137369 -0.07710172762439 -1.11797896691392

C 0.90245846260825 -0.15462930335015 0.13315900502063

C 1.70122703832476 -0.24845986125446 1.27437960941805

C 3.09220138012887 -0.27494648339192 1.17127585357810

C 3.70139138618316 -0.19985711007341 -0.07924186741545

C -0.60780390455527 -0.12338870658417 0.25566090087446

S -1.06630959300996 1.66716287955004 -0.09081014179289

C -2.85401814008146 1.57055926192169 0.14309909901496

C -1.31359427179290 -1.13481126104052 -0.58562281503181

C -2.50011133652718 -1.68103864020621 -0.15066114241347

N -3.50250935904823 -2.17494222260942 0.24206450498004

H -0.86954956923976 -0.27411941498323 1.30616663372658

H -1.11917435207570 -1.15610746781980 -1.65419206888912

H -3.26350239626753 2.57060755158217 -0.01901112379204

H -3.29920558018482 0.88386527330489 -0.57907026017470

H -3.10098926696969 1.24785885384970 1.15780977948480

H 1.22903556859901 -0.30376521291343 2.25212053309601

H 3.69856486016620 -0.35303268064158 2.06928819818229

H 4.78415838727662 -0.21910479728373 -0.16239776508552

H 3.37794319177451 -0.03928984558584 -2.20403051807237

H 0.91431308865495 0.00141527400496 -2.01442253748502

0 imaginary frequencies

SP = -840.457788747131

U = -840.27362884

H = -840.27268463

G = -840.32337078

**12 adduct**

C 1.48970050792289 -1.35103801169486 0.38510057543810

H 0.56977858258451 -1.93216925315217 0.29733678180113

H 1.67686050315052 -1.10141112621528 1.43192862758853

S 1.40660761017380 0.14949938797896 -0.61913719821433

C -0.04113602588733 2.44709244444365 -0.28090801031983

H -0.17772561369523 2.46674240262859 -1.36556944543448

C 0.04933210406334 1.00934542209040 0.25587528517650

H 0.32325896148141 1.04869728231099 1.31314225706964

C -1.26215826826525 0.27098053132427 0.11540678686235

C -1.77433426671533 -0.44336267441067 1.19862911705117

C -1.95382726501316 0.25202691891934 -1.10036639162616

C -2.96532750594286 -1.16015118026769 1.07634988618637

H -1.23723280577642 -0.43752171351734 2.14335449724321

C -3.14217227863102 -0.46042565502775 -1.22341438304523

H -1.56022290626140 0.78644103995221 -1.95994553962236

C -3.65209898049442 -1.16951554828072 -0.13420314461431

H -3.35251263423077 -1.71111156795275 1.92842327026442

H -3.67168254203656 -0.46576675241321 -2.17163821154121

H -4.57903784592077 -1.72672334399719 -0.23229924387442

H -0.89751123795838 2.95319165909513 0.17255033515528

C 1.15571371078720 3.22618797052593 0.03583394216826

N 2.08821154088093 3.85355007677121 0.29802763332327

H 2.32401665578435 -1.94535830911105 0.00695257296412

0 imaginary frequencies

SP = -840.976805824780

U = -840.77806462

H = -840.77712041

G = -840.82767362

**13**

N -3.10712316136080 0.21075132347641 0.11663326543260

C -1.78687388972616 0.52777675193600 0.06293481662155

C -1.02363747963722 0.10019796643736 1.27256467463216

C 0.26831895277097 0.38702032176712 1.40492670814200

O -1.25616828083934 1.11421383992448 -0.88446040180396

H -3.41185321628180 -0.26087577119157 0.95855792604824

H -2.93753678938341 1.39977516794351 -2.35440560116790

H -1.56271544265850 -0.44871492156847 2.04076797285226

H 0.80444219642122 0.93770035990129 0.63694343088446

H 0.82144425313117 0.07856210082028 2.28680579023482

H -4.84193042910078 1.76842026793321 -3.86999265384254

C -3.92619858041473 1.08032543180784 -2.06008829120760

C -5.01190558323526 1.28488705742756 -2.91242538922369

C -4.13287015342627 0.46149886856887 -0.82487940759071

C -5.42193486039229 0.04901086607229 -0.46335403707540

H -5.57718919819386 -0.43624260046877 0.49653894020112

C -6.49235824775161 0.25919254706008 -1.32175122702521

H -7.48535967725312 -0.06529377064741 -1.02567097453560

C -6.29414003443499 0.88222635478958 -2.55445138982053

H -7.13035037823314 1.04836783801030 -3.22638415175605

0 imaginary frequencies

SP = -478.681072602565

U = -478.50928152

H = -478.50833731

G = -478.55350594

**13 TS**

N -3.18336629310381 0.03618630465161 -0.03513828448743

C -1.86770016024621 0.47170813815797 -0.04857521533312

C -1.03328219358658 -0.09247124969847 0.97650295495859

C 0.31006106079369 0.22250874812863 1.04325604069288

O -1.47354184882168 1.29645344987330 -0.90678479834128

S 1.81527131741010 -1.07108806476703 -0.34710607380391

C 3.23540050018571 -0.02345065569099 0.10265044935369

H -1.45172943171146 -0.87201590926434 1.60771025167087

H 0.66753960221544 1.11572759645153 0.54329105620982

H 0.88343488914370 -0.08522080303034 1.91008238412460

H 3.19810166005112 0.94561384390777 -0.40544800728861

H 3.25407439588461 0.16215377335970 1.18309517176907

H 4.17850007485975 -0.50788516003233 -0.16657016808995

C -4.24854454918890 0.41584634935350 -0.87058325998982

C -5.54826680883585 0.22731314790904 -0.37819707022573

H -5.68163053557482 -0.16194911427036 0.62805816744219

C -6.65304632318270 0.53252445066720 -1.16354912345564

H -7.65054597557952 0.37820393995852 -0.76220915217831

C -6.48517427408936 1.03757455151978 -2.45318422556490

H -7.34766186012172 1.28143132938279 -3.06565513253278

C -5.19476369508833 1.21782276624516 -2.94451500864385

H -5.04593021763863 1.59866188255501 -3.95103487970585

C -4.07779049930057 0.90658480801738 -2.17036669761043

H -3.08394739186464 1.03687750355579 -2.57453344727939

H -3.44811744260930 -0.51763262694081 0.76756706830930

1 imaginary frequency: -291.20 cm\*\*-1

SP = -916.947428448375

U = -916.73468525

H = -916.73374104

G = -916.78802783

**13 carbanion**

N -3.33375390487096 0.64841821000190 0.52835193452155

C -1.92570692517528 0.90054991532696 0.36552281220092

C -1.06620978070077 -0.06840462557731 0.81321548701872

C 0.41289625154138 0.12830128001944 0.83201291177474

O -1.60868313011301 2.04775998312663 -0.13564326105052

S 1.20644069587951 -0.57558198723168 -0.67051634342157

C 2.93979805608957 -0.21401073121235 -0.29448531114937

H -1.46932348465716 -1.01579471387244 1.16076022953106

H 0.67144815174609 1.19046537574948 0.86693838308423

H 0.87801513264352 -0.36600856113083 1.69075539552781

H 3.10227916064377 0.86358124971576 -0.20931066205573

H 3.24556938135646 -0.70317230337871 0.63415732398154

H 3.55378606227586 -0.59843661623996 -1.11210452135836

C -4.22501076496463 0.65733731557285 -0.55719141478748

C -5.56294015416040 0.29974182976328 -0.31960358011728

H -5.86557184241841 0.03313281353078 0.68996571261599

C -6.49055370581210 0.28384819013484 -1.35342545019519

H -7.51811960442321 0.00145917849532 -1.14110135230120

C -6.11319085013835 0.63170117493018 -2.65157192184819

H -6.83896921599996 0.62497871175035 -3.45888102208329

C -4.78715885654433 0.98251184481529 -2.89154439458771

H -4.46998304274203 1.24623968790644 -3.89700531244597

C -3.84523263744622 0.99404063290690 -1.86342379906476

H -2.81741612685647 1.26247966604046 -2.07476465847648

H -3.53049186515279 -0.10397352114359 1.17542481468656

0 imaginary frequencies

SP = -916.968348631956

U = -916.75413949

H = -916.75319528

G = -916.80629389

13 adduct

N -2.96087200935979 0.01101512318450 -0.03266989896827

C -1.86053196202498 0.76465976406876 0.22169034020348

C -0.99654612462603 0.26517333139441 1.36408993333750

C 0.49155844591044 0.35631549911391 1.05127364451426

O -1.58493258003566 1.79723200636600 -0.39303509477554

S 0.93686276589222 -0.83211403042388 -0.24958678110622

C 2.66167450554213 -0.34470689793476 -0.48946718605816

H -3.13736571384544 -0.75243158770135 0.60753971628198

H 0.74647429644339 1.36270958659127 0.71148081031054

H 1.07073659721139 0.13471118236337 1.95044143768989

H 2.72612304152403 0.69145291938694 -0.82941708950740

H 3.22804901516618 -0.46596428404746 0.43680368598461

H 3.08912137419782 -0.99671568527550 -1.25386823920658

C -4.02978539913726 0.32697096542812 -0.91148020320369

C -5.30888546183054 -0.10560640761148 -0.55160350953450

H -5.44692866932620 -0.64402320816679 0.38214624327813

C -6.39290931114274 0.15761339587225 -1.38135307919067

H -7.38303713362725 -0.18061236633240 -1.09110833181455

C -6.21075923963810 0.85667023937129 -2.57399593742266

H -7.05766264840918 1.06850297857452 -3.21925520622148

C -4.93185076622099 1.27368733390176 -2.93363671612215

H -4.77623634463028 1.80709440024809 -3.86673287275213

C -3.83604342002847 1.00684002327196 -2.11451489109406

H -2.84378147974476 1.31769687896598 -2.41272733331867

H -1.21675375820396 0.91431041301682 2.21906514011092

H -1.27622002005593 -0.75296857362634 1.64820341858542

0 imaginary frequencies

SP = -917.485847192501

U = -917.25712543

H = -917.25618122

G = -917.30980268

**14**

N -2.99880683792908 -0.56873035960063 -0.35724130664457

C -1.90556653580840 0.16691343920890 -0.08960947697330

C -0.88827504925108 -0.50241397499000 0.77326439338403

C 0.24793522469174 0.10406916785452 1.10425470897705

O -1.75931628743013 1.31716113047728 -0.53122113765345

H -1.11500740207317 -1.50837298470586 1.11783295864689

H 0.47192974047517 1.10922239453590 0.75774301523867

H 0.98395357646688 -0.39027122008634 1.73110470571460

H -3.73188317005976 -0.18248599687190 -0.93503338938916

H -3.10190325908215 -1.50319159582187 0.00956552869922

0 imaginary frequencies

SP = -247.470784434541

U = -247.38513005

H = -247.38418584

G = -247.41819050

**14 TS**

N -3.22606689426252 -0.43069986064147 -0.10865742301793

C -1.97903906729015 0.14027718460475 -0.00274007269483

C -1.01625661206111 -0.53553460835658 0.81863229961037

C 0.25376152862097 -0.02208170879538 1.00719901195941

O -1.76285088253024 1.23137811762929 -0.59915358536172

S 1.93033827556233 -0.55679108343978 -0.64430457214357

C 3.17477177766075 0.44573570163596 0.22919524220127

H -1.27385837241561 -1.52245435468376 1.19415745257515

H 0.43341491886642 1.02850777792648 0.80773910607256

H 0.89274311889529 -0.46471079250715 1.76302597409922

H 2.96286482822485 1.51640525757172 0.13961777014405

H 3.19750047038166 0.19463602161864 1.29615343991651

H 4.17588503230901 0.26817798859325 -0.17416160668626

H -3.81494080141927 -0.09617221529970 -0.85768324066679

H -3.33569732054237 -1.39904342585627 0.15460020399256

1 imaginary frequency: -308.00 cm\*\*-1

SP = -685.736016351316

U = -685.60964571

H = -685.60870150

G = -685.65277194

**14 carbanion**

N -3.16893777329150 -0.47423874583393 -0.13658514985150

C -1.87873966980051 0.12148381661508 -0.02741010774334

C -0.89902771174047 -0.53992999550531 0.67561836891158

C 0.45499737941799 0.04338325689912 0.89543397796470

O -1.76968309586166 1.29211150736949 -0.57489838869515

S 1.65083957826789 -0.45923591882221 -0.41663869721964

C 3.14294200426042 0.36683731934051 0.19032110734252

H -1.09889349003801 -1.54345975613229 1.04366919365271

H 0.42635349025433 1.13700428503419 0.89286531595328

H 0.88975818976110 -0.28179591949335 1.84592257812943

H 2.99645815471379 1.44916312554473 0.23884620896471

H 3.42033720493064 -0.00632026744222 1.17990088086873

H 3.95838259150078 0.15492158964201 -0.50504659774698

H -3.60097719819254 -0.23278636077522 -1.02067847813408

H -3.15177565418225 -1.47987893644060 -0.01328721239697

0 imaginary frequencies

SP = -685.756648113416

U = -685.62731239

H = -685.62636818

G = -685.66817038

**14 adduct**

N -2.57029286521069 -0.51601780444426 -0.81026857365901

C -1.80841661810711 0.18370616017947 0.04500048647756

C -0.96068124757171 -0.62684783142565 1.00466046666065

C 0.47078744814656 -0.11111532040203 1.09040639356469

O -1.81195142309087 1.42335410243675 0.06898160025628

S 1.33587441370295 -0.37771504738152 -0.48554546345960

C 2.90382328389480 0.42417306388024 -0.07755192625068

H -1.42776183176609 -0.53139142196144 1.99088234929136

H 0.47674238315035 0.95722799795113 1.31887183499953

H 1.00507387060015 -0.63986222449448 1.88303483640387

H 2.74920530577048 1.48253262206128 0.14445567750166

H 3.37807333074579 -0.06700341405317 0.77527600195281

H 3.55930073122907 0.33570242417541 -0.94631854834200

H -3.18633455609466 -0.02765475608062 -1.44518720770149

H -2.54952335550222 -1.52451778172669 -0.81936102799000

H -0.98074886989682 -1.68558076871440 0.73362310029436

0 imaginary frequencies

SP = -686.275619432178

U = -686.13226807

H = -686.13132387

G = -686.17357492

**15**

N -3.17090635324895 0.34407601939886 0.08694315799514

C -1.86327021742896 0.48668206586002 -0.26656251951453

C -0.90420013170037 0.00874883563234 0.77001867965205

C 0.40863800667788 0.14392440969016 0.60566644380795

O -1.50387232826138 0.96911863505090 -1.34302642012501

H -3.36277751790519 -0.19815254200434 0.91991986456131

H -1.31942637260545 -0.44490742484965 1.66601541691779

H 0.81995573358482 0.60340286115492 -0.28883783139854

H 1.10482009510845 -0.20066976189500 1.36420502681066

H -3.44959164200292 2.47948544199630 -1.52523753799813

C -4.28646868315318 0.64244425274661 -0.73262094326841

C -5.37900806399876 -0.18524246927141 -0.69620757706008

C -6.51168885313185 0.11834529117240 -1.49029825703370

C -6.52485422256726 1.26221603659508 -2.31260895695894

C -5.39124008605862 2.11230684230822 -2.31589252719303

C -4.30343758771933 1.81434710865806 -1.53978683890284

H -5.38281001999114 -1.07657386418071 -0.07506377456622

N -7.61399544504311 1.55721181578775 -3.08989649041436

C -8.62028337988208 0.72447913509457 -3.02655418040474

N -8.71334255374440 -0.40973051536128 -2.27440702813948

H -9.48845086442243 0.94934218000040 -3.63935098696892

C -7.67228967739487 -0.69276974382446 -1.52483809786141

H -7.71914841097350 -1.59277979029037 -0.91512896537275

H -5.40537142413729 3.00726518053062 -2.92908965656379

0 imaginary frequencies

SP = -664.516574921642

U = -664.31886910

H = -664.31792489

G = -664.36847805

**15 TS**

N -3.22121507838850 0.25339710630353 0.14569619517563

C -1.88409482001953 0.63113255215080 0.10675853826354

C -1.05419996567854 -0.00124557910414 1.09451908342904

C 0.30920326199071 0.20915314118671 1.11084561487972

O -1.47793041993359 1.45403216636717 -0.74406062884022

S 1.65159386442117 -1.20912841569081 -0.35070064559527

C 3.14845788818624 -0.20788906915613 -0.07767873489512

H -1.50530341425028 -0.75246176440293 1.73730410811882

H 0.71992905884661 1.06821821630159 0.59241236603032

H 0.89255939725630 -0.15285360345059 1.94903381646461

H 3.18761007545885 0.65357399417170 -0.75188333429670

H 3.17582082805300 0.16811032050350 0.95234994234903

H 4.05427931549549 -0.80060281467691 -0.23561173702835

C -4.24728143699033 0.59381409984867 -0.74335509096942

C -5.36364444769380 -0.29856949173152 -0.78560535310321

C -6.43774962121658 -0.07280213813458 -1.59860605099094

C -6.45739376912915 1.07241202712235 -2.43618149581365

C -5.36133767761125 1.95654262219658 -2.38968096645945

C -4.25838044319658 1.72260615905512 -1.53217924014811

C -5.44104684654216 3.08617709329388 -3.24045878878073

N -6.46435502660403 3.31171914724702 -4.03478765797593

C -7.46487578933664 2.38722229655404 -4.00070924309279

N -7.52153789208125 1.30651515969773 -3.26497068339605

H -5.34440194817525 -1.17852004232748 -0.14803021006386

H -7.27636609051177 -0.76112207290801 -1.61774757855493

H -3.44203722602457 2.43096971027246 -1.51562578991832

H -3.43438010913261 -0.51199906024690 0.77063848060608

H -4.62777159051538 3.80934065261245 -3.25061302096514

H -8.30397007667642 2.58060758694468 -4.66279189442853

1 imaginary frequency: -277.97 cm\*\*-1

SP = -1102.785111003891

U = -1102.54574931

H = -1102.54480510

G = -1102.60367107

**15 carbanion**

N -3.26517626430985 0.67795876623586 0.60858582957623

C -1.87358829413757 0.80268623830429 0.25031205963086

C -0.97959045869342 0.13547426752015 1.05616107924361

C 0.49002972942434 0.24060607305440 0.82948814489323

O -1.58665778701706 1.54254480176948 -0.75783131171130

S 1.11552721061913 -1.05500329206425 -0.32419904002425

C 2.85288828245083 -0.55525227240639 -0.42468031840009

H -1.34631703992687 -0.50660426960121 1.85264324461646

H 0.75606764757990 1.20456377088552 0.38502341239406

H 1.05295831054199 0.12769159542609 1.76097805504463

H 2.94123181906686 0.45729929137695 -0.82751204950264

H 3.32894171509261 -0.59765141400287 0.55859778531087

H 3.37022957733508 -1.24566999576691 -1.09466515245009

C -4.29745793119020 0.73690196117051 -0.33983546446376

C -5.26039730932767 -0.24815645887940 -0.37887319241714

C -6.33555285800968 -0.15760660988781 -1.29627300698166

C -6.43694827211957 0.93081605963773 -2.18637399001112

C -5.45146644239925 1.94757940974451 -2.12159219693864

C -4.42704605148288 1.85785722930634 -1.21811249300839

H -5.19847719800869 -1.10747496275121 0.28412849946459

H -3.69817720085597 2.65397609363981 -1.14990796478993

H -3.40397844682828 -0.08327156757609 1.26199815814116

N -7.46548731181996 1.01086047122334 -3.08725030157436

C -8.33434475661955 0.03283976086141 -3.07347174693617

N -8.33546536393819 -1.06230713597074 -2.26209173471850

H -9.15327249369437 0.08617204912107 -3.78538696800501

C -7.34985197387195 -1.14037783883033 -1.39488393712183

H -7.32658164817971 -2.00594847792509 -0.73559818054340

H -5.53454918967989 2.80478645638483 -2.78221721871737

0 imaginary frequencies

SP = -1102.805490393029

U = -1102.56490578

H = -1102.56396157

G = -1102.62324401

**15 adduct**

N -2.89529043190893 -0.37084354718262 -0.03302421998645

C -2.01759714178879 0.49516523953940 0.53685526181977

C -1.02337797475871 -0.12432744238797 1.49828479642867

C 0.40685004018585 0.27425854373931 1.14676410265604

O -2.02308990275311 1.70665203147680 0.30951770910737

S 0.87593703195024 -0.43830007548680 -0.45912443930198

C 2.41674990829548 0.46658693896422 -0.73175903715656

H -2.89123742384412 -1.32279785856442 0.30853285912610

H 0.48944361142337 1.36165167264695 1.08093579399192

H 1.09288782720021 -0.08214593232089 1.91790038186854

H 2.22690705160254 1.54025630080757 -0.79743383971393

H 3.13162754296591 0.26479488636834 0.06911848373137

H 2.83948115260588 0.12205776420528 -1.67785834961113

C -3.94743676937893 -0.02212513769276 -0.91615654196942

C -5.14491838969501 -0.68396096422077 -0.82893770719877

C -6.18606165127311 -0.36387662651786 -1.73342960900441

C -6.00732540424887 0.63558782728350 -2.71114632295264

C -4.75367911377072 1.29048846622393 -2.79250741180897

C -3.74678640592678 0.96158512573536 -1.92503840826002

H -5.30595936569290 -1.44839433524429 -0.07419956960728

H -2.78107229347783 1.44316345340694 -2.00964464193999

H -1.26293738935427 0.26377624845042 2.49358549142877

H -1.13032895101277 -1.21182006621680 1.52927362742524

N -7.01749216730778 0.95783944018383 -3.57880035840516

C -8.13552463068113 0.29167958992400 -3.44879837952453

N -8.41639199595842 -0.69170924067354 -2.54623601290272

H -8.94208342080243 0.53945754686311 -4.13274628538991

C -7.45059393679739 -1.00187223932147 -1.71188103280674

H -7.64711424493938 -1.78270929418252 -0.97997747499147

H -4.59936516085800 2.04019168419374 -3.56149886505166

0 imaginary frequencies

SP = -1103.321659869739

U = -1103.06682900

H = -1103.06588479

G = -1103.12483496

**16**

N -3.97165870124689 0.08090946645111 0.39741550335018

C -2.70868091123631 0.56906042359175 0.54853815293978

C -2.01179171505795 0.07740835507623 1.76466634373932

C -0.72884145719173 0.35969615948557 1.99027110981043

O -2.19935672585380 1.35293099293038 -0.25884980195697

H -2.58647042552498 -0.53252557477616 2.45846325863261

H -0.19398589121502 0.96736666221850 1.26355553589687

C 0.02789328345518 -0.14754510703779 3.18108108108938

C -4.81898004906327 0.38090257384970 -0.69894623311088

C -5.49442906574204 -0.62540592665393 -1.33747577336173

C -6.37557256092829 -0.30507668766485 -2.40042161703779

C -6.55218003621075 1.03204097635712 -2.80963659136604

C -5.84916562808673 2.05530779469910 -2.12516834353970

C -5.00981831471721 1.73518649921621 -1.09274846147915

H -5.36503714985569 -1.66175888656624 -1.03905884070695

H -4.48966273171859 2.51759595427253 -0.55309925845638

H -4.25495445228442 -0.67738168538120 1.00405143397372

H 0.65573925630730 -1.00011176952504 2.86208682815839

H -0.68185995064563 -0.53012780557876 3.91845406044656

N 0.85970298453922 0.88073485311482 3.82351576000396

C 2.02601456425810 1.17869948432531 2.98779421512787

C 1.33290483925781 0.35131331440930 5.10481944727288

H 0.48395069680725 0.14319997234600 5.76108084517849

H 1.97324126105343 1.09002853181984 5.59333023609031

H 1.91209472543969 -0.57879068313420 4.97769574870213

H 1.72236518113305 1.59511985444312 2.02556207695914

H 2.63261713579481 0.27646820296073 2.80076870866141

H 2.65421653837501 1.91897036905150 3.48903772261840

N -7.39752259236435 1.34403445833195 -3.84119456605315

C -8.01628423937919 0.34398361080542 -4.41423118180627

N -7.91946270802633 -0.98019588968270 -4.10389142953217

H -8.68845139476609 0.58210386704296 -5.23354623324974

C -7.11128539321878 -1.28229339815691 -3.11286787372854

H -7.01548198711572 -2.33177222771543 -2.84152328615891

H -5.99606738497108 3.08808126507403 -2.42335557710747

0 imaginary frequencies

SP = -837.937875935117

U = -837.63245502

H = -837.63151081

G = -837.69141480

**16 TS**

N -3.41088823461747 -0.00996204437155 0.03308501931446

C -2.12171755767765 0.49487888032431 0.18785405903769

C -1.32731461033985 -0.18126870030751 1.16838337098259

C -0.00866739412009 0.18203238390534 1.38425408829378

O -1.72621739354033 1.46611998719691 -0.49922574385610

S 1.52487714801905 -0.80704644372985 -0.21588007755439

C 2.89336376565431 0.36041293117414 0.06972480111416

H -1.75053888676993 -1.04220898365300 1.68030442862982

H 0.31185876665941 1.13676308702357 0.97985564951914

C 0.72597959266718 -0.28666087788956 2.62218250088255

H 2.50321628618326 1.32251137321235 0.42527459635335

H 3.60202268730177 -0.01237853191692 0.81565670985417

H 3.44493173961887 0.55194815135074 -0.85548489297250

C -4.44996962998491 0.41165950044064 -0.80256231684500

C -5.67819516012444 -0.20798258475721 -0.68749589982799

C -6.75485870858697 0.18100302246625 -1.51532815973908

C -6.60013623971794 1.20788954106199 -2.46988519338878

C -5.33436835123644 1.82981893226686 -2.57841088771990

C -4.29167308612790 1.44240290857080 -1.77878881291694

H -5.82967048659761 -1.00061086918499 0.04073348946088

H -3.33031875664526 1.92224743208929 -1.88113228557048

H -3.64818029368831 -0.77639092101486 0.64811050361002

H 1.80666555843042 -0.13677608062188 2.48899801997432

H 0.55298655831220 -1.35730037095764 2.75845722026320

N 0.28400028070408 0.40467126193889 3.85132899672281

C 0.54881325306866 1.84002970648159 3.73550363484022

C 1.06773214771029 -0.12718158316607 4.96669476311750

H 0.89719049681472 -1.20293921855495 5.06400189153490

H 0.76291040736584 0.35583771357575 5.89896456557341

H 2.15005031525674 0.03956498303229 4.82877348715215

H -0.07969837109401 2.28470675613214 2.96053609014942

H 1.60491959537870 2.04594597777566 3.48937020913341

H 0.31461958423101 2.33215924649793 4.68306729985212

H -5.19587310974648 2.61741200562276 -3.31238388328940

N -7.64283305288123 1.59291215005305 -3.27131569362239

C -8.77324039520643 0.95710067953159 -3.10639742024388

N -9.03506065690683 -0.05101409828968 -2.22469616866531

H -9.60717226818627 1.25401458714650 -3.73588745459865

C -8.03808901357199 -0.41920172228286 -1.45316363032476

H -8.22308252600802 -1.22121416817285 -0.74104787423058

1 imaginary frequency: -273.85 cm\*\*-1

SP = -1276.203719145804

U = -1275.85627977

H = -1275.85533556

G = -1275.92479922

**16 carbanion**

N -3.64834402321087 0.77924255513770 0.76572806208812

C -2.25917956589018 1.14129522729741 0.64836551078679

C -1.34316751862587 0.19350738396160 1.01480929351436

C 0.11835103801670 0.47904421326894 1.12769535197477

O -2.02513512197759 2.35111562454314 0.26045034934982

S 0.94267445340302 0.06639015210608 -0.47400169936844

C 2.59199361438766 0.78534147595602 -0.24620112088696

H -1.68994961862310 -0.80393742704770 1.27346477158231

H 0.28395146838059 1.55251226257152 1.25424148486117

C 0.80723528536250 -0.30207874423453 2.24978827906113

H 2.50668369740248 1.79488820966054 0.16507559103751

H 3.22357670973752 0.17708751175749 0.40340442150448

H 3.06152625526541 0.85106312484390 -1.23070261188002

C -4.54443165691185 0.87297703436503 -0.30237619742927

C -5.87677531668625 0.56583345828752 -0.10987225240943

C -6.78942964789848 0.64055456407922 -1.18657834265658

C -6.36394746569451 1.04414857083850 -2.46909071490715

C -4.99051223859156 1.33633224690978 -2.65793693037646

C -4.11120506807827 1.24948043307551 -1.61165918596098

H -6.23536710941411 0.26520238134259 0.87092466772135

H -3.06172103776647 1.46279849620892 -1.77577003575030

H -3.82318736791817 -0.01439154238820 1.36708316329010

H 1.88690585133356 -0.07590563477267 2.23434699225896

H 0.69826754788016 -1.37183516082882 2.04326297026252

N 0.27539785254460 -0.04524393399711 3.59626526802421

C 0.40748024139023 1.37083777515416 3.93712498994367

C 1.05304848830793 -0.83913495237667 4.54707617394690

H 0.97129234129590 -1.90133798621080 4.29978149055060

H 0.66824503018658 -0.69127497444978 5.55981215075229

H 2.12255490542599 -0.56514652000100 4.54035692640115

H -0.25119368551200 1.98041890013395 3.31438682432892

H 1.44310133629357 1.73258032715761 3.81199036795634

H 0.11583979811106 1.52178856739188 4.97999465697834

H -4.64378366800348 1.62100809340355 -3.64651679215918

N -7.24937096461146 1.13764961081994 -3.51054254898820

C -8.49554479333727 0.83870112612889 -3.24980318981569

N -9.01738559605216 0.43851602892105 -2.05454104348045

H -9.20607105032203 0.91185441772365 -4.06821697487082

C -8.16941208864599 0.34556237018738 -1.05500618776846

H -8.56163531095376 0.02745673307376 -0.09087392946742

0 imaginary frequencies

SP = -1276.223899613215

U = -1275.87533897

H = -1275.87439476

G = -1275.94409203

**16 adduct**

N -3.46846177151033 0.09078325683887 0.24927863224045

C -2.33700572610069 0.76236497508226 0.58636253504603

C -1.61083829710965 0.24794789598993 1.80911200938957

H -1.74532766839943 1.00671760267903 2.58554082646949

C -0.11679498492161 0.06783094530077 1.54995513059642

O -1.93657536083151 1.74919480703589 -0.03574574055014

S 0.09509559685334 -1.29460935977388 0.35167257221472

C 1.72741149615711 -0.89231886432102 -0.31702888475405

H -2.05752587258563 -0.68127481364754 2.17516555205786

H 0.27169074879525 0.96295198792454 1.06063673336264

C 0.66609629535007 -0.22826490256849 2.82967081033388

H 1.72372867587947 0.10727959888357 -0.75710304464965

H 2.50047368042408 -0.95953709918832 0.45025131142348

H 1.94398528917314 -1.62301668179821 -1.09935638872592

C -4.29901486810528 0.41405233780883 -0.85468505488974

C -4.77996262782842 -0.58561958707702 -1.65774256531742

C -5.65259245259301 -0.25779812880487 -2.72498827292736

C -6.01199232487682 1.08127681172847 -2.97598355110989

C -5.50160748926771 2.09611811747779 -2.12677624267957

C -4.67767222781187 1.76616503127606 -1.08482319972208

H -4.50463522100340 -1.62214695819896 -1.48550219957664

H -4.31255958250208 2.53677785744929 -0.41709789131028

H -3.63040285331142 -0.80038895809965 0.69906064954762

H 1.72669455850991 -0.37296782849178 2.56179429903382

H 0.30481624722497 -1.17127442611966 3.25140791083744

N 0.54442945905345 0.80620956668607 3.86409658855184

C 1.04031236760471 2.09122862577587 3.37133133603077

C 1.34092829935375 0.39555511759869 5.02025992877869

H 0.98114014395096 -0.56573709315680 5.39773898086449

H 1.24623162837577 1.13653155244557 5.81853279207044

H 2.41092970160047 0.29082331775410 4.77085474982213

H 0.38904596905934 2.48636434676299 2.58829294541011

H 2.06476985647137 2.01256527626784 2.96771688188171

H 1.04972895953512 2.81364006451354 4.19168376108494

H -5.79009934380986 3.12720196268636 -2.30217922961875

N -6.84904276253148 1.40062205449767 -4.01228365894692

C -7.28182524781694 0.40562855168763 -4.74299773210519

N -6.99468697133971 -0.91924156703364 -4.59631375188134

H -7.94730359815994 0.64957855615798 -5.56610980284581

C -6.19372694140686 -1.22873558870879 -3.60173507360208

H -5.94614477954855 -2.27899836132098 -3.46095465183573

0 imaginary frequencies

SP = -1276.740731383606

U = -1276.37777750

H = -1276.37683329

G = -1276.44600491

**16H**

N -3.81963896266616 0.01038574666233 0.30530454649807

C -2.50485007592455 0.34833836259341 0.36732936584821

C -1.82001277534656 -0.12032213922983 1.60575327510602

C -0.53261877452920 0.14164403555325 1.81358031847609

O -1.93130909725093 0.99271295814871 -0.51362976710947

H -2.40930496150404 -0.67449201892830 2.33245597346566

H 0.03075121241167 0.69126562847756 1.06441905103032

C 0.18591957075570 -0.33875496554157 3.03645073258547

C -4.69164183797369 0.34124911911883 -0.76343185703542

C -5.55172213037229 -0.60399001829029 -1.25707376604572

C -6.45806131713505 -0.24917926578651 -2.28667887280210

C -6.47074958043313 1.05758831703660 -2.81317879446369

C -5.57518009839183 2.01836216722250 -2.27974790986443

C -4.71363322540947 1.66844043132681 -1.27583697167477

H -5.55146345365965 -1.61738904181920 -0.86613555234658

H -4.04630529420260 2.40845260023278 -0.85040440980884

H -4.16681746910635 -0.64370644904362 0.99497777734031

H 1.04539751376932 -0.96007102814223 2.77145613035600

H -0.48465584574396 -0.90679822834538 3.68136706808733

N 0.72786689685639 0.79539354668488 3.86264265370401

C 1.80683039091918 1.55457029404844 3.16487650416801

C 1.20558236573209 0.29085323528558 5.18323367716149

H 0.37513466764193 -0.19860355385426 5.69080508283281

H 1.56192388774703 1.13856558701293 5.76728343159595

H 2.01586949316599 -0.41636472029798 5.00503485069034

H 1.40810194908815 2.00027237280905 2.25551311204698

H 2.61329395886387 0.85900876474463 2.93190339760029

H 2.15922270070638 2.33642644261110 3.83655594408469

N -7.34147365858836 1.40204795501237 -3.81294827006748

C -8.14720860360826 0.46295845463789 -4.23727469099951

N -8.22504576223944 -0.82587195078870 -3.79823275328035

H -8.84083305362296 0.72728519906531 -5.03021416926662

C -7.38946738926804 -1.16045396119773 -2.84120736524355

H -7.42835847482747 -2.18290785470852 -2.47088825172066

H -5.59452329044664 3.03123619931597 -2.66810627297077

H -0.04481947540697 1.44383777837318 4.04020678202189

0 imaginary frequencies

SP = -838.405627895221

U = -838.08328855

H = -838.08234434

G = -838.14387136

**16H TS**

N -3.45176253779197 0.21470231865500 0.21892640396501

C -2.11723279629687 0.58755671169198 0.21536956758606

C -1.30918495521257 -0.08825142408864 1.20094564419524

C 0.03315246702629 0.18812562489328 1.31337361173451

O -1.67831939626469 1.43768200686997 -0.58673082790634

S 1.53172897291115 -1.00253707461178 -0.22895034479806

C 2.94000020488856 0.12842696566247 0.00857829317242

H -1.76113498722254 -0.88270603941546 1.79020950554672

H 0.41295076819368 1.08927077770117 0.84511658831843

C 0.77814287200126 -0.29969107162952 2.52940303585288

H 2.59117288687556 1.09915640553364 0.38446528092930

H 3.66744801306297 -0.26694564331256 0.72421988074582

H 3.46022881816384 0.31314281817580 -0.93571268514655

C -4.48034715057887 0.56811711032471 -0.66630009723620

C -5.63185805838773 -0.19041688157898 -0.66005221435055

C -6.70465614018170 0.13930989375639 -1.51848927119921

C -6.61632799195689 1.24222559131607 -2.39168659164631

C -5.42989074468308 2.01264900039520 -2.37935272906186

C -4.39760344069664 1.69624916237179 -1.53616883999826

H -5.72342067544142 -1.05016152225586 -0.00157413888071

H -3.50537553602015 2.30438144172723 -1.52614313201793

H -3.68374513141367 -0.54026513127429 0.85036798636274

H 1.84964825122104 -0.11789688483960 2.46888207659410

H 0.59224004743250 -1.35879638657512 2.70473689330544

N 0.30448360417786 0.42357058105073 3.77157647168398

C 0.52184615370252 1.89449314123385 3.68323655281807

C 0.95826349779369 -0.14280614827527 4.98377725741086

H 0.74386089636645 -1.21022116428786 5.02994258756599

H 0.56041249008425 0.36318249255505 5.86293349558663

H 2.03255374349728 0.02590337587787 4.90270454636503

H -0.06511754519948 2.29252423675868 2.85688148140767

H 1.58531066218857 2.07232099979973 3.51885016334924

H 0.19988272016387 2.34655435542554 4.62089152147160

H -5.35375606679658 2.87148471160375 -3.03863126811315

N -7.65216504669003 1.56605675303765 -3.22847047006948

C -8.71124619523915 0.80170536797612 -3.17170466442725

N -8.90446182810988 -0.28847061918255 -2.37343568621704

H -9.53907204835339 1.05001634677710 -3.82961218733934

C -7.91398131890690 -0.59916823298643 -1.56901921124176

H -8.04342820968262 -1.46453368926914 -0.92192992013398

H -0.70340926862436 0.26385972241221 3.84866543381620

1 imaginary frequency: -227.14 cm\*\*-1

SP = -1276.679041285940

U = -1276.31586967

H = -1276.31492546

G = -1276.38458940

**16H carbanion**

N -3.48989976725752 0.96241002550337 1.06786726868127

C -2.10626467643212 1.29477448770661 0.91197057329281

C -1.23134101728985 0.22693773541307 0.96856948507302

C 0.24784528560480 0.42127315392650 0.95061395388410

O -1.79807080016796 2.52656098885768 0.76002135686528

S 0.97804185084079 -0.21526201081577 -0.61020945487267

C 2.71092603878118 0.29091414192666 -0.42977919929641

H -1.61642185138815 -0.78553815349679 1.07055127539050

H 0.48252164685533 1.48714925270539 0.97396702638486

C 0.91281057701395 -0.28584621291454 2.13540668223875

H 2.76794881464977 1.34184004650431 -0.13460583344651

H 3.24546352019863 -0.32635528628090 0.29433983410058

H 3.18753766078983 0.17685559638487 -1.40603027040499

H 1.97120658573888 -0.04466589974969 2.24665664145358

H 0.79257077335567 -1.36704164916150 2.04209220720060

N 0.23874994282019 0.10788713313687 3.41612260715435

C 0.44311958790392 1.54459482975077 3.75453002783720

C 0.65107582410224 -0.77419475310181 4.54044184629980

H 0.42658264419539 -1.80700325160362 4.27564641973441

H 0.09681401260091 -0.48258945511423 5.43237714097801

H 1.72220979295224 -0.64765251769755 4.70253258470518

H -0.01561053152203 2.16363146186031 2.98530584670149

H 1.51539744395881 1.73481204801137 3.81450943654811

H -0.03235578577321 1.73953467717595 4.71549477024828

H -0.76625033402414 -0.01784989609569 3.23802581850596

H -3.66788123317939 -0.02429655007026 0.93364481098335

C -4.56683468028718 1.76428303864568 0.67930757767517

C -5.66336354771214 1.18510072251477 0.07427694387142

C -4.60846145743631 3.16163221120551 0.98101057158788

C -6.79590798577528 1.96817447590503 -0.25183078822282

C -5.68894145246009 3.93241353415136 0.64640703615618

H -3.76710669300988 3.60670220703034 1.49388667947583

C -7.95615483599737 1.43672229202417 -0.86635156081108

C -6.81837168015530 3.35181421458405 0.01685119963144

H -5.70476324998882 4.99180520842893 0.88246842671462

C -8.91227014559433 3.49840255959995 -0.87071327261713

H -9.78147855360976 4.09632995254262 -1.12948357334253

N -7.90776983254101 4.11693100205104 -0.30502969408200

N -9.00030133351946 2.17284123225125 -1.17689393278440

H -5.66724330731316 0.12330836281131 -0.15827322187271

H -8.00275724992794 0.37465904349253 -1.09969524762079

0 imaginary frequencies

SP = -1276.702687548405

E = -1276.33845499

H = -1276.33751078

G = -1276.40755874

**16H adduct**

N -3.48461086236712 0.08725177993234 0.26223759305540

C -2.34919615984201 0.74657728763870 0.60271922924658

C -1.62978581547043 0.21548866413210 1.82561616516081

H -1.79711609843536 0.96084473840710 2.61164200153601

C -0.13351428490139 0.05731719074369 1.55896782772180

O -1.93186589146065 1.73083519151279 -0.00933256175352

S 0.08833754737947 -1.29531284854833 0.35542656793842

C 1.71752448904674 -0.87292773976034 -0.30814047189713

H -2.06553420000724 -0.72666375252002 2.16971812548068

H 0.25072528496883 0.96218675253565 1.08567794934435

C 0.66601430002304 -0.27620792812963 2.81521330214818

H 1.70339976999502 0.12823607135828 -0.74346483897535

H 2.49131358132976 -0.93928968642974 0.45866529145087

H 1.93856425985221 -1.59924242882855 -1.09307276740053

C -4.30559445113243 0.41477655767231 -0.84874086506441

C -4.79927153043380 -0.58648259029711 -1.64207392635350

C -5.65742629211069 -0.25664570533600 -2.72022837820114

C -5.99078044917664 1.08534924810259 -2.99062001690707

C -5.46966001019976 2.10130469396282 -2.14946561242708

C -4.65897832620487 1.77001973436265 -1.09733469366891

H -4.54378132567792 -1.62554363414221 -1.45504270876848

H -4.28560024913734 2.54264987700135 -0.43665101602134

H -3.66004005887662 -0.80072371400296 0.71369694703225

H 1.72324629478881 -0.40103988055995 2.57598924435401

H 0.29241000606263 -1.19157178629217 3.27657584456507

N 0.61145473910503 0.78549816741335 3.88045743800859

C 1.01529023432765 2.13341380224855 3.38624507280385

C 1.44800479907311 0.37473706320133 5.04702443112523

H 1.11676989687309 -0.60700315301129 5.38389533024079

H 1.32005243241624 1.11255490239349 5.83821279266660

H 2.48864942251585 0.33789537746756 4.72381522355935

H 0.27396851728924 2.49709995079293 2.67668416404276

H 1.99371355367244 2.04441495608951 2.91252110006669

H 1.06594873411142 2.80600045081117 4.24178902661729

H -5.73883720686561 3.13500230097440 -2.33947068069853

N -6.81347348702226 1.40673403709404 -4.03788739273466

C -7.25816515878731 0.41063228845768 -4.75972987860958

N -6.99598656149679 -0.91734927423287 -4.59431835133508

H -7.91243133182591 0.65589991659059 -5.59139931208601

C -6.20890332441971 -1.22879942399831 -3.58955548294747

H -5.98142210061494 -2.28149724648008 -3.43371672581149

H -0.35267268636373 0.85074979167257 4.21694501349568

0 imaginary frequencies

SP = -1277.210613435970

U = -1276.83168532

H = -1276.83074111

G = -1276.90042464

**17**

N -3.07710543193879 0.13025422904698 -0.16990124194035

C -1.79881892017227 0.61020725030154 -0.21094449288912

C -0.88114625996823 -0.05667396051848 0.75752925468331

C 0.39011472425544 0.32086667150467 0.86154023701556

O -1.43248116202821 1.50398299300224 -0.97309368421333

H -3.24366488717356 -0.63093705261697 0.47613469070869

H -8.61429627232223 0.91080587037717 -2.93803344647323

H -1.28972507322458 -0.85163281144540 1.37659932959374

H 0.79286392957725 1.11896378693554 0.24387926207533

H 1.05943748604824 -0.15863780323370 1.56918451602848

H -6.58327721966764 4.09086231717768 -4.60241149059056

H -3.34465730309650 2.23847867627975 -1.91146728638824

H -7.39998184516629 -0.60360690376433 -1.29024536476376

C -4.19265055272090 0.52288706773976 -0.92701268209321

C -5.36002466089929 -0.28453211627300 -0.75479160396355

C -6.51206026603650 0.00733395152057 -1.42084905656636

C -6.55496235349247 1.12148338402023 -2.30079637172704

C -5.40496468047191 1.91961853311851 -2.46940779130353

C -4.21147284753743 1.61082411431039 -1.77173766384634

N -5.43050140998802 3.00000447465193 -3.31313462314784

C -6.55956750629764 3.23507278196591 -3.93338845821217

N -7.72219929338864 2.53258417138865 -3.84388158023035

C -7.70077159083730 1.49431658637623 -3.03370841054372

H -5.31310660345248 -1.13377621186590 -0.07907204121241

0 imaginary frequencies

SP = -664.519148319434 (-664.51914817)

U = -664.32124243 (-664.32122861)

H = -664.32029822 (-664.32028440)

G = -664.37098702 (-664.37095363)

**17 TS**

N -3.18892639137346 0.01952028137847 -0.06944353600920

C -1.86163576193668 0.44150439369345 -0.03869523961697

C -1.04915063127871 -0.22486074199843 0.94080003537677

C 0.28629962566666 0.08697556589995 1.07494564165557

O -1.45387841170343 1.32813434803299 -0.81819840592625

S 1.87869874852359 -1.06561292034357 -0.39863735253648

C 3.20333893399826 0.08480839834101 0.09202035815488

H -1.48695972280769 -1.04619311575406 1.50129993026525

H 0.66013277538997 1.01406116583900 0.65587033307926

H 0.84245389259400 -0.30412603717543 1.91821412048095

H 3.12426452018261 1.03979315890663 -0.43754576061333

H 3.15650428405750 0.29206468115561 1.16796614669422

H 4.19061230639952 -0.33591358020624 -0.11996327754678

C -4.24768138208369 0.46649520891972 -0.85232793859305

C -5.48587844767701 -0.23284649702899 -0.66344939864403

C -6.60100522671233 0.11152864752366 -1.36469163126219

C -6.54658301655550 1.18028044882531 -2.30125616049689

C -5.33050177950809 1.87173650220732 -2.49164318241290

C -4.17782021328068 1.50850754526648 -1.75826270889114

N -5.26102976519548 2.90619451773348 -3.39060625106319

C -6.36223392506086 3.19978049460650 -4.03688466741656

N -7.57912166739766 2.60233136972320 -3.92818988682960

C -7.64858174287317 1.60634570675570 -3.06546698889054

H -5.51765872954919 -1.04774242500868 0.05412192650312

H -7.53624511939995 -0.42042820619624 -1.21783144311240

H -3.26130431595433 2.05490026691985 -1.91757618245402

H -6.30818457501812 4.01895700540774 -4.74903203697479

H -8.60825995423722 1.10541492666102 -2.95318972146390

H -3.41759430720839 -0.72367511008558 0.57684127854436

1 imaginary frequency: -269.03 cm\*\*-1

SP = -1102.787714358178

U = -1102.54847165

H = -1102.54752744

G = -1102.60678960

**17 carbanion**

N -3.04623679476125 -0.06656965100757 -0.34621557280512

C -1.70868199720461 0.44725640184910 -0.29681679882801

C -0.93670479774127 -0.01983650273010 0.74199949271847

C 0.51209680357766 0.31404859169270 0.84663176645477

O -1.34809986663376 1.26385909234406 -1.21879614884465

S 1.56228432552253 -0.93324985096335 -0.01387457527269

C 3.20168250058041 -0.25738737806516 0.35115719838796

H -1.35979213675701 -0.73325031965476 1.44450570830982

H 0.73299183710908 1.28427086712239 0.39296131973475

H 0.84905085430052 0.33955118736276 1.88729058381250

H 3.31041860985401 0.74659156891690 -0.06717376112968

H 3.37634421586628 -0.22366811400378 1.42977955453008

H 3.94913260905509 -0.91064477532691 -0.10491138166893

C -4.14937292998918 0.40056123405346 -1.01598318463185

C -5.36503238162210 -0.34430603898307 -0.80573237140689

C -6.53060738904643 0.01648799847510 -1.40511785058240

C -6.56817567603238 1.14846181465983 -2.26837267897747

C -5.38018024156583 1.88850387036836 -2.48013456750829

C -4.17553043459178 1.50913570870113 -1.85419233894827

N -5.39954675852096 2.98323185808225 -3.31030286018879

C -6.54728716225678 3.28115644433939 -3.86993414877046

N -7.73650953346106 2.63953244134055 -3.73423638152558

C -7.72225993191720 1.58580028956809 -2.93422821304826

H -5.33158094849273 -1.20761540603245 -0.14671323893008

H -7.44041695127458 -0.55229348824446 -1.23543316559022

H -3.28179571235679 2.08742390809359 -2.03327626381819

H -6.55865029145799 4.14743992422959 -4.52662244956333

H -8.65871693966985 1.04722726597339 -2.80039818279960

H -3.23395688051197 -0.81132494216103 0.31009551089047

0 imaginary frequencies

SP = -1102.810502096137

U = -1102.57019533

H = -1102.56925112

G = -1102.62798480

**17 adduct**

N -3.00224905042150 0.18353603278675 0.11962939880311

C -1.91279716332952 0.91322308754760 0.49256391688465

C -1.02908269536620 0.25219509864483 1.53284878162472

C 0.43432372482551 0.25289908344808 1.10368549191643

O -1.65839614141216 2.03085486299547 0.04789729786889

S 0.65415317023044 -0.80958948064226 -0.35517339371607

C 2.33597703122434 -0.32616200000519 -0.80808203018316

H -3.09000590880440 -0.72803104270695 0.54902415876540

H 0.75197020217820 1.26628538577597 0.84736061136091

H 1.06051996534778 -0.11379064140870 1.91962003207600

H 2.37662860499940 0.73587095453248 -1.06024340053781

H 3.03275805704924 -0.54044527142453 0.00537146936863

H 2.62477521499056 -0.91065591014161 -1.68411411128978

C -4.02641253931114 0.51946527759212 -0.78210609252288

C -5.04155239359178 -0.47326757160951 -0.93969074439774

C -6.09727160009935 -0.26320543294030 -1.77617343813505

C -6.18580987991157 0.95335828965606 -2.50428227940658

C -5.17838761670876 1.92931576171054 -2.35642848215624

C -4.08590907286870 1.70353819434697 -1.48434341568280

N -5.24747551881763 3.10792203732152 -3.05414749505637

C -6.28454125965848 3.26698314394714 -3.83768963135847

N -7.31235829761992 2.39927416214366 -4.04632714611416

C -7.24530062181724 1.26402113481361 -3.38162381352263

H -4.96017983620829 -1.39840284687387 -0.37674983415045

H -6.87255538057431 -1.01395394925492 -1.89446043487431

H -3.32690495921914 2.46420366996748 -1.38455778218279

H -6.34312364721983 4.19985326396814 -4.39154466343909

H -8.05098887466066 0.54727232368050 -3.52775718423758

H -1.13037411969833 0.84214441647583 2.44969486198355

H -1.37152439352651 -0.76264703434693 1.75409035231168

0 imaginary frequencies

SP = -1103.324108089609

U = -1103.06881275

H = -1103.06786854

G = -1103.12687736

**18**

N -3.73049506444843 0.19845382154691 0.08569581076392

C -2.61475601784986 0.86832558736115 0.50650872465172

C -1.88360940816398 0.17102907164003 1.59364312672493

C -0.68651990398928 0.58623443216846 2.00709877249957

O -2.24890685588663 1.94102727623499 0.02333250526541

H -2.34124628497922 -0.72183134581473 2.01379612392798

H -0.25462621815281 1.47581512006690 1.55366741744846

C 0.12464784043594 -0.15549816229745 3.02601548459763

C -4.62222089295943 0.52690209289803 -0.94719467193751

C -5.58007058720421 -0.48840562897577 -1.25746918991830

C -6.50825042593988 -0.29798547731411 -2.23681209604941

C -6.52470323413973 0.92587513673135 -2.95880012900405

C -5.57942614632391 1.92621796556594 -2.65469533280519

C -4.61963536429282 1.72204732253026 -1.63299491865529

N -5.58211600397214 3.11304452929563 -3.34241009861113

C -6.49224003095272 3.25142977323247 -4.27368713872350

N -7.44506568947257 2.35419210159310 -4.64725495514474

C -7.44540705293626 1.21402688421019 -3.98747530067895

H -5.55254812284103 -1.41823626855657 -0.69704042063806

H -7.23651469349968 -1.06740826727385 -2.47367634993335

H -3.90951809480068 2.50457655867498 -1.41318962194682

H -6.49654776649464 4.19029265381883 -4.82054874087453

H -8.19541811113951 0.47471838744440 -4.26129081690926

H -3.90789186193939 -0.68931701424360 0.53727037648382

H 0.89502838172698 -0.74452882033104 2.49436761727455

H -0.52041251060944 -0.86830247740460 3.54543362606807

N 0.75571572512838 0.71786736429271 4.02546841860376

C 1.87372167055444 1.44603715283525 3.41964316104548

C 1.27936856291028 -0.12542864623129 5.10270122561080

H 0.46176966041785 -0.66392036512604 5.58868737727819

H 1.77434918493485 0.49861976681940 5.85090582303902

H 2.00952349374425 -0.86382975566648 4.73037982591287

H 1.52375680467142 2.10458529294080 2.62233734694678

H 2.62636751646292 0.75878544392978 2.99770236736054

H 2.35869450200116 2.06628249340389 4.17728565032655

0 imaginary frequencies

SP = -837.940539079532

U = -837.63400589

H = -837.63306168

G = -837.69498110

**18 TS**

N -3.39474741628927 0.11720404587893 -0.00492229621772

C -2.08248248279143 0.57696941439156 0.12539932003602

C -1.31432540012380 -0.10669299746699 1.12012765705949

C 0.00526974339236 0.22626777831857 1.36095610933613

O -1.66310702590009 1.51231254823446 -0.59112866381301

S 1.56297089203690 -0.77838294334901 -0.23993894475050

C 2.94635346241527 0.35388636882168 0.10945992160676

H -1.76627587753820 -0.95182895468536 1.63357226050889

H 0.36128900418018 1.17367524890620 0.96919326753509

C 0.70581509154417 -0.29177300512974 2.59899866262893

H 2.56743956462165 1.31026895041020 0.49187126834146

H 3.63511505969181 -0.05653524086073 0.85440757945045

H 3.51810530824558 0.56760169665310 -0.79848637536853

C -4.39732495929659 0.52230873302628 -0.87704355001879

C -5.67066272014367 -0.11083077725385 -0.68354154227726

C -6.73477289010940 0.19447233364574 -1.47638736136659

C -6.59294534642831 1.15748801406598 -2.51331175484979

C -5.34099933248167 1.77926795008190 -2.71143252621246

C -4.23994053909139 1.45575719659577 -1.88543408602651

N -5.18471331972557 2.70790779010442 -3.70989513155561

C -6.24097451048906 2.97379464263686 -4.43813575291679

N -7.48621286010031 2.43805819816922 -4.32957205896176

C -7.63827179759095 1.54172107642643 -3.37275488112787

H -5.77034231158363 -0.84358039121771 0.11216422745431

H -7.69682058846033 -0.28581083068938 -1.32413750298013

H -3.29356500804837 1.94494566552402 -2.05633692542821

H -6.11845315595684 3.71052183428369 -5.22765649762979

H -8.62293269522418 1.09238278541942 -3.25849740784079

H -3.65729475400516 -0.61581439225940 0.63999417910502

H 1.79125553287818 -0.15247952621282 2.49759643480266

H 0.51544274629841 -1.36385312999314 2.69253156949991

N 0.23949941189952 0.36081547002824 3.83939548698423

C 0.55150371005926 1.79018350912882 3.79416767623625

C 0.95881417751001 -0.24353145373392 4.96085775856427

H 0.74319184325923 -1.31450734742233 5.00918616706132

H 0.63608438950851 0.21523772635473 5.89934474960227

H 2.05124683199674 -0.11449699551174 4.87071545104665

H -0.02481748378507 2.28276973648041 3.00750119681896

H 1.62400811911168 1.97236852060091 3.60737898938102

H 0.28499758651408 2.25337075159848 4.74779332628190

1 imaginary frequency: -255.92 cm\*\*-1

SP = -1276.208157097691

U = -1275.86044242

H = -1275.85949822

G = -1275.92913607

**18 carbanion**

N -3.63308681138828 0.88041403111067 0.69532818238223

C -2.22389994594354 1.20007860540004 0.62089347433649

C -1.35689719441458 0.22398805185522 1.02429047593090

C 0.11401446845655 0.45926797271964 1.13939791026800

O -1.93654644946862 2.39369082962573 0.22661785491986

S 0.92561956520307 0.00857329196470 -0.45737022929391

C 2.57997620232006 0.72120999163388 -0.24832855844669

H -1.74455057670883 -0.75565934764117 1.29146495188246

H 0.31467981364092 1.52761003938370 1.25698777349577

C 0.77541724117201 -0.33373205375946 2.26875224241831

H 2.50175557215449 1.74500705268507 0.12752186427485

H 3.20428587519209 0.13033639660325 0.42396272258366

H 3.05288923259851 0.74864414315037 -1.23302626273604

C -4.49019648348666 0.95829880306597 -0.38180541060715

C -5.84680642011665 0.53870489526609 -0.17029101018319

C -6.76389857402727 0.59066565499768 -1.17457122981796

C -6.38530629607723 1.07451721100471 -2.45953716555194

C -5.04661510404440 1.47917643477183 -2.67995870631841

C -4.10553482696143 1.41091957396971 -1.63491346703599

N -4.66615779175706 1.93700286225971 -3.91759528751466

C -5.59492268219275 1.98048549481938 -4.84187959981580

N -6.90247289229362 1.62856461366219 -4.73184954277511

C -7.27062353498538 1.18153864547307 -3.54310995157346

H -6.12591298340625 0.17724564581113 0.81555687861276

H -7.78919788270125 0.27261397892124 -1.00854731670239

H -3.08691881311777 1.72387875674033 -1.82462685658347

H -5.29205904801064 2.34340485179254 -5.82069557172254

H -8.31158882756037 0.88822333012033 -3.41954597082695

H -3.87818017476923 0.17135496540132 1.37311104909737

H 1.86272598732350 -0.14780796888832 2.24716926424545

H 0.62617504532204 -1.40115485680830 2.07625792615837

N 0.25715001484113 -0.03945355485762 3.61275041166154

C 0.43993313501266 1.37582063869039 3.93332486914212

C 1.01054608145608 -0.84644575915386 4.57205891936966

H 0.89386356501988 -1.90836072930569 4.33798326337007

H 0.63321244023088 -0.67369545871021 5.58363218654533

H 2.08829573387092 -0.60725951315298 4.55936926864821

H -0.20073232753910 1.99955062056006 3.30589615607187

H 1.48670200713851 1.69982961802675 3.79803960727135

H 0.15961466001764 1.55076224079092 4.97551988481905

0 imaginary frequencies

SP = -1276.229085751903

U = -1275.88000551

H = -1275.87906130

G = -1275.94752682

**18 adduct**

N -3.47737236623073 0.25534720288642 0.27369381639161

C -2.42680632678204 0.98542445386540 0.74431289846039

C -1.68159471245418 0.37536840009011 1.91125602242314

H -1.74853058685893 1.09493133913631 2.73100667378527

C -0.20674871523729 0.15169758655399 1.57150816634854

O -2.09676574736878 2.07462129108984 0.27597587839140

S -0.10250786139484 -1.14212273223337 0.28595259884486

C 1.51994756474948 -0.77120426436995 -0.42315427917797

H -2.14793700240774 -0.55715652286540 2.24260692123154

H 0.19624245237009 1.06005200295873 1.11869121308582

C 0.61872181740368 -0.25110958728483 2.79329885803589

H 1.54387355293539 0.25071555096800 -0.80770773693852

H 2.31752292223482 -0.91416281892952 0.30755562957968

H 1.67374881160765 -1.46509259439726 -1.25243899644316

C -4.28806217028525 0.56831749230494 -0.83681490886158

C -4.77417126283867 -0.53255310247527 -1.59997932998052

C -5.58100255381748 -0.31950816910113 -2.67999595976040

C -5.94307048608570 1.00567386792022 -3.03906176304174

C -5.46744886143254 2.09383788345662 -2.27785450536539

C -4.63106062094914 1.85958432473317 -1.16165553396770

N -5.81940791887762 3.37816569708472 -2.60501332758794

C -6.59964017896398 3.52498097869117 -3.64538605506490

N -7.10819432045741 2.55084736995500 -4.45087482694948

C -6.77449325484918 1.31698506928350 -4.13740666445606

H -4.48538608440701 -1.53862137623197 -1.31068869350384

H -5.95242284131446 -1.15072472491077 -3.27153243962401

H -4.28943585200813 2.70087677099881 -0.57476613123529

H -6.88173922279777 4.54057822153400 -3.90880364040956

H -7.16560590107635 0.51541249670391 -4.76088174074600

H -3.55323577251429 -0.69118854115671 0.62344999168555

H 1.65798162674618 -0.42699611154812 2.46719377999352

H 0.23283466526218 -1.19969818807433 3.17912282442111

N 0.59280735398835 0.72708707089389 3.88691177605504

C 1.13187102910446 2.01286208074735 3.44384306116229

C 1.41402616293745 0.21201570232944 4.98229880406954

H 1.01961086505237 -0.74949208286619 5.32290015544756

H 1.39167878063378 0.91066122572506 5.82286192420555

H 2.46558662337791 0.06718438831956 4.68005586360396

H 0.46708365957049 2.48488017759670 2.71678917211415

H 2.13140738729848 1.90765820741984 2.98723282476094

H 1.21532534613685 2.68429396319811 4.30228767901667

0 imaginary frequencies

SP = -1276.742293153132

U = -1276.37892537

H = -1276.37798116

G = -1276.44755935

**18H**

N -3.60965666621047 0.08502349625742 0.01150654390623

C -2.38915088182537 0.62869622323388 0.28639581335377

C -1.68351975870659 -0.04312453448246 1.41701864087404

C -0.44948987682857 0.32116516857261 1.75425404075032

O -1.90902813205739 1.57993474642917 -0.32761204338938

H -2.20576654482420 -0.83576779306600 1.94685693221899

H 0.04728755275290 1.10817398601787 1.19354530318082

C 0.30788410751411 -0.34115521261636 2.86406178656749

C -4.54988012656144 0.47181843977843 -0.95791444334065

C -5.70217559564883 -0.36854548690397 -1.05318928389691

C -6.69267307955983 -0.09010059022943 -1.94670164226109

C -6.57955428165808 1.04631056097935 -2.79213273481470

C -5.44205501524134 1.87390401619435 -2.69942922724588

C -4.41707388239282 1.57725411799055 -1.76849204872429

N -5.31907600955904 2.97589255803394 -3.50593799750541

C -6.30010390101806 3.20360768567679 -4.34285986529766

N -7.43680091529659 2.47411972167687 -4.51318765256923

C -7.55642484197197 1.41393741371104 -3.74089231680635

H -5.77334965916446 -1.23245561980126 -0.39902779272526

H -7.56965061564924 -0.72553792029052 -2.02226026239982

H -3.55638173375335 2.22572891087864 -1.71205181129884

H -6.20709540023184 4.07674428194627 -4.98267715833731

H -8.45353530574809 0.80833460065434 -3.85247800347551

H -3.87874664825819 -0.71017686051018 0.57680402257797

H 1.28768227939514 -0.68305592818574 2.52148365294861

H -0.24870915966035 -1.18513071900365 3.27206724293153

N 0.57056740612673 0.59794139453488 4.01003786836051

C 1.37835873320583 1.78697508080480 3.60932078667127

C 1.22194615480888 -0.13280154468668 5.13591078588020

H 0.58403237420391 -0.96701920819857 5.42603644078246

H 1.34828924562974 0.55810191117017 5.96852895833752

H 2.19040333172602 -0.49468444022910 4.78971607097194

H 0.81705932745186 2.37992445009421 2.88959505641155

H 2.31165828204744 1.43121880945434 3.17191607607803

H 1.57576420485179 2.37861151921134 4.50235817042287

H -0.33748896788819 0.93610076490263 4.34188309086218

0 imaginary frequencies

SP = -838.408472982961

U = -838.08604624

H = -838.08510203

G = -838.14727017

18H TS

N -3.14469834278856 1.20325710877386 2.33045507967783

C -1.83813274590332 1.69153189959159 2.46967025366596

C -1.02803165327592 0.93532172428030 3.38704587756255

C 0.31406400331826 1.23707526083888 3.53927439479436

O -1.45832106260633 2.68452269652483 1.83004866477208

S 1.66337538226677 0.21419644058956 1.88264351405390

C 3.22286349671821 1.11619786403595 2.16161727674544

H -1.44126750919520 0.03913415282666 3.84166103101005

H 0.64612245793557 2.21241991882045 3.19229743119155

C 1.09647608321184 0.69402428645319 4.71088598817403

H 3.00993627680308 2.10770655736863 2.57741937930168

H 3.87762180336007 0.58440316547615 2.85778912236445

H 3.76069923749587 1.25579278380734 1.22057284902593

C -4.10317253605441 1.54123571952071 1.38310978012654

C -5.22799316783250 0.65446725506134 1.29604112977698

C -6.22332880288135 0.86301807621088 0.39051485222951

C -6.15197694647041 1.97451955136896 -0.49474542747013

C -5.05100133696206 2.85707227423175 -0.40685968864505

C -4.03276986877283 2.64448825505239 0.55178497562449

N -4.96489001547060 3.93337480871890 -1.25282579948879

C -5.93346868321644 4.08484389093748 -2.12215822746686

N -7.03079957143134 3.29757224794736 -2.28761941548460

C -7.12155248635232 2.26265287545540 -1.47526184722194

H -5.26963975765519 -0.19818475353601 1.96849874314342

H -7.07052016601655 0.18583398723439 0.33039574250765

H -3.20135349000690 3.33076072284072 0.60195305276956

H -5.86291648404547 4.93698118395819 -2.79536217882330

H -7.99006704658135 1.61353355332852 -1.58279145911578

H -3.34534009546380 0.36578006600729 2.85827554932530

H 2.16749029797559 0.75385700781002 4.53528045582369

H 0.82341949774288 -0.33496180305292 4.95081626461746

N 0.84482414758450 1.51416157566045 5.96546645951755

C 1.95982284226110 1.32809141606061 6.94236138786288

C -0.47021884108888 1.21916854338961 6.60821784425046

H -1.26114262381662 1.39457012138671 5.88299985161405

H -0.58296027861939 1.87604060957807 7.47049902017820

H -0.46043666371092 0.17476636894998 6.92246119504569

H 2.00433952840812 0.27043567557981 7.20502704863698

H 1.75074213421088 1.93157972164047 7.82511259293115

H 2.89052063460763 1.64596801960221 6.47364652402840

H 0.84283235231834 2.49810916966927 5.68790071136658

1 imaginary frequency: -317.60 cm\*\*-1

SP = -1276.678743033517

U = -1276.31597438

H = -1276.31503017

G = -1276.38481393

18H carbanion

N -3.51433688647510 0.74891256131963 0.66275919288060

C -2.12158008395900 1.10309079841375 0.57800937616554

C -1.22528452656668 0.14320471149556 0.97784573861689

C 0.23613254712083 0.43358732185397 1.08117461828026

O -1.85584073694747 2.29411327999803 0.18509560354879

S 1.12998427374356 -0.18229147550796 -0.40109424128933

C 2.77818937790906 0.52680899953265 -0.13666887138449

H -1.57332033183945 -0.86005531805843 1.21232031501609

H 0.40257986300806 1.51297349851526 1.09204625939518

C 0.84275556473233 -0.20982641179580 2.32698236577484

H 2.69313171323548 1.58452036407287 0.12593267646551

H 3.33461936092298 -0.00317897006396 0.63821892843589

H 3.32461227458341 0.44456902643066 -1.07896189006340

C -4.41568975198842 0.89033542464353 -0.37508596862774

C -5.75168919260056 0.42135988818023 -0.14037710580202

C -6.70971348530014 0.51922446795958 -1.10267297194733

C -6.39443758401254 1.09772497298786 -2.36484350951528

C -5.07656412148897 1.55146504749547 -2.60746519551400

C -4.09341535095499 1.44044675733280 -1.60520845579070

N -4.75562218881405 2.10040013405177 -3.82465912462479

C -5.71899727837600 2.17542846574355 -4.71038102009296

N -7.01083254845879 1.77438828745436 -4.57813412866106

C -7.32223089796691 1.24274797677476 -3.40878061944147

H -5.98191963851013 -0.01555939838711 0.82731583563927

H -7.71952971664363 0.16323646856188 -0.91990404264619

H -3.09165814108623 1.79250477992921 -1.81263782133263

H -5.46399027538872 2.61153644058653 -5.67282282402368

H -8.34866281112700 0.90886018413795 -3.26828340280223

H -3.72486679852848 -0.01062545822029 1.29620295601514

H 1.88687798594995 0.06480489439291 2.48535102049370

H 0.75674229617592 -1.29636690590008 2.26712887395249

N 0.09512259547786 0.21029069909825 3.55858767762418

C 0.24637993547702 1.66394777684545 3.84980893974340

C 0.48731063384015 -0.61716457883977 4.73164855368964

H 0.30733575195165 -1.66545483846933 4.49514122792091

H -0.11317663016515 -0.31253623352667 5.58839257895031

H 1.54615818517893 -0.44873493184854 4.93184376969715

H -0.20392625452666 2.24006153187857 3.04308087289800

H 1.31025969721889 1.88744563622802 3.93641966131549

H -0.26595577921092 1.87938369261721 4.78702922939468

H -0.89725104559004 0.04338043208563 3.35640492164536

0 imaginary frequencies

SP = -1276.706716956142

U = -1276.34241977

H = -1276.34147556

G = -1276.41134770

18H adduct 1

N -2.80621684145296 -0.40471793981601 -0.34294161049022

C -1.80978052053591 0.05550653430833 0.45819241466987

C -0.89831795122159 -1.03726309589800 0.98160603685891

H -1.46224499077855 -1.60717424593634 1.72866559579064

C 0.41709866873315 -0.54321321985376 1.59072703859129

O -1.67244608850528 1.24966504711340 0.73715851307219

S 1.56749030216142 -1.93871547232417 1.84992750451876

C 1.89000644659170 -2.42887546934936 0.13988387785796

H -0.69580484721628 -1.71838082861764 0.15204093176320

H 0.91037584099976 0.14147145565111 0.89596192378083

C 0.24742010334184 0.11693297583055 2.96726168012647

H 1.03610225164615 -2.93752796284249 -0.30999933656416

H 2.16765244503586 -1.55720667359463 -0.45688015201213

H 2.73412648892666 -3.12121426056391 0.16721275296722

C -3.85818920375782 0.30539281398149 -0.94968527159244

C -4.68709387387240 -0.46934446042124 -1.81816611986060

C -5.74559842475774 0.10200772997265 -2.45919943867501

C -6.02979725638736 1.47984260601388 -2.26050310482141

C -5.21365634935044 2.24309441336071 -1.40117713334807

C -4.11321142820519 1.64227439788311 -0.74239442639244

N -5.47709695809071 3.57251061007124 -1.19389733706265

C -6.50678410965163 4.07273220538851 -1.82960302814533

N -7.35424409071702 3.43043641114760 -2.67968713917637

C -7.10384456854769 2.15311518804375 -2.87968082866380

H -4.45673425839608 -1.52136692476426 -1.95808187301685

H -6.37725129114437 -0.48253289630781 -3.12107484430871

H -3.50309062742791 2.24557241374966 -0.08798557548237

H -6.71986490923972 5.12570016961352 -1.66735157758792

H -7.76328168439581 1.60996429829039 -3.55372689822207

H -2.79162499959458 -1.39850930061280 -0.53710260802848

H 1.13364050087449 -0.01553435720672 3.59064887661051

H -0.61039749516946 -0.31288641710935 3.48685704487477

N 0.01946925829497 1.59467477985298 2.87704297661936

C 1.27384492693352 2.34185021125334 2.58669094878751

C -0.62806827431483 2.10863607546120 4.11417589438291

H -1.59593345482397 1.62119356111215 4.22968413550767

H -0.75698708352016 3.18625978543673 4.01525798068349

H 0.01608344865182 1.88080716615170 4.96461938833215

H 1.72765484169944 1.95633453996562 1.67479096943925

H 1.95317210542922 2.21459253046001 3.43034049635984

H 1.02362226439116 3.39443364792483 2.45641006225880

H -0.63313231263562 1.72964795718004 2.08333025959740

0 imaginary frequencies

SP = -1277.212340218465

U = -1276.83360526

H = -1276.83266105

G = -1276.90251249

19

C -1.95643331769231 0.46895154493548 -0.43753003084148

C -0.93811380469178 -0.30210343293785 0.34388513546096

C 0.21228183165059 0.26179007870108 0.70229287020617

O -1.58382679834345 1.33153200654952 -1.25709874950981

H -6.15628205252651 0.47669444706779 -1.98728310373924

H -4.93004524916782 -0.77109978326301 -2.22677808090451

H -1.14830407069799 -1.33665564680323 0.59389526786850

H 0.43375196023669 1.29873733278787 0.46432041941581

H 0.96072018511713 -0.29937865699706 1.25398839257875

H -6.67242224371708 -1.64041583609931 -0.69377255281312

H -5.21447339635578 -2.12368748561382 1.32360124492560

H -4.23098084898695 0.11498174031266 1.59897510269857

N -3.25793052390463 0.17448910048446 -0.24278760467256

C -4.29895543617418 0.88001779205845 -1.00017135863155

C -3.77532659940730 -0.59587127112600 0.89720397335827

C -4.82285740310870 -1.60704529818561 0.44147708433742

C -5.94773029098109 -0.90825872755893 -0.32391776051419

C -5.37035128932520 -0.09532167414481 -1.48369083129327

H -4.74844340221705 1.63901610757676 -0.34636186708525

H -2.95907309658561 -1.08763051891897 1.42004887351606

H -4.34548842757076 -2.36029005194815 -0.19687738890837

H -6.48356121773781 -0.23593199888351 0.35897132089465

H -3.83042450781228 1.39156023200622 -1.83820035634741

0 imaginary frequencies

SP = -442.984776408718

U = -442.77092764

H = -442.76998343

G = -442.81435283

19 TS

C -1.92479734813582 0.30001689352226 -0.21161633263294

C -1.04938467036433 -0.23967933048012 0.79629256555737

C 0.26120129860095 0.19914480145772 0.89042271581512

O -1.51865173095054 1.16148478890408 -1.04314486822953

S 1.91327320606796 -0.87363803148178 -0.49384702117998

C 3.25163974918983 0.04338947014478 0.33296708135130

H -1.36073591756501 -1.07749196331954 1.40541330197903

H 0.53817739277670 1.14889207284529 0.44744967152309

H 0.84295688139901 -0.09221306840704 1.75813224224871

H 3.10126118661184 1.12508129693993 0.24399952017460

H 3.30223303506380 -0.20462516503670 1.39892600598989

H 4.22208885943768 -0.19585728458619 -0.11123945423525

N -3.23688663128215 -0.14697122004073 -0.30496806370017

C -4.14936855663986 0.66001930996365 -1.12796705331366

C -3.89645218723617 -0.76192064083100 0.85604837604812

C -5.12365265820514 -1.57334856065092 0.44944839002300

C -6.10457986450379 -0.73290118789637 -0.36365586105850

C -5.37697775731113 -0.13273381777415 -1.56395712486617

H -4.46787325757105 1.54631004848403 -0.55667372741041

H -3.19883629807683 -1.41914822181736 1.36803167552806

H -4.80290252977569 -2.44008093592566 -0.14165381562402

H -6.50023989417364 0.07612038189874 0.26487250910740

H -3.60467606903686 1.01121763754197 -2.00140854775742

H -4.19505958322411 0.02572310521241 1.56510548947949

H -5.59643011379898 -1.95707389719338 1.35964443427298

H -6.95661059120824 -1.33874835985604 -0.68911626675655

H -5.06651499759351 -0.93484260598236 -2.24508825523559

H -6.03585095249471 0.53627448436450 -2.12772758709800

1 imaginary frequency: -251.00 cm\*\*-1

SP = -881.248483440807

U = -880.99291820

H = -880.99197399

G = -881.04353121

19 carbanion

C -1.82047381958575 0.23191856171204 -0.48221651449690

C -1.06050431408407 0.03852831881242 0.65003147885058

C 0.37649600354429 0.43895882299948 0.71462510553683

O -1.41484467527846 0.87926289928701 -1.53397299851684

S 1.48976652525464 -0.93910277847903 0.20832940738091

C 3.09634773814073 -0.15946420081233 0.50503937220964

H -1.45243471179791 -0.50657512646567 1.49868216431067

H 0.59595977475355 1.28604068807332 0.05968821552596

H 0.67076374811968 0.71230084773586 1.73291215986615

H 3.22106692640040 0.72728501390710 -0.12201368291154

H 3.20296566909063 0.12146188269655 1.55628596545068

H 3.87855512649878 -0.87925684192901 0.25322350667446

N -3.14870290186334 -0.30547910313918 -0.57497581613179

C -4.13111727408500 0.69098269060687 -1.03141206097024

C -3.65132981540550 -1.03859109075323 0.58798501189739

C -4.97577582755422 -1.73435387965318 0.28118936684045

C -6.02653841448828 -0.74023725807359 -0.20905716744189

C -5.46770279379680 0.05102510435708 -1.39102124494395

H -4.29158863364886 1.44192673875527 -0.23596827236935

H -2.91239984245810 -1.78882989693386 0.87419331192846

H -4.81032654650767 -2.50267488113917 -0.48460704288713

H -6.27572682869559 -0.04565695704789 0.60436188785715

H -3.71790833604789 1.21021513119437 -1.89440544336660

H -3.78662665867873 -0.36082992423587 1.44907355156689

H -5.31810464609984 -2.24825342757153 1.18605725721500

H -6.95071946006638 -1.25817938857987 -0.48712062219076

H -5.32983515327455 -0.61584804049802 -2.25146183312447

H -6.16482885838574 0.83841109517407 -1.69836006375976

0 imaginary frequencies

SP = -881.270096922048

U = -881.01355875

H = -881.01261454

G = -881.06426733

19 adduct

C -2.09077969316017 0.75134983145320 0.19103091505064

C -1.22479346600878 0.04636056084039 1.22587317355263

C 0.26908310959046 0.13804643304214 0.94612453648998

O -1.58050952917590 1.43541227219207 -0.71131277839395

S 0.77276122159332 -1.08081198827343 -0.30568707294539

C 2.50852915289753 -0.60323165601242 -0.47398796499026

H -5.33587998154757 0.24783978843177 -2.44812750470819

H 0.53977193604849 1.13663308662879 0.59770964501502

H 0.82120292342257 -0.07065107663170 1.86549299003851

H 2.59347411102896 0.42072195159040 -0.84545154262871

H 3.02835275470721 -0.69283674693247 0.48293944499592

H 2.97296037793526 -1.28086698815676 -1.19333470172818

N -3.43367591469776 0.65584490043214 0.33642615018204

C -4.30709742809378 1.10101684685811 -0.75816607067804

C -4.08058642651589 -0.35437559392126 1.18622414824082

C -4.42129976344656 -1.59346562699633 0.35995519688031

C -5.29868320458095 -1.21269893695369 -0.83701987338573

C -4.65857320830202 -0.08590430086970 -1.65510707706202

H -5.21367209113659 1.51725248124417 -0.30670727876519

H -3.45235184382062 -0.59176149198486 2.04182041307149

H -3.48786842643121 -2.05266125718339 0.01009950804452

H -6.27667781179013 -0.87608112663338 -0.46831346849796

H -3.80934726776085 1.89425303925530 -1.31200720029209

H -4.99839446188136 0.09739689411135 1.57732163165416

H -4.93163493495545 -2.32372821355592 0.99658479386346

H -5.47643450819341 -2.08761792194061 -1.47054085969432

H -3.74016486355658 -0.44771005087014 -2.13417785056641

H -1.43739691820311 0.50477292486898 2.19770579324302

H -1.52808384396499 -1.00107803403273 1.30919290401392

0 imaginary frequencies

SP = -881.790694183671

U = -881.51978418

H = -881.51883998

G = -881.57086532

**20-29 (Shuhua)**

20

N -3.18504309636931 -0.04994906520053 -0.01035670470469

C -1.92063464373491 0.39805920057888 -0.00376948520627

C -1.01889891124107 -0.26194339857452 0.98545437171522

C 0.24654862734428 0.11904863829954 1.13338616974766

O -1.53505880773380 1.29877337877913 -0.76969553073635

H -1.44430914680345 -1.06331755131575 1.58477649983445

H 0.66598204553688 0.92372996079977 0.53554822721559

H 0.89512231817142 -0.36281585003201 1.85881099251247

C -4.19671272667995 0.50112810223574 -0.89935630370909

H -3.44394514647145 -0.77644433608595 0.64099958029790

H -3.90011156915618 0.38254960657259 -1.94452284360668

H -4.35586119056823 1.56380243368262 -0.69726582697428

H -5.13007775229420 -0.03562111973950 -0.73200914638593

0 imaginary frequencies

SP = -286.810338130889

U = -286.69469625

H = -286.69375204

G = -286.7317865

20 TS

N -3.17344438441652 -0.18431125942295 -0.10954869041333

C -1.88098611129200 0.27852855885097 -0.05254484430124

C -1.03691424441634 -0.27848473884981 0.96644015006910

C 0.29969107011968 0.07716598352140 1.06487558393277

O -1.50177609665404 1.14302994137788 -0.89315232560092

S 1.85992076762014 -1.07529084122555 -0.30404263489017

C 3.17180743242354 0.12097265113431 0.09730011063183

H -1.44057894928968 -1.08530871029166 1.57311857650652

H 0.62614355900812 1.00748691256851 0.61170871316766

H 0.85408451395124 -0.21642791632528 1.94943898918501

H 2.96901310517877 1.09896678836122 -0.35169993496220

H 3.25676825046015 0.25728034182481 1.18153223992824

H 4.14186017858164 -0.22312617100423 -0.27237783290408

C -4.18848909851188 0.51827348906927 -0.87874992663697

H -3.49315395830076 -0.69886465249467 0.69785770900849

H -3.92925428395203 0.53268462765119 -1.93948742304974

H -4.32318860922324 1.55284508692277 -0.54107667073686

H -5.13550314128676 -0.01142009166819 -0.76559178893410

1 imaginary frequency: -295.62 cm-1

SP = -725.073220992461

U = -724.91569609

H = -724.91475188

G = -724.96008648

20 carb

N -3.03667900064847 -0.39115371396538 -0.48246357457306

C -1.73269852850514 0.18558012309170 -0.40388679606054

C -0.94850475792309 -0.13341488411670 0.68344067611390

C 0.47881590941515 0.28453630959895 0.78083669906973

O -1.38700282806100 0.94718478989416 -1.39087489202965

S 1.62233881141206 -0.98786477098172 0.08903500385611

C 3.20990664534870 -0.17637771775219 0.40305251713273

H -1.34538994593029 -0.80266739395246 1.44351967826109

H 0.66268934039685 1.20904744215664 0.22667800024518

H 0.78876879028716 0.44332435255774 1.81845572757400

H 3.26943788798537 0.77936788405089 -0.12437359439214

H 3.35721844656273 -0.00995429408109 1.47348790895886

H 4.00651381825671 -0.82811908810519 0.03684419651715

C -4.09727964068849 0.50177257695003 -0.95112665501335

H -3.28840151749932 -0.79221509769122 0.41334652935283

H -3.92625631673483 0.78492598994624 -1.99069045016594

H -5.05239712206645 -0.02597612406663 -0.90049009791113

H -4.17807999160763 1.42100361646622 -0.35279087693579

0 imaginary frequencies

SP = -725.091837596543

U = -724.93362085

H = -724.93267664

G = -724.97910282

**20 adduct**

N -3.02169041103466 0.10920090782664 0.18766552409853

C -1.95463010671014 0.84849845602038 0.51700919626912

C -1.01322982665182 0.26671560891797 1.55254816463056

C 0.43544274664106 0.28973158924512 1.07680522043342

O -1.75098041342938 1.96770239398867 0.01475505277761

S 0.65099280655163 -0.83170874354737 -0.33786338225046

C 2.33408924559989 -0.36856141238743 -0.80706526797132

H -3.12415713867873 -0.80475281299185 0.60238878524872

H 0.71481890774243 1.29937387069438 0.76631126218839

H 1.09795242298327 -0.02160595850009 1.88739062237690

H 2.37620339451341 0.68174209537969 -1.10447825849734

H 3.02864500531446 -0.54715709553049 0.01699728659667

H 2.62593648087531 -0.99000920641537 -1.65622098832634

C -4.00448195213513 0.56123240341280 -0.78685669542582

H -1.09843041416284 0.89310839199775 2.44661483584076

H -1.31730438887517 -0.74685118859978 1.82961157526376

H -3.54510794388774 0.70061475051258 -1.76911117078335

H -4.78463142428335 -0.19575010335152 -0.86354404287235

H -4.45543699037251 1.50547605332794 -0.47195771959749

0 imaginary frequencies

SP = -725.615154450200

U = -725.44251265

H = -725.44156844

G = -725.48827215

**21**

N -3.16347089692454 -0.12005372201784 -0.09438510716497

C -1.98016175693730 0.47528809827706 0.09634743956357

C -1.07108290723212 -0.22312967864347 1.05962930614080

C 0.13507766483278 0.26731384809354 1.30894833466816

O -1.65663388684732 1.52588202760238 -0.47720209146173

H -1.43680868439146 -1.12556190758371 1.54098738219798

H 0.50672847064510 1.16842941773067 0.83099014215093

C -4.16658879922255 0.43876606822311 -0.98990322112532

H -3.37141394428122 -0.96871726148425 0.41194564758756

H -3.76533876537726 0.54013718341687 -2.00112483895032

H -4.49445760033306 1.42111558378174 -0.63999116725381

H -5.02140455974215 -0.23628033977030 -1.01161706952641

C 1.08356055496417 -0.36059424471931 2.27556626005741

F 1.43787149468893 0.51776960572282 3.24411292802547

F 2.23477328377413 -0.73984348949150 1.66964243588495

F 0.59135033238391 -1.44952118913781 2.89505361920571

0 imaginary frequencies

SP = -623.994264445643

U = -623.87027489

H = -623.86933068

G = -623.91652

**21 TS**

N -3.36502754451394 0.01110491521180 0.01578495137771

C -2.10267660402592 0.47593691209384 0.19572002628701

C -1.30427602502612 -0.20242487675250 1.19723620043112

C 0.00027507822745 0.15873549570627 1.41008761242664

O -1.68739704426962 1.44641573316514 -0.48917316180054

S 1.59895909074104 -0.87077229148442 -0.13209549234248

C 2.90725322220057 0.39511016619380 -0.08023205698542

H -1.73127804983745 -1.06844569481579 1.69370160048628

H 0.36405178076595 1.12081302703466 1.06621125037913

C 0.64527492141363 -0.29069979506670 2.69103091885380

H 2.49617592250862 1.35509775482187 0.25512583509845

H 3.71635517492310 0.11858516575797 0.60154993571663

H 3.33692750376384 0.55408989611399 -1.07401543526723

C -4.29035736997471 0.61765250784288 -0.92507196715132

H -3.67899847897516 -0.75910561353834 0.58544644337761

H -3.90056430014521 0.57827855657635 -1.94631723299912

H -5.22842216516403 0.06291303883083 -0.88891563126637

H -4.49177506277882 1.66277089215409 -0.67049972263224

F 0.05901059621114 0.34230811862578 3.75524549396022

F 0.50767485406428 -1.61168136155571 2.93593064481878

F 1.95681449989138 0.00231745308417 2.79324978723133

1 imaginary frequency: -194.19 cm-1

SP = -1062.261861176438

U = -1062.0959178

H = -1062.0949736

G = -1062.14755823

**21 carbanion**

N -2.92647591363330 -0.39857157550773 -0.50769111172713

C -1.65560506112089 0.19295838737613 -0.28135295154109

C -0.93701004951857 -0.22900703287178 0.82145951115584

C 0.48283421923225 0.18609299562249 0.99639767880746

O -1.25763214767804 1.05945075896253 -1.14675175608324

S 1.62711715593020 -1.07718901133128 0.29649512576766

C 3.18684867212495 -0.17339025649744 0.09314148536663

H -1.33757208412639 -1.00414711589869 1.46784359447859

H 0.68070030318809 1.12289782623982 0.46844234152030

H 2.99167625610566 0.82006227332313 -0.31801599665713

H 3.73945171676227 -0.08537643063605 1.02836363804001

H 3.78752453470107 -0.73547306186619 -0.62579603813822

C -3.97054254380498 0.48509859416891 -1.02551207511602

H -3.24386505389256 -0.88205470557726 0.32386618934580

H -3.71899254832339 0.82603892107227 -2.03068102129903

H -4.90600758780554 -0.07541796655634 -1.08557439806479

H -4.13529697035464 1.36810882768892 -0.39198866283273

C 0.80001746092487 0.45001852043231 2.45590165747420

F 0.07882952809210 1.49099854145840 2.94250167070045

F 0.53285172911247 -0.60760004949123 3.25790524499160

F 2.09914838408438 0.77150155988907 2.67604587381085

0 imaginary frequencies

SP = -1062.283572215095

U = -1062.11711394

H = -1062.11616973

G = -1062.16997221

**21 adduct**

N -2.95170882175349 0.10658477585010 0.15173694005757

C -1.83302257523147 0.75612704160341 0.49089677852500

C -1.01807984908017 0.14212904466832 1.61379564026843

C 0.46430335724776 0.11796474563008 1.24229327939574

O -1.48639012391915 1.81599827018521 -0.05396440529287

S 0.73843935269549 -1.03153456706403 -0.13859559646407

C 2.08664401528788 -0.19558457764826 -1.01064609668358

H -3.16373364476925 -0.76658700295815 0.61090084099540

H 0.78260433614165 1.11514354968779 0.92884123266328

H 1.78044490527943 0.80831104355212 -1.31022839737681

H 2.98805803909152 -0.15272632210722 -0.39924745413728

H 2.28988776462313 -0.78817892542171 -1.90526577728298

C -3.84484683168692 0.59370926057719 -0.89056544433944

H -1.16565752578087 0.77094003689888 2.49737509329998

H -1.37785746544319 -0.86189138181412 1.85139480507329

H -3.33826051061189 0.61532788170536 -1.85911336547169

H -4.69854849515196 -0.08074162703622 -0.95112687905879

H -4.20134905350277 1.59932811199438 -0.65536188727114

C 1.31706173257289 -0.25029443214360 2.44258689549084

F 1.01624792463989 -1.46592260761873 2.94905361619738

F 1.16003500177846 0.63723624166702 3.45339823894816

F 2.63472846757305 -0.26533856020782 2.14784194246358

0 imaginary frequencies

SP = -1062.801257999021

U = -1062.62038229

H = -1062.61943808

G = -1062.67406772

**22**

N -3.17772157081411 -0.08140643115999 0.07498167509156

C -1.92604904466275 0.40153516559071 0.02496175047696

C -0.97866285165335 -0.18891658217375 1.01549551491840

C 0.28529477777471 0.21753050843028 1.09021932802414

O -1.58776808225681 1.27363168813601 -0.79346318671895

H -1.36784399474938 -0.96092081036732 1.67531345123497

H 0.66747589459276 0.99065125224127 0.42910916554319

H 0.97053834777185 -0.21322739285647 1.81402814014546

C -4.23424138894506 0.39339712900547 -0.81939337858829

H -3.41209286332228 -0.77147382029691 0.77535340022673

H -3.86009868175340 0.37080700770918 -1.84539327071446

H -4.48097471447303 1.43110148588622 -0.57478676486457

C -5.45489802412944 -0.48371447334093 -0.68664184834415

C -6.37643537885605 -0.25521412331263 0.33819672114627

C -5.65664952615803 -1.55550758665177 -1.55743117659073

C -7.48511958885985 -1.08483480605459 0.48942269590434

H -6.22406148850477 0.57998790860265 1.01711027625216

C -6.76713146561771 -2.38515021505052 -1.41086821630088

H -4.94219666573543 -1.73767850109934 -2.35587998195649

C -7.68228093719318 -2.15213394234273 -0.38584863565802

H -8.19617903310163 -0.89646051082684 1.28844005690239

H -6.91720709464251 -3.21398196233169 -2.09641243817523

H -8.54769662471051 -2.79802098773631 -0.27051327795479

0 imaginary frequencies

SP = -518.030889799618

U = -517.82886014

H = -517.82791593

G = -517.8765626

**22 TS**

N -3.16594145942787 -0.14398774199677 0.07302161409221

C -1.89229195835925 0.37043919324341 0.04448813792305

C -1.00571863864978 -0.04521958574084 1.09480687994800

C 0.34031867986494 0.28462161905758 1.06910746483924

O -1.56285329395404 1.14515706815858 -0.89730414634709

S 1.76562735302532 -1.14213031856431 -0.19561162587306

C 3.19557527234120 -0.03613473377450 0.01590472343857

H -1.38047633201806 -0.76646579102035 1.81698465393699

H 0.66369820751466 1.12619309334006 0.46567769469458

H 0.94286061297488 0.09966039522396 1.95155740134184

H 3.10456302938412 0.85949843134531 -0.60736566683979

H 3.28294084950352 0.28619032755309 1.06003318308425

H 4.12659238433155 -0.54191465286877 -0.25537732547466

C -4.23470444433555 0.39918026137581 -0.76152739386010

H -3.45254505647839 -0.60186264802194 0.92694054249584

H -3.88314053377712 0.44566024245407 -1.79333953970750

H -4.49274039515669 1.41922939577467 -0.45096068950845

C -5.45217479758479 -0.48988992442046 -0.67356035773333

C -6.37702514064259 -0.31983063140146 0.35936527171563

C -5.64759706481310 -1.52022765712261 -1.59567819917768

C -7.47878995892061 -1.16622855045417 0.47059553726263

H -6.23304841658258 0.48289801046012 1.07835794233795

C -6.74999519392321 -2.36621915304115 -1.49015130171722

H -4.93166740121027 -1.65765864030476 -2.40201140961946

C -7.66752864562491 -2.19142838843516 -0.45506572379985

H -8.19151465235893 -1.02324550800137 1.27763774325703

H -6.89310123267264 -3.16157204360728 -2.21588226705054

H -8.52732177244965 -2.84971206921074 -0.37164314365906

1 imaginary frequency: -292.21 cm-1

SP = -956.294211670244

U = -956.05019967

H = -956.04925546

G = -956.10529063

**22 carbanion**

N -2.86284740977001 -0.74435153736070 -0.65520882605560

C -1.61983505906678 -0.03712289757458 -0.58548585182037

C -0.87870545529084 -0.16352343299367 0.56734383416399

C 0.49591380477631 0.39489284324192 0.71447671418742

O -1.29623209687620 0.64717452362313 -1.63528051618291

S 1.79239757534394 -0.84611545947828 0.29414688397234

C 3.27442314267960 0.10302078742999 0.71980673413006

H -1.27049593161231 -0.77532630087502 1.37691517885124

H 0.65292231710936 1.25892168239370 0.06307817672897

H 0.69649777068965 0.70774379295341 1.74416029374767

H 3.35299140790864 1.00243876667939 0.10363420400818

H 3.26201548721808 0.38574549018355 1.77590488906966

H 4.14864882871831 -0.52566541849701 0.53581152141731

C -4.00073815205959 0.04680161658041 -1.15219754482614

H -3.09214672970139 -1.11197514041839 0.26237647587964

H -3.87031424141253 0.23533192132516 -2.21862931385605

H -4.05265350027262 1.02092517598887 -0.64448130997711

C -5.28885870820414 -0.70558421981733 -0.92126964796391

C -5.88932136020442 -0.69546483808235 0.34100948628052

C -5.88149926793837 -1.44898388738033 -1.94397090365798

C -7.05563924601700 -1.41904722946342 0.57995002692638

H -5.43802656156427 -0.11351926788409 1.14136051781124

C -7.05085352409694 -2.17170044969758 -1.71063242266155

H -5.42332839879925 -1.45933377983795 -2.92972923127702

C -7.63966355686978 -2.15963417489501 -0.44746628196386

H -7.51213797996940 -1.40127478343149 1.56544623346355

H -7.50252029392067 -2.74378041285838 -2.51608395938594

H -8.55099286079731 -2.72159336985395 -0.26498536100973

0 imaginary frequencies

SP = -956.313931246699

U = -956.06886265

H = -956.06791844

G =-956.12418771

**22 adduct**

N -3.06334076029882 0.27147518841362 0.51396175678101

C -1.90864556939719 0.94076774283534 0.63542113730306

C -0.89412893158679 0.37984385494183 1.61198791508169

C 0.49513753810933 0.28639524663065 0.99090125672877

O -1.68453205641068 1.98217222569262 -0.00429297970657

S 0.51179170108054 -0.95514745857787 -0.33747873190280

C 2.15449854820007 -0.61478174584903 -1.01204199759699

H -3.19667510109602 -0.58565438592300 1.03172218200195

H 0.78536321415704 1.25140049066006 0.56900399326254

H 1.22482258915822 0.00586334030550 1.75363139108457

H 2.20458033784029 0.40147946514198 -1.40957130968312

H 2.92167824560729 -0.75021509261258 -0.24623184285612

H 2.33493275389822 -1.32312508109659 -1.82316654450308

C -4.12065342134798 0.71843625643159 -0.39444982174602

H -0.85378462111560 1.07307714209932 2.45889477564638

H -1.21882675311353 -0.59141858542944 1.99523143008642

H -3.70979008739810 0.79275643201163 -1.40545832856720

H -4.45462729651711 1.71551264610629 -0.09578681019877

C -5.27713264032622 -0.24928201793550 -0.36837768018371

C -6.40737629980560 0.02034328453210 0.40451030661417

C -5.21889390779574 -1.44017863497938 -1.09762893258636

C -7.46639021264654 -0.88526959442273 0.44990561535277

H -6.45843646026907 0.94618794458933 0.97152574085044

C -6.27406665056300 -2.34772802765078 -1.05238467821643

H -4.34307948135261 -1.65336529071953 -1.70533170747470

C -7.40053461890075 -2.07181034043364 -0.27732185392459

H -8.34214184874848 -0.66296519621923 1.05253341416985

H -6.21924011569208 -3.26928939049483 -1.62441231421191

H -8.22450809366901 -2.77848041804772 -0.24329538160524

0 imaginary frequencies

SP = -956.835975788976

U = -956.57684113

H = -956.57589692

G = -956.63260676

**23**

N -3.18555440223649 -0.05353799217435 0.06487826961760

C -1.91711868762889 0.38540436227831 0.05496643261611

C -1.00606449100500 -0.30289534639301 1.01581435250282

C 0.27290919160794 0.04294825399001 1.12839923985338

O -1.53719969189007 1.29281062180527 -0.70441454446746

H -1.43593532323411 -1.09585024099621 1.62307087304532

H 0.69644291551841 0.83828798622466 0.52103709325132

H 0.92898988861475 -0.46004899735846 1.83237382654495

C -4.22086413827202 0.51581585332429 -0.79829904531328

H -3.44890257923341 -0.77613389101887 0.72066966901664

H -3.84801356632691 0.54374165110366 -1.82430203301398

H -4.43093578986088 1.54395988671217 -0.48782535174434

C -5.47010593104939 -0.32723053169845 -0.71455410592264

C -6.34787086553154 -0.18768104373311 0.36722859294456

C -5.73071583081214 -1.27474284192190 -1.69573107983220

C -7.46947013559897 -1.00206791571917 0.44970638546361

H -6.15033314656653 0.55765386603143 1.13224730532050

C -6.86342284880279 -2.09038758319354 -1.60662262036906

H -5.05895231674312 -1.39506915176656 -2.54079782718109

C -7.73938889948994 -1.96048981069948 -0.53039276175818

H -8.15496624591659 -0.89699082309620 1.28549282828905

H -8.62154733448744 -2.58289805483875 -0.44405074636808

O -7.02903296170603 -2.99190373457266 -2.62755427940060

C -8.18026404886365 -3.83830958787030 -2.57751868081086

H -8.12671086567463 -4.46604624852326 -3.46687001913053

H -8.16313978289877 -4.46844168254946 -1.68281878101543

H -9.10083211191170 -3.24689700334605 -2.60013299213812

0 imaginary frequencies

SP = -632.622578293537

U = -632.38520978

H = -632.38426557

G = -632.43896527

**23 TS**

N -3.00872379956094 -0.45311086593836 -0.20844402391395

C -1.77007327746738 0.13807628564796 -0.10527694359971

C -0.92903257151143 -0.30087620065069 0.97225403432901

C 0.35893711919504 0.18795838255987 1.11894505060205

O -1.43653270259942 1.00704658345603 -0.95812284435102

S 2.10184743145348 -0.87939506961055 -0.11662648288744

C 3.30538769829890 0.39386876161730 0.37671246294492

H -1.28334138548064 -1.12133214580335 1.59139681221989

H 0.62010018609332 1.12444782942253 0.63783351534055

H 0.89668589107448 -0.02034451763160 2.03722516777735

H 3.13011573612483 1.33722637288421 -0.15069186918214

H 3.23998397334991 0.59182263566699 1.45315704940124

H 4.32827291837447 0.07256850543886 0.16063089321588

C -4.05363337366702 0.15721393004392 -1.03100661840596

H -3.32817292837455 -0.95609377615771 0.60807425996152

H -3.75945247352269 0.12060369208887 -2.08161649838149

H -4.18268278214584 1.21210777231254 -0.75981936708074

C -5.35729538661145 -0.58046979992717 -0.83633634491202

C -6.07990844396013 -0.43216969763007 0.35482415460378

C -5.84246724861071 -1.42058294161012 -1.83037816867513

C -7.27194662492019 -1.12133690941361 0.52812342407003

H -5.70797205696383 0.22726088469601 1.13416030357195

C -7.04903441177146 -2.10696831059530 -1.65217632575530

H -5.29604176849998 -1.54875463649150 -2.76053556676300

C -7.77146066300215 -1.96316625035797 -0.47000204316926

H -7.83645191612708 -1.00580439727231 1.44877581294443

H -8.70714806449459 -2.48561405476729 -0.31313435700299

O -7.44241768736044 -2.89947441601153 -2.70186416869195

C -8.68139746431806 -3.60092570994424 -2.57183194554387

H -8.81054655788360 -4.15100430275332 -3.50394172999585

H -8.64742085181154 -4.30301479839129 -1.73291126366680

H -9.51317651329895 -2.90176283487704 -2.44039637900394

1 imaginary frequency: -196.18 cm-1

SP = -1070.886158232573

U = -1070.60657921

H = -1070.605635

G = -1070.66645219

**23 carbanion**

N -2.81230616801085 -0.70516778408447 -0.57963109718134

C -1.57021988857380 0.00097601986620 -0.50089642274325

C -0.82996526391122 -0.13543240762280 0.65216481168730

C 0.54877693212354 0.41432061657373 0.79493148085756

O -1.24190701351425 0.69149203958618 -1.54463307665959

S 1.83555322379949 -0.82116621485466 0.32854592302764

C 3.32713853449160 0.12818772300755 0.71820988697461

H -1.22039742258415 -0.75604443107508 1.45560769402416

H 0.70137027836410 1.29082062734458 0.15923732612403

H 0.76396343423284 0.70512295887832 1.82800706690246

H 3.38155696980096 1.03574331247949 0.11128292430470

H 3.34887988980626 0.39751432598181 1.77758601259858

H 4.19722179212446 -0.49419951066656 0.49689424786278

C -3.93868195170868 0.06960646348888 -1.12259774862546

H -3.06092618579943 -1.06049143440524 0.33764813144214

H -3.75959478783971 0.26965112711123 -2.17927555953395

H -4.03565689974832 1.03826067378129 -0.61090333882355

C -5.22375180643060 -0.70674541786688 -0.96117985200817

C -5.88210923877324 -0.72915338513187 0.27549148186577

C -5.74999114773607 -1.42750709759637 -2.02669656670345

C -7.04747505205111 -1.46932859095664 0.42496522776158

H -5.47887299799804 -0.16376256430898 1.11141445762614

C -6.92844022525300 -2.16470999071511 -1.87225170110772

H -5.25590933825269 -1.42210770318290 -2.99433543868737

C -7.58532498664554 -2.19226289481601 -0.64352288670170

H -7.56023483358760 -1.48694197152447 1.38240435708251

H -8.49889249486317 -2.75704531306496 -0.50392117486544

O -7.36450767736505 -2.83191210892372 -2.99118384094377

C -8.58924207767209 -3.56172795438005 -2.88656725977833

H -8.76275475629441 -3.99454585817956 -3.87180589377508

H -8.50670874014588 -4.36199677820112 -2.14444308252799

H -9.41859009998426 -2.89644647654177 -2.62654608947577

0 imaginary frequencies

SP = -1070.905760707155

U = -1070.62550225

H = -1070.62455804

G = -1070.68626051

**23 adduct**

N -3.11421576513121 0.34572570725831 0.40590730089555

C -1.93443603617435 0.96763357345870 0.53389676623173

C -0.97861965184878 0.40258980213668 1.56664793368727

C 0.42911723445049 0.23162138055452 1.00760064117596

O -1.64328147726589 1.96875008480129 -0.14215239942837

S 0.45020085911503 -1.06504478155851 -0.26651971961100

C 2.13001333116265 -0.81440185033206 -0.88763519707579

H -3.31472219138807 -0.45673524501756 0.98583443086607

H 0.77354850947296 1.16642440803476 0.55931779334779

H 1.11608407457159 -0.04392104311404 1.81073448124652

H 2.23442896649956 0.18177659247207 -1.32347160778517

H 2.86102523362054 -0.94623061268586 -0.08665912395070

H 2.31418804053168 -1.56227187677170 -1.66158015837360

C -4.15064639379409 0.82039198942394 -0.51250445142282

H -0.94391172397657 1.12540989905182 2.38895765428547

H -1.35679604697331 -0.54014206975002 1.97259327552071

H -3.75053666561050 0.83665022847201 -1.52915609112013

H -4.42862498574852 1.84346597249543 -0.24334145487286

C -5.35142589838634 -0.08921097543678 -0.43123504635166

C -6.24698234147000 0.02896633307922 0.63909479083033

C -5.54365644029032 -1.08204703116881 -1.38277398063271

C -7.31541716570371 -0.85137410913292 0.74081485689780

H -6.10312021498696 0.80841285034993 1.38181619906822

C -6.62365718215640 -1.96500929460912 -1.27406736891358

H -4.85630818409020 -1.18925712075830 -2.21712947624865

C -7.51449711173075 -1.85763343266509 -0.20786443129716

H -8.01340046437570 -0.76311764583384 1.56820342375818

H -8.35519326287631 -2.53263701810974 -0.10536867593004

O -6.72174075223617 -2.91047569004511 -2.26368679174529

C -7.80270614212713 -3.84160322403631 -2.17786108707951

H -7.70006996508110 -4.49701406904029 -3.04255155239438

H -7.73590702013301 -4.43340334461600 -1.25963372034940

H -8.76673316586897 -3.32528838690659 -2.22022721322880

0 imaginary frequencies

SP = -1071.427645633830

U = -1071.13319382

H = -1071.13224961

G = -1071.19420652

**24**

N -3.27961660781725 -0.01481343550750 0.16712917447211

C -1.97939264076993 0.07585106991047 -0.21068167564087

C -0.95704706454753 -0.41422084446952 0.76336493645357

C 0.29562336112969 0.03150441978822 0.70803030128082

O -1.64124994454805 0.53454001561103 -1.31315302777926

H 0.60607802076065 0.76192937311127 -0.03389679952527

H 1.04316301728972 -0.32062045675886 1.41264570389914

C -4.31580167895460 0.38939842138467 -0.74123343940585

C -5.27425777021025 -0.53962040419087 -1.13923298696339

C -6.30849376836354 -0.14789482555810 -1.98687964029675

C -6.37994031663359 1.16608584671548 -2.44362819075979

C -5.41777116520194 2.09178382078011 -2.04163913303553

C -4.38872252483476 1.70826152525225 -1.18632201005831

H -5.21309118357980 -1.56323813089284 -0.78205059680318

H -7.05492047519640 -0.87448475884138 -2.29318747052611

H -3.64468109472499 2.42769601745675 -0.86150150071352

H -5.47124543230488 3.11945964711758 -2.38807667196415

H -7.18409404545695 1.46968347687740 -3.10701853717387

H -1.25412139864229 -1.13378170067639 1.51788716544081

C -3.70053127261292 -0.59426882511639 1.45314063165363

H -3.56754821235469 -1.67901286615713 1.47030636336660

H -3.14420795981018 -0.14244791449854 2.27546240228949

H -4.75612984261546 -0.36678947133772 1.59353500178968

0 imaginary frequencies

SP = -518.012547129081

U = -517.81096076

H = -517.81001655

G = -517.85864802

**24 TS**

N -3.35134761856716 0.17620400813557 0.35981712691854

C -2.01325054089024 0.47452449789581 0.15904635204069

C -1.05530480946985 -0.02988295680920 1.10835292946950

C 0.29340081721760 0.21770991186664 0.93953234261782

O -1.68237755233731 1.16449041435145 -0.84256610344015

S 1.50455498705897 -1.31935907104855 -0.50795135100321

C 3.04137423228599 -0.35002497932316 -0.38414720622689

H 0.61525846647846 1.02869563571071 0.29673878234138

H 0.97976686584328 -0.04390798652432 1.73655845798147

H 3.04054167782641 0.49954681669532 -1.07458347807031

H 3.16717862761369 0.04203772574373 0.63243410338322

H 3.91697546642554 -0.96565801600580 -0.61016257525758

C -4.29901785886719 0.47805571348973 -0.66831200584385

C -4.96541235729605 -0.55836243701760 -1.32282456441417

C -5.91809025906736 -0.27274946465051 -2.29893554029194

C -6.20300177448296 1.04860254439494 -2.63516967884294

C -5.53495842379734 2.08390489875290 -1.98147176452996

C -4.59204173968210 1.80240552193932 -0.99690250801460

H -4.73884999946550 -1.58928391180942 -1.06764456356369

H -6.43234548669532 -1.08724389066868 -2.80056581942386

H -4.08246772875511 2.60701008569007 -0.47767334328649

H -5.75539445491352 3.11759516019677 -2.23158122785419

H -6.94278749108046 1.27148870140950 -3.39810175642794

H -1.37241536788393 -0.71904437297133 1.87991760438991

C -3.77633187985426 -0.76939175041205 1.39510560976771

H -3.41343509739578 -1.78525041768041 1.20577166297823

H -3.42640432952265 -0.44276083790656 2.37621499407566

H -4.86581637072578 -0.78435154344490 1.41910352052766

1 imaginary frequency: -266.88 cm-1

SP = -956.279522434285

U = -956.0364957

H = -956.03555149

G = -956.0916839

**24 carbanion**

N -3.02509648418585 -0.85606127914328 -0.79118650924445

C -1.70257547356518 -0.25105760515997 -0.81902442715302

C -1.05265538191831 -0.06597804368390 0.36828790962426

C 0.34652010063498 0.45225094696836 0.44050457966881

O -1.26141256138992 0.05793902527515 -1.99487315610913

S 1.56756459874880 -0.92083991697631 0.46299796277107

C 3.09642752304870 0.03442955128046 0.62845823558030

H 0.58612997252558 1.08579652845721 -0.41772059932266

H 0.50996897087764 1.03485963983165 1.35216689736684

H 3.23269978474863 0.70129506122606 -0.22680069597492

H 3.08976528014004 0.62049163752660 1.55114035538424

H 3.93323657192811 -0.66691813298514 0.66355200460765

C -4.11605366487096 -0.03585467866485 -1.11980028847675

C -5.42572336706005 -0.55163476251863 -1.12269969165233

C -6.51185134319263 0.25510872488607 -1.45044197271247

C -6.33541548865355 1.59694362988602 -1.78131256558170

C -5.04309543306179 2.11928170106548 -1.76957740369138

C -3.94907935702238 1.32479901032409 -1.43994485219765

H -5.60344239945412 -1.59141864649442 -0.87501631275063

H -7.50853472179665 -0.17793448819747 -1.44530802094982

H -2.95854535778410 1.76359651605008 -1.43290150495906

H -4.87758578483087 3.16586814178554 -2.01136708198303

H -7.18512522997655 2.22226267141542 -2.03707287463618

H -1.53264245182112 -0.36340185947887 1.29478197275052

C -3.26622810608771 -1.91028106693709 0.19240663118877

H -3.65050845574189 -1.52018238400078 1.14521612787024

H -3.97909703820260 -2.64260955658662 -0.19232231901300

H -2.32864470203622 -2.43275036515087 0.37885759959546

0 imaginary frequencies

SP = -956.301215800905

U = -956.05719985

H = -956.05625565

G = -956.11229426

**24 adduct**

N -3.07706239774132 0.22600350586854 0.37791936692314

C -1.96195604401205 0.98769925446487 0.47298150905976

C -0.89816453386922 0.60864197684409 1.48685034090111

C 0.43967164674251 0.35688828318066 0.79225049909269

O -1.78559514207422 1.98135654904656 -0.24936588020433

S 0.32053955656429 -1.08882008804757 -0.30473235028563

C 1.95667054100959 -0.99641385046618 -1.06876695687158

H 0.72757165990170 1.22529716970344 0.19559102705306

H 1.21351413355819 0.17496671807826 1.54126680335471

H 2.07072419265358 -0.06373234236664 -1.62568918038327

H 2.74015760804646 -1.07387679722503 -0.31155789640924

H 2.04772946925372 -1.83679650221418 -1.76002934112228

C -4.02579846422114 0.51461361654143 -0.66393507254754

C -4.14696782819433 -0.36880042190242 -1.73474193339783

C -5.08942791027811 -0.12429570459378 -2.73080896893110

C -5.89930409362631 1.00790041387735 -2.66499335135387

C -5.76841151535488 1.89162484514275 -1.59452804030793

C -4.83631462877256 1.64476292983850 -0.58926392450220

H -3.51097167143875 -1.24791473740040 -1.78092749288813

H -5.18533649830513 -0.81701843036650 -3.56142896365357

H -4.73534177610420 2.32397919943280 0.25117506854537

H -0.78654787412013 1.46826379505129 2.15471008246064

H -6.39872842888471 2.77386975722365 -1.53659472242150

H -6.63149780716196 1.20034515911353 -3.44328461889778

H -1.17525190176129 -0.25010880073679 2.09591826513744

C -3.27579168217268 -1.02357355972273 1.12978583881213

H -4.27777120250490 -1.38816879637573 0.90804135928270

H -2.55235755671708 -1.78991945588139 0.84036634524512

H -3.21297985041500 -0.84277368610836 2.20379218830993

0 imaginary frequencies

SP = -956.818007792666

U = -956.55958843

H = -956.55864422

G = -956.61513122

**25**

N -3.16528046299823 0.45861332421633 0.29460284861522

C -1.88569227118396 0.27616850573297 -0.11598246035653

C -0.98648611619143 -0.27725518192457 0.93866363310580

C 0.30554428332152 -0.48645696257168 0.70294260430922

O -1.49292488995020 0.54189124026698 -1.25757244107158

H 0.74522722450301 -0.25962707306702 -0.26443822764915

H 0.95632505984086 -0.88902364223956 1.47318760536777

C -4.24868824055651 0.89975277449817 -0.51497263710226

C -5.48689707083753 0.28614232443831 -0.36262687281112

C -6.59140084298387 0.70710049362788 -1.10330452617123

C -6.44524067445687 1.74993609618919 -2.01544355855456

C -5.20271866934063 2.37208964245076 -2.16680467126162

C -4.11228416373690 1.95848333460923 -1.41717589393985

H -5.59742047868681 -0.53115243170917 0.34434864344619

H -7.54315665158263 0.21093923173459 -0.95917646101188

H -3.16044782192327 2.46312553404760 -1.52817863703727

H -3.40661481279329 0.10745036258875 1.21228891959204

H -5.10516804646261 3.19067389974798 -2.87304014707383

H -1.42814794106683 -0.49959766757232 1.90678929570254

O -7.46137922993607 2.23217607946163 -2.80198262246830

C -8.73606729233469 1.59383066944177 -2.69099129318049

H -9.38848415634173 2.10707311819516 -3.39725951350327

H -8.66637722811740 0.53471093884308 -2.95863635469143

H -9.13821950618378 1.69695538899392 -1.67823723225438

0 imaginary frequencies

SP = -593.271824658462

U = -593.06498823

H = -593.06404402

G = -593.11472755

**25 TS**

N -3.25654199409201 0.14723327925604 0.11359812800160

C -1.92115049635432 0.51487792447738 0.03069222104112

C -1.05957860581246 -0.12226440139182 0.98802132544397

C 0.29786532931329 0.13494527198369 1.00304374026949

O -1.53643330934373 1.34515101435492 -0.82657047721793

S 1.70017227872997 -1.14813376840967 -0.49785223657527

C 3.15408506771816 -0.14475621698250 -0.05466475438956

H 0.67030640304984 1.03230745910519 0.52142390140964

H 0.89281226630281 -0.22646385377555 1.83384645852262

H 3.04783472621047 0.88727718639346 -0.40561916041596

H 3.29700884479669 -0.11993013123138 1.03168125273092

H 4.06408533390553 -0.55715623598697 -0.49991366728886

C -4.29667859799952 0.46287680563643 -0.78347016491907

C -5.30595010748776 -0.49094802448497 -0.96854468153886

C -6.38757682890335 -0.23094464613683 -1.80071291677217

C -6.46137985150100 0.98591826952425 -2.47197610883230

C -5.46903612946092 1.94167003674648 -2.29514540536270

C -4.39205206962454 1.69009116468802 -1.44706807981513

H -5.23663474985546 -1.44513113578086 -0.45301833979399

H -7.16809053240846 -0.97281534336007 -1.94009940167652

H -3.63617929171596 2.44900863402830 -1.29891438266548

H -3.44330607025294 -0.64690742148143 0.71014736058288

H -5.54470920798171 2.89236408179366 -2.81444773759928

H -1.48110533657288 -0.90111219399564 1.61830700469578

O -7.52306199843375 1.24055647743641 -3.33706096073975

C -8.66449575735529 1.78822767437325 -2.66212516016857

H -9.43156867104649 1.95269878786074 -3.42042898237801

H -9.03736509116584 1.08737728514761 -1.90724250302304

H -8.40627555265829 2.73998202021185 -2.18488627152555

1 imaginary frequency: -269.37 cm-1

SP = -1031.534142626240

U = -1031.28546382

H = -1031.28451961

G = -1031.34354333

**25 carbanion**

N -2.96084421212779 -0.79869660805823 -0.91139447464667

C -1.77297014279393 -0.00910833269647 -0.79667672128574

C -1.02302757059271 -0.16667064435888 0.34431555513761

C 0.33656211905254 0.42954666241423 0.49595026949191

O -1.48628710279840 0.74137444884737 -1.80858926960175

S 1.65362118722602 -0.72878358936043 -0.06808975796363

C 3.11703534950361 0.27246768749336 0.29592311481121

H -3.05861021989841 -1.48008279931420 -0.16995637838714

H 0.44287075488983 1.34545482052114 -0.09161868749267

H 0.55876876447655 0.66932310174603 1.54022320551635

H 3.09674507400992 1.20829493745105 -0.26869626672975

H 3.18118062521583 0.49374703343897 1.36452409302074

H 4.00198342849781 -0.29618565782038 0.00119276517393

C -4.20351795255952 -0.23473690458456 -1.29041617081772

C -5.26312821407326 -1.10239567469413 -1.59786942847312

C -6.51147451746582 -0.61348268214596 -1.94882990258522

C -6.72829959822092 0.76461321151493 -2.02888379044033

C -5.68855686197364 1.64046300380410 -1.73311310443835

C -4.43895791281784 1.13761321594030 -1.35580697484509

H -5.09980010794393 -2.17580486836537 -1.55299250647088

H -7.32715552146299 -1.29307855434574 -2.17710124530105

H -3.64523851695869 1.83433313437410 -1.11249573070570

H -5.82861492342215 2.71395712740708 -1.77778812398849

H -1.38106785880066 -0.83979262622968 1.11951565635505

O -7.99491715493376 1.16070839201167 -2.40740949067963

C -8.26000461441217 2.56349846358739 -2.42340762830527

H -9.30356374470974 2.66843237749450 -2.72113025921828

H -8.11743738043817 3.00037654023484 -1.42942408794095

H -7.62029317446746 3.07661478369295 -3.14895465918934

0 imaginary frequencies

SP = -1031.557204628478

U = -1031.30768005

H = -1031.30673584

G = -1031.3653304

**25 adduct**

N -2.98026362133967 0.06783949560695 -0.03631748745151

C -1.93938467691726 0.82377684367396 0.39081218363685

C -1.04110188737460 0.15355916731189 1.41391213628545

C 0.43128942482060 0.25151755600571 1.02896934654097

O -1.72738574676614 1.97900415638240 0.01285614413586

S 0.75437250751824 -0.72823625320239 -0.46789313132346

C 2.47999201011256 -0.26259556576179 -0.74140856905468

H -3.03462720185213 -0.86562592462864 0.34868853998799

H 0.70425583236651 1.29139734695147 0.83440703312770

H 1.05194257502413 -0.12543695909932 1.84478048928778

H 2.56611352260601 0.81141255766606 -0.92125501616249

H 3.09608550886065 -0.54538832747875 0.11521054209998

H 2.83295839675925 -0.79958062058421 -1.62424753658402

C -4.03990757608355 0.41043243080003 -0.91202219262111

C -5.02351144088096 -0.56626123371025 -1.10864101213851

C -6.10792291132875 -0.31962028497231 -1.93840850553179

C -6.21284021257162 0.90980352070678 -2.58449551774948

C -5.23703177611201 1.87973635605451 -2.40421384922639

C -4.14575331361431 1.63754583645583 -1.56984943189090

H -4.93445867092335 -1.52411226081407 -0.60329735073360

H -6.87213920038887 -1.07594029451029 -2.08779103395326

H -3.39016058130153 2.39773546546161 -1.43852497959179

H -1.19413304045717 0.68788240290368 2.35747741140106

H -5.32863793966350 2.83229666433307 -2.91696332715678

H -1.33340060614216 -0.88808184269717 1.57411846456114

O -7.28748286431221 1.15938562840616 -3.43177776475990

C -8.43110918005983 1.67226943234124 -2.73188463992532

H -9.20996846367860 1.83643006920183 -3.47786181161275

H -8.78060037990527 0.94955576617204 -1.98663071012883

H -8.18418848639439 2.61929887102395 -2.23974842346821

0 imaginary frequencies

SP = -1032.072594004750

U = -1031.80850624

H = -1031.80756203

G = -1031.86722496

**26**

C -1.76024159286780 -0.27960692769398 -0.29305765804395

C -1.19103154725512 0.40791698948092 0.90448824891371

C -0.06046629350850 -0.01164853832799 1.46715802473841

O -1.13756836213359 -1.18599619341033 -0.88434494170495

H -1.71696481853775 1.26830513489264 1.30373827810018

H 0.47966389101378 -0.87181061413351 1.08162298524147

H 0.35184970097016 0.49645045633157 2.33379001972615

C -3.84515550778780 1.11584563034218 -0.06501184197943

C -3.59353973052432 -0.46743655117096 -1.90866492946298

C -5.18798713335454 0.90444738360139 -0.75019433472875

H -3.48303983738205 2.13235552766890 -0.24101197340300

H -3.91965671899542 0.93979113565116 1.00859606936410

C -4.79972734049811 0.43843175621317 -2.15201008274747

H -3.89005746540445 -1.49959742969979 -1.69868889176100

H -2.88915771266227 -0.47555711915793 -2.74203618497856

H -5.78503143025047 1.82021104101235 -0.75355465281445

H -5.61963417997336 -0.07351116484459 -2.66016288261582

H -4.50760987757816 1.30900779841781 -2.74701584436693

N -2.96502732398906 0.12706809219472 -0.71779011662262

O -5.88311288884549 -0.12683834121549 -0.03174830613498

H -6.67350383043548 -0.35282806615225 -0.53510098471910

0 imaginary frequencies

SP = -478.898604239016

U = -478.70964223

H = -478.70869802

G = -478.75427214

**26 TS**

C -1.85945321379143 0.69713512041702 -0.03827747646102

C -0.98983402213372 -0.43680857806343 0.12723013347372

C 0.26527316768352 -0.29104912453606 0.69971954734928

O -1.56721710275716 1.86395430241816 0.37240420866808

S 2.04384702395160 0.39650466324722 -0.72643242782121

C 3.24589017627662 0.34645156892946 0.63924303969008

H -1.26482197502528 -1.38276171316753 -0.32506580028708

H 0.46381325172491 0.57287189863918 1.32472833716324

H 0.81995817500905 -1.18380498143265 0.96748076933935

H 2.84104829758813 0.84750893912356 1.52654169759596

H 3.49781873926158 -0.68201981606041 0.91786306882116

H 4.17384166401842 0.85730002466975 0.36646930059723

C -4.05060537927369 1.58728166614136 -0.75894689246128

C -3.57033773135245 -0.76402261187362 -1.16856505860345

C -5.34142711004826 0.85754316368418 -1.10221962625412

H -3.79301847317541 2.30510613196296 -1.54542756255013

H -4.13893650495736 2.12839607105931 0.18546432881132

C -4.85787090532536 -0.35865059118624 -1.88953518021075

H -3.77180846494359 -1.45246531808741 -0.33989708585653

H -2.85689652139020 -1.24098451645202 -1.84408298779972

H -6.02990579365877 1.48834022800671 -1.67153917540470

H -5.60130111562759 -1.15887597257575 -1.91926392706407

H -4.63644610331196 -0.05036135538062 -2.91607302481466

N -3.05352720963501 0.51603981234471 -0.67008027657551

O -5.95934496113298 0.46382842045849 0.13568179535324

H -6.68573790797338 -0.13245743228635 -0.07741972469841

1 imaginary frequency: -241.07 cm-1

SP = -917.162769175536

U = -916.93176676

H = -916.93082255

G = -916.98441124

**26 carbanion**

C -1.65333643695925 0.33598538111178 -0.79202140914451

C -0.92373372990988 0.73836871950014 0.31442154833524

C 0.56540950799419 0.65551227631202 0.34106309196654

O -1.13769742692018 -0.01574095853248 -1.93222566008241

S 1.15780217240474 -0.96255290374316 1.00716592715654

C 2.94696444404662 -0.69261589551954 0.93815270973198

H -1.42751339376053 0.97549316913049 1.24449129916036

H 0.99820901664230 0.76304803163842 -0.65713872752491

H 1.00373853743227 1.42490756244798 0.98457124766121

H 3.27379720108408 -0.51294776376615 -0.08953023974302

H 3.23769529016323 0.15442109748033 1.56524008563364

H 3.44382137165119 -1.59131094822238 1.31125754607196

C -3.76784204457355 0.81767436072771 0.43710926600387

C -3.84386569791148 0.49333465586144 -1.94590999444395

C -5.22712156297464 0.77979974011819 0.01986591260687

H -3.47601099191951 1.85797885393204 0.64512911468455

H -3.58747666117266 0.22698437830686 1.33920477242149

C -5.15194394185025 1.13747613717898 -1.46228650076472

H -4.02999379023790 -0.45315037268247 -2.46330270840202

H -3.31116342748854 1.14814447749509 -2.64154886586395

H -5.83576100988265 1.48265643902902 0.59673991771127

H -6.03015749379616 0.79424509517786 -2.01506812191153

H -5.09648016906649 2.22655082758793 -1.55274330714936

N -3.05707979772687 0.27087844696992 -0.71729278009386

O -5.72070698788115 -0.55684775534732 0.22357882120784

H -6.60755297738686 -0.59929305219270 -0.14992294522912

0 imaginary frequencies

SP = -917.180423355506

U = -916.94871845

H = -916.94777424

G = -917.001354

**26 adduct**

C -1.80455948242217 1.54047291379858 0.35098675395640

C -0.95342124305107 1.04939439671008 1.50551060818779

C 0.40781779144209 0.54699647517494 1.03246237525523

O -1.35125838295165 2.39403037457765 -0.43856378476914

S 0.20594367234007 -0.95894353351414 0.03401699264336

C 1.91640585110391 -1.16694670907555 -0.51415326958733

H 0.90442950061301 1.30665094834600 0.42459940681508

H 1.03900969872915 0.32293368114526 1.89523054310588

H 2.23834847044163 -0.30804951026382 -1.10736203439320

H 2.58341449714020 -1.29646250668825 0.34117325744292

H 1.95892887971145 -2.06390506271598 -1.13536016194997

H -0.79791079085527 1.91609156495977 2.15681613765348

H -1.45921922341431 0.28664026714375 2.09740291646373

C -3.69867703396569 0.02559379686106 1.04925737413926

C -3.94538628953615 1.57862606161954 -0.82124827332738

C -4.96411869534430 -0.30174030694658 0.25905131485665

H -3.93311585787261 0.42651546753628 2.03949834874653

H -3.05167233192719 -0.84396895125018 1.16416248169685

C -5.30834270136635 1.02788690649621 -0.41111617937325

H -3.66381694966426 1.18932576826236 -1.80600765402146

H -3.91611306075984 2.66870463718393 -0.85141146813875

H -4.74266427173624 -1.03908102223426 -0.51951780684291

H -5.76448843105690 -0.68333032579924 0.89561671037955

H -5.77838020926089 1.70237386149111 0.31404861125011

N -3.04872552302780 1.06508964429598 0.21907587632097

O -6.13564418700139 0.91475328742965 -1.56598102011334

H -7.02178369630734 0.67534787545585 -1.27318805639707

0 imaginary frequencies

SP = -917.701668805689

U = -917.45522525

H = -917.45428104

G = -917.50775723

**27**

N -3.77053226000118 0.16097366355659 0.17091151406823

C -2.56900566490015 0.69099145210002 0.45197821366544

C -1.83459528033649 0.03604915978823 1.56854635331681

C -0.60690505979684 0.41738398648123 1.91725832299116

O -2.11561312563505 1.66053970969902 -0.18367485448650

H -2.33990118851230 -0.77692791064985 2.08563983589916

H -0.13831472569933 1.23124410339552 1.36821446972501

C 0.18302733110300 -0.24464618654536 3.00614398730398

C -4.61218623840279 0.67622190200203 -0.89818981559835

H -4.08884444258441 -0.63046915002061 0.71024002505213

H 1.01724778094236 -0.80476156932947 2.54442521806038

H -0.45153538144751 -0.97204907758034 3.51820657534989

N 0.70544180909975 0.69778402993997 4.00801145319695

C 1.76886373012321 1.51865452251221 3.42277841502159

C 1.27357371983030 -0.08199744281973 5.11030746831788

H 0.49707258221020 -0.69535434608170 5.57467297690772

H 1.67917884545839 0.59280448632749 5.86822771615550

H 2.08464136467040 -0.74748986369745 4.76934929726964

H 1.37766078368978 2.15341451912687 2.62548815323891

H 2.58242880146872 0.89915579628809 3.00912661248268

H 2.18952745442993 2.17066204872700 4.19221736454213

H -4.10967232661154 0.59186426735566 -1.86557437655549

H -5.53070855039056 0.09051485941962 -0.92413259681956

H -4.86384995870784 1.72543704000495 -0.72317232910533

0 imaginary frequencies

SP = -460.231641165149

U = -460.00761756

H = -460.00667335

G = -460.05682062

**27 TS**

N -3.35405593636697 -0.09895269038141 -0.08174211505882

C -2.08567850815629 0.40309408594720 0.10766718208973

C -1.27355722386773 -0.24593682570098 1.09122325100617

C 0.04145366209963 0.13689212639681 1.32907880557236

O -1.70949886008517 1.38407125256646 -0.59830212722366

S 1.59195220257255 -0.80715695774019 -0.19056665985573

C 2.96116223132618 0.35058449777407 0.12457952691664

H -1.68527672867645 -1.11502294277820 1.60017346799291

H 0.34383557685243 1.11137819455406 0.95630188099511

C 0.73729093920525 -0.31728014509007 2.59761259215540

H 2.56716476785763 1.30956582610624 0.48401432946620

H 3.65893586473605 -0.03119085749199 0.87603294629049

H 3.52406857098921 0.54891707570584 -0.79216137300976

C -4.36053148648685 0.66785455128254 -0.79985437031185

H -3.69096514725168 -0.72155823008229 0.63772133391983

H 1.81811668782411 -0.13329325863824 2.51330395284694

H 0.59287066924532 -1.39433262698089 2.71640136736838

N 0.22437670794291 0.34449762750038 3.81472641002422

C 0.45037277937326 1.78784739086366 3.72875703117538

C 0.97219059273061 -0.18074182324805 4.95716736534117

H 0.82707628336491 -1.26203300367019 5.03321921067468

H 0.61312947950019 0.28060829443600 5.88112513145727

H 2.05476252684107 0.01668481215786 4.87046373222411

H -0.15570894026770 2.22373082778812 2.93121160060267

H 1.50984685922266 2.02906426994498 3.53363177674408

H 0.15880768863857 2.26030483964036 4.67053003930085

H -4.05448092057141 0.83614724729084 -1.83454916103756

H -5.28946089924211 0.09554121636348 -0.80809153774537

H -4.55319943935018 1.64171522548359 -0.33367558992197

1 imaginary frequency: -305.86 cm-1

SP = -898.493173696220

U = -898.22735779

H = -898.22641358

G = -898.28225757

**27 carb**

N -3.65808361900350 0.67621158502785 0.80036772534878

C -2.28129328517333 1.05512597078363 0.71356949415303

C -1.33293173246003 0.10285120114542 1.00192158307404

C 0.12147305576612 0.41366365383061 1.11536213735226

O -2.05279137734845 2.29413155674949 0.41033042006177

S 0.95826157139709 -0.03984149052959 -0.47183193970182

C 2.63559738466354 0.61224908647007 -0.24062426487729

H -1.65367042152448 -0.91360236691948 1.22274756608791

H 0.26885221400949 1.49253744858332 1.20783978115567

C 0.82271875852707 -0.31254242773993 2.26681819173150

H 2.59317385607249 1.62855005433419 0.16045232342927

H 3.23763064011434 -0.01666498520438 0.41730977812357

H 3.11207833479751 0.64773284484108 -1.22346699336606

C -4.50987082493508 1.15828176967768 -0.28802665635477

H -3.72593393321595 -0.33277208075209 0.86789453714212

H 1.89339037467933 -0.04651961275652 2.26199332698088

H 0.75696564898440 -1.39147261831832 2.09062281540223

N 0.26051799236758 -0.03723384271202 3.59761945395188

C 0.29928743756774 1.39592075084873 3.88606463114644

C 1.07128193357342 -0.74507234258454 4.58723125506945

H 1.05772833912195 -1.81898342336389 4.38033255937782

H 0.66373914979288 -0.58305144367482 5.58895759177378

H 2.12237898922014 -0.40698025508896 4.58324287089413

H -0.38857109116930 1.93907061874891 3.23403590637115

H 1.31145245584341 1.81879765809690 3.75918084636525

H -0.01445308024872 1.56610865084182 4.91959041790637

H -4.13930197224513 0.86655959274338 -1.28181274568182

H -5.51400169093509 0.74696363486502 -0.16145325892224

H -4.58762510823944 2.24598081205644 -0.25826935399534

0 imaginary frequencies

SP = -898.510138141418

U = -898.24339195

H = -898.24244774

G = -898.29920521

**27 adduct**

N -3.53427931295501 0.22591654197838 0.32799141014625

C -2.40055340292731 0.86193765423520 0.64923746049021

C -1.63916682940716 0.33269987131732 1.84532921991893

H -1.72975100101624 1.08633185243127 2.63284389856622

C -0.15746657344569 0.12272412615823 1.54012157889045

O -2.00638689206697 1.85884233316910 0.01780921109271

S -0.00232103779536 -1.18686425194742 0.27478142338397

C 1.62623256565091 -0.78705598460278 -0.40519206327374

H -2.09055132631020 -0.59200766425611 2.21814855963415

H 0.24563466658221 1.02903562084494 1.08371764611464

C 0.64728849612745 -0.25776111527502 2.78382633244131

H 1.63534229538732 0.23185161796727 -0.79871915104233

H 2.41211570974511 -0.90440567733665 0.34274952798939

H 1.81371595121574 -1.48417093290529 -1.22480342149208

C -4.37383742058233 0.65627286540413 -0.78049378364495

H -3.80051271792373 -0.58807587380306 0.86114151188389

H 1.69772063178523 -0.41362839874215 2.48388206878534

H 0.27213537860425 -1.21302602712077 3.16370691613632

N 0.57736929210046 0.72078511556292 3.87566463884701

C 1.09908784907301 2.01672262612580 3.44224354077930

C 1.38697985572250 0.22419132137877 4.98821529103261

H 1.00692343438531 -0.74563636045717 5.32155595832334

H 1.33287034302659 0.92241856558751 5.82770359746081

H 2.44743805941502 0.10186542088437 4.70765994079061

H 0.44324912743802 2.47129624816479 2.69618329418958

H 2.11235162196664 1.93242812714023 3.01223471982795

H 1.14572638044262 2.69272836895978 4.29999910766323

H -3.82905610961229 0.59982413718174 -1.72669148375028

H -5.24072845304086 -0.00200452292042 -0.83059233035895

H -4.71557058158522 1.68376439487509 -0.63225462082591

0 imaginary frequencies

SP = -899.034076371654

U = -898.75309326

H = -898.75214905

G = -898.80927125

**27H**

N -3.77507375413690 0.17903587874590 0.21547283717114

C -2.55034219405295 0.67897393859597 0.43363856420390

C -1.79029670462942 0.02354025329523 1.53769402690076

C -0.53859619318565 0.37323737964316 1.82021368710997

O -2.08832997840142 1.61976351159086 -0.23402119082044

H -2.29588225259720 -0.75869461926561 2.09889971047205

H -0.05167619155894 1.14996240119044 1.23637654995626

C 0.24735225930566 -0.30834135353441 2.89788593104427

C -4.64644703025939 0.69885196458863 -0.82771921890887

H -4.09292942806376 -0.59240196456034 0.78388156301786

H 1.14220865055639 -0.79009727660890 2.49539388073245

H -0.36251254172153 -1.05308644301100 3.40922979855469

N 0.72969483088023 0.65732334858312 3.94662295904898

C 1.80339684018782 1.56254057468784 3.44190432031006

C 1.19033859625310 -0.07951615879880 5.15923683508974

H 0.36266625689362 -0.67437137234807 5.54349033412954

H 1.51360923656424 0.64822129625549 5.90255717863025

H 2.02174740239710 -0.72272640212912 4.86845238576787

H 1.42315735739303 2.14784641054739 2.60652376723798

H 2.64454598202919 0.94434174524406 3.12719729492957

H 2.09942024949921 2.22541093881273 4.25418695664412

H -4.18370507659553 0.58777464859886 -1.81183652101615

H -5.57878876910986 0.13546250394779 -0.80735909952373

H -4.86512688380034 1.75631758322852 -0.65873958854153

H -0.06643066384669 1.24063121270027 4.21981703785925

0 imaginary frequencies

SP = -460.699508185831

U = -460.45963650

H = -460.45869229

G = -460.50938583

**27H TS**

N -3.35522830696547 -0.04676073810668 0.07493976670237

C -2.07451784101303 0.42161147645152 0.15115814201648

C -1.21420909038760 -0.20211530235631 1.12473298150719

C 0.11046440206083 0.16896410533349 1.26446311128610

O -1.70698308929175 1.34877041868036 -0.62149536331923

S 1.67135222152572 -0.84719435232277 -0.22137079097494

C 3.01132982658908 0.35294325920787 0.06026336563209

H -1.60209311989729 -1.05700439331366 1.67552399456322

H 0.41722278202415 1.12578581537648 0.85455243022994

C 0.83887463033375 -0.28626316332120 2.50566480435898

H 2.59673561827102 1.30973526429756 0.40271859246089

H 3.72353584100777 0.00336197483680 0.81374150477156

H 3.56229617904078 0.54733950059231 -0.86419314575525

C -4.37503662861491 0.63235374223790 -0.70703537227533

H -3.65887312406450 -0.67907272411876 0.79972718856009

H 1.89608949353456 -0.02561273793518 2.50193621982934

H 0.72368822395296 -1.36016310344845 2.64855296767381

N 0.25291484678989 0.36880596254014 3.73772218440631

C 0.47341084956814 1.84128135109404 3.74424295449515

C 0.78566739511971 -0.26325361478209 4.97623242249359

H 0.54248917784038 -1.32532085244048 4.95804806037443

H 0.32450640411566 0.21740059825690 5.83867075789801

H 1.86670528731511 -0.12102990466123 4.99615526935027

H -0.00950255028968 2.27780310614131 2.87123294051431

H 1.54833341950028 2.02421403350104 3.71761400875806

H 0.03930741263690 2.25180628783527 4.65540105778147

H -4.11485793000125 0.63922799858055 -1.76833309355816

H -5.31535127112908 0.09280960314948 -0.58686987084878

H -4.52048924251609 1.66766921299100 -0.37902517822915

H -0.75778181705604 0.20890717570279 3.70802808929709

1 imaginary frequency: -266.16 cm-1

SP = -898.969238895038

U = -898.68777836

H = -898.68683415

G = -898.74316153

**27H carbanion**

N -3.53868612208250 0.50215632938951 0.93954499804995

C -2.19823597688158 0.96268741209857 0.81754662943528

C -1.18676365983809 0.02943693061517 0.95090829959736

C 0.25603903390830 0.40929362565667 0.98692555105425

O -2.03948390969742 2.22750456853146 0.63362995858052

S 1.10397281951778 -0.10796213588992 -0.55877054160761

C 2.76227920579677 0.58855926754315 -0.32231105618667

H -1.43792963035584 -1.02650303263973 1.03547818563890

H 0.35598892805072 1.49536488926166 1.03031194745087

C 0.96560027612878 -0.23166922203112 2.18229936224904

H 2.69208784625657 1.63328995363599 -0.00849112349370

H 3.34604951220169 0.02189990190372 0.40512289929722

H 3.27255745764087 0.54873497787852 -1.28744338766449

C -4.51489137810808 1.10799730808092 0.03376944721431

H -3.56784080935336 -0.50803235850955 0.86919144686104

H 1.99222790197642 0.11230570092512 2.31792757297914

H 0.95536056020665 -1.31871606696510 2.08247915804162

N 0.22586822045768 0.09138751617387 3.44637074781305

C 0.31999136492344 1.53393251027619 3.80880838221566

C 0.66399095726969 -0.77602740463192 4.57204878523214

H 0.53359327969995 -1.81840512613059 4.28303023647717

H 0.05573255351586 -0.54697406957721 5.44670912927257

H 1.71477487866774 -0.56729782434552 4.77711139757975

H -0.17488309664187 2.12929617963463 3.04317213532729

H 1.37484702464841 1.80051953365095 3.88284469539264

H -0.17820932660981 1.67977845741170 4.76681741835255

H -4.23541447523725 1.00772959309059 -1.02470189314671

H -5.48113396428418 0.62092738692077 0.18243054824462

H -4.63690181829658 2.16861857559058 0.25707190795686

H -0.76158765348074 -0.10383337754909 3.23116716178536

0 imaginary frequencies

SP = -898.989073388029

U = -898.70706512

H = -898.70612092

G = -898.76346913

**27H adduct**

N -3.54233431415303 0.24484360947452 0.30101405898140

C -2.40343376466671 0.85641134721034 0.64469186422445

C -1.66749985643209 0.29357812352774 1.84451805148670

H -1.79660044375368 1.02895842004166 2.64693469239356

C -0.18103796008916 0.09998392938722 1.54575400662540

O -1.97867426541183 1.85363216369210 0.03755472903212

S -0.01358808969014 -1.21152139267642 0.28805060379697

C 1.62231218829227 -0.81236554898639 -0.37427166462015

H -2.11974740461900 -0.64393401845753 2.18082763981075

H 0.22347294238488 1.01013227048323 1.09978018961821

C 0.63255733579971 -0.30566690838012 2.77155245183093

H 1.63509162679837 0.20546166817660 -0.76935169127769

H 2.40113052510515 -0.93211196664057 0.38081006743952

H 1.81445168478639 -1.51241360765744 -1.19007986473277

C -4.35691379464888 0.70395340680564 -0.81524559585486

H -3.82869528983311 -0.57362005972531 0.81697665230925

H 1.68092441691486 -0.44897189134274 2.50564728058523

H 0.24292668221888 -1.22862805912757 3.20332737812245

N 0.63026652647522 0.71098969491960 3.88148563417095

C 1.03972361205235 2.07233607150358 3.43195155506288

C 1.49781764716875 0.23727756110913 5.00076684091042

H 1.16064521235138 -0.75238420363848 5.30765273694315

H 1.40962755914622 0.94292138881329 5.82621239697570

H 2.52626809522978 0.19681615258966 4.64112667624530

H 0.28367101780762 2.47637973113454 2.76085970722771

H 2.00248725997105 1.99021306247635 2.92609600841381

H 1.12549751168052 2.70745710942774 4.31287881126163

H -3.79621727140852 0.65363263689071 -1.75233413429355

H -5.23164979521033 0.05862230675357 -0.88956596032343

H -4.68626608236132 1.73386122247004 -0.65663613015577

H -0.32121351190562 0.77615577974531 4.25201500778970

0 imaginary frequencies

SP = -899.504263338488

U = -899.20725978

H = -899.20631557

G = -899.26368768

**28**

N -3.77579213233520 0.20515660978317 0.17875822625181

C -2.54807050465147 0.68699442141069 0.41959588728897

C -1.84009954416289 0.06311822370255 1.57573791973693

C -0.58045213239671 0.37843668623005 1.86235932613921

O -2.04101519114775 1.58826315649817 -0.26980129921317

H -2.38942214311372 -0.66350991947809 2.16976662638759

H -0.05361469673701 1.09894424730041 1.24246974777488

C 0.16602818067554 -0.28179135196206 2.98103828082507

C -4.59561764214516 0.69288866514522 -0.92015312907729

H -4.12965780786299 -0.53523659814632 0.76675903279874

H 1.03636869416094 -0.82125999952434 2.59915232167338

H -0.47735439832749 -0.97577964612263 3.52269354371091

N 0.69852795769519 0.69420425298950 4.00558537152002

C 1.74328993671492 1.58218407094968 3.40907670222063

C 1.31595107948181 -0.09929300358862 5.11288877118748

H 0.54549693836782 -0.72646148737987 5.56109785124084

H 1.71733491074474 0.59566108243801 5.84995931980489

H 2.11364166562625 -0.71338807931668 4.69481685740798

H 1.29100757363752 2.20920018462119 2.64275218970034

H 2.52545817763369 0.95450145820177 2.98186346036473

H 2.14836932633464 2.20718091379525 4.20467640170587

H -4.10166610784759 0.52058872501727 -1.88006309393374

H -5.54301276465332 0.15503167894586 -0.90585227212502

H -4.79152636157555 1.76270085522989 -0.81208757211305

C -0.41263964075100 1.52556624696497 4.55931844894258

H -0.81979590940576 2.14884111700780 3.76452259269911

H -1.18119426541357 0.85898550941902 4.95098262630102

H -0.00454319854585 2.14827197986811 5.35508586077926

0 imaginary frequencies

SP = -500.041130595585

U = -499.77248905

H = -499.77154484

G = -499.82445668

**28 TS**

N -3.38333824634124 0.01121370842734 -0.16040260493784

C -2.12031166059506 0.48695386426698 0.07029848175339

C -1.32621397138004 -0.22940888407747 1.02825042051416

C -0.01471436863570 0.13146798383057 1.29592141261040

O -1.72457846962971 1.50736276570045 -0.56313556656011

S 1.56404440086734 -0.79292320652163 -0.17782794248487

C 2.95387520260872 0.30689377681402 0.23731852818828

H -1.74723687340952 -1.12850215048724 1.47055697237015

H 0.30369213533658 1.11863628539403 0.97494535826495

C 0.67197509279582 -0.38166582622193 2.54026938040156

H 2.57631021696888 1.26433115747837 0.61767138006167

H 3.60892218681603 -0.12763875138532 0.99864050226403

H 3.55739429942769 0.51982882269114 -0.64934801286806

C -4.35406711672585 0.76533239351707 -0.93518044182155

H -3.72957415317235 -0.69791040707251 0.46758903753680

H 1.74629972147381 -0.21812117132470 2.49332434474088

H 0.47357472426512 -1.44252772884844 2.69574010920017

N 0.23197117932874 0.31803826508073 3.82484234582425

C 0.31447280196374 1.80060923427410 3.67120537040710

C 1.17353519851639 -0.11081558181859 4.90414113632551

H 1.14261111352420 -1.19809416300306 4.97861867369673

H 0.85323243506635 0.34234581193966 5.84231674799221

H 2.17796931889421 0.22375291871375 4.64563327503210

H -0.44024896136507 2.12759312699175 2.95769113239644

H 1.31340035548505 2.05940038401558 3.31857841957967

H 0.12730426361422 2.25341095682575 4.64509264706235

H -4.00500295888272 0.91472411268294 -1.95990547260296

H -5.28353317951143 0.19537913056161 -0.97017452668594

H -4.56092872809876 1.74696996494671 -0.49386053891681

C -1.15363255491223 -0.06344096732085 4.23081961391812

H -1.85220990087541 0.27272982223423 3.46850549507814

H -1.19617096303015 -1.14755847903741 4.33710220062325

H -1.36782254038763 0.41963283073235 5.18476212103572

1 imaginary frequency: -300.11 cm-1

SP = -938.307148635888

U = -937.99698468

H = -937.99604047

G = -938.05514070

**28 carbanion**

N -3.67664834771412 0.71686427344904 0.67851675044832

C -2.29811699241297 1.08388532391857 0.69650027762460

C -1.37371134242636 0.07977479871527 0.87582681385383

C 0.07656060027335 0.35828189576688 1.06363082608285

O -2.03883306900985 2.34604948760200 0.58882842972262

S 0.98395750618440 -0.09188607840188 -0.48393230845669

C 2.65430345316697 0.54048820649281 -0.16432979506451

H -1.70671461307426 -0.95376317000250 0.93052418001845

H 0.24134836436107 1.42990908406778 1.18815489463767

C 0.74562566617584 -0.40529493193619 2.20748111692321

H 2.60175511372307 1.55037472738480 0.25074514248930

H 3.22249581625109 -0.10616619540096 0.50687476100224

H 3.17339392887556 0.58694812223351 -1.12458008225755

C -4.50111662233466 1.38968422915702 -0.32606550809085

H -3.75964997490839 -0.28818324061459 0.57965645613103

H 1.81239634650337 -0.18181245882096 2.23356329611395

H 0.61403114630513 -1.48262673003293 2.08884537090347

N 0.24706078702497 -0.07361862393747 3.60427381853037

C 0.08116824803503 1.39918314365532 3.78675294458205

C 1.27573708824833 -0.57007417561278 4.57117484175775

H 1.43186714797739 -1.63436143782386 4.39293838769225

H 0.90696035547167 -0.40550878551751 5.58364497444567

H 2.20163380685072 -0.01808145568236 4.41078150523239

H -0.74607233156718 1.74355497598492 3.16763432656111

H 1.01020213088665 1.89260299321762 3.49989050122253

H -0.13620577578800 1.58484756911586 4.83905366194854

H -4.11430028756385 1.26465972735883 -1.34785917662014

H -5.51177860013582 0.97721136480726 -0.28787655868892

H -4.56716983870640 2.45733732205655 -0.11273476586726

C -1.04774795818738 -0.75608353915906 3.91465701502407

H -1.80949790668129 -0.38507648595915 3.23467557208321

H -0.91020414732996 -1.82989919047089 3.78707344539673

H -1.30772969847410 -0.52722074561095 4.94867888461768

0 imaginary frequencies

SP = -938.323559993375

U = -938.01205896

H = -938.01111475

G = -938.07028471

**28 adduct**

N -3.67092301474068 -0.05129111077370 0.04143162489764

C -2.70425091181606 0.63223151868911 0.66522149818189

C -1.95094796843492 -0.10582959923052 1.75373059492160

H -2.30556968798674 0.29729681440596 2.70647007105011

C -0.43887977462717 0.09687763264659 1.63090630312739

O -2.45328972550696 1.81948309272689 0.39713391989275

S 0.11031323069285 -0.82788317033036 0.15791257621159

C 1.72889439497529 -0.06441202494948 -0.09503222874128

H -2.19519781720339 -1.17211153800454 1.74532903555370

H -0.23832686956486 1.14960732068821 1.42751348772906

C 0.32158055175186 -0.38575661238137 2.87360855155096

H 1.62427656285681 1.01155698578987 -0.24871989383505

H 2.39654764633093 -0.25850526429018 0.74711545965323

H 2.15936918988201 -0.51250258849076 -0.99297919123542

C -4.50470433187000 0.54953453546837 -0.99001679803976

H -3.81794774565198 -1.01750809301786 0.29263297018994

H 1.26482498703221 -0.85863637423362 2.60259818835843

H -0.27749001140971 -1.10865879140765 3.43015172949440

N 0.70091250398280 0.69882154427400 3.85776616662922

C 1.72453821380078 1.61634225396448 3.26792031754758

C 1.30287117971165 0.02638480670614 5.05237458713495

H 0.54848471833813 -0.61746420535423 5.50412948040600

H 1.61723656258655 0.79668923561978 5.75609552441274

H 2.15970422483193 -0.56125687455393 4.72267187582796

H 1.30000667248004 2.13744556921876 2.41192719474929

H 2.58586075329081 1.02097220534494 2.96600729371483

H 2.01005622747413 2.33741435950828 4.03351260895140

H -3.90086944256614 0.86097147924438 -1.84637524494835

H -5.23062080135274 -0.19314299103558 -1.31948786126469

H -5.03773382899044 1.41986518928232 -0.59911898567025

C -0.48461956194405 1.49240346687214 4.30174904615409

H -0.89193638207157 2.04065168220905 3.45350987814906

H -1.22514318727113 0.80878568742438 4.71637370394928

H -0.15102655701020 2.19462385797013 5.06593651529564

0 imaginary frequencies

SP = -938.842670639807

U = -938.51666358

H = -938.51571937

G = -938.57495332

**29**

N -3.27062210627630 0.06273805866639 0.07650725117983

C -1.94557266577809 0.29450731074685 -0.11079292521003

C -1.03738600756699 -0.31522664637864 0.92563887953283

C 0.27463725286800 -0.12211955604632 0.78633617672900

O -1.51185699735498 0.95428256513026 -1.06045964960630

H 0.67663935054474 0.45226279184512 -0.04180387413119

H 0.97628798527750 -0.53874318247639 1.50319064969283

C -4.32495786651846 0.46438432535562 -0.78586412641421

C -5.40231641098133 -0.40969875949026 -0.94692208052515

C -6.47904813100842 -0.04590017653251 -1.74911135979895

C -6.48512275171971 1.18716588781714 -2.39981140767857

C -5.41114842953426 2.05772344773773 -2.22847899301810

C -4.33247757822140 1.70769872011636 -1.41896984059335

H -5.38970153378835 -1.37139906286813 -0.44158268778306

H -7.31273634042946 -0.73128489955943 -1.86833365534428

H -3.51173281512719 2.39807594970700 -1.27384948131234

H -3.53249387347240 -0.59129689702664 0.80096309735662

H -5.41172378590256 3.02583332306376 -2.72042855823179

H -7.32293982424795 1.46923407397156 -3.02995917784554

C -1.62590781681173 -1.10719336508626 2.06477553404958

H -2.31213750107416 -0.49903531451080 2.66401896804431

H -2.18080914309739 -1.98025729693489 1.70315368178234

H -0.82887300977904 -1.46375129724754 2.71978357912556

0 imaginary frequencies

SP = -518.032317172856

U = -517.83104558

H = -517.83010137

G = -517.87790366

**29 TS**

N -3.27728695895727 0.21621883476581 0.21600916329003

C -1.93838513050392 0.59375319418605 0.15916552777915

C -1.07553155495991 -0.01496969172324 1.13296823982929

C 0.28982400052374 0.21664102336558 1.02542676077774

O -1.55785944478170 1.41650984474919 -0.71426710365354

S 1.47563635023765 -1.25164263803566 -0.41280599872804

C 3.01606108871734 -0.30463780670911 -0.20845888365434

H 0.63584893092319 1.07084168838717 0.45511504060900

H 0.93381463351036 -0.07840114133411 1.84733178981908

H 2.96831357160813 0.65504122551877 -0.73326732136990

H 3.20882538443975 -0.10302286429455 0.85152908729963

H 3.87116724911896 -0.86171383143518 -0.60193810397294

C -4.27914580818127 0.52701812770579 -0.72686941309312

C -5.20958260506170 -0.46973262804780 -1.04689035337742

C -6.24992551867694 -0.20760458587250 -1.93180012385875

C -6.37207714407206 1.04969010015049 -2.52213285226424

C -5.44938263836889 2.04283950154386 -2.19983229791198

C -4.41333824440647 1.79537429697365 -1.30145977745601

H -5.10888553037963 -1.45303159255812 -0.59462207041148

H -6.96274014875094 -0.99311525842877 -2.16558887350520

H -3.72005523737250 2.58414286648298 -1.04054634468953

H -3.47324994875315 -0.60566857976180 0.76881577569399

H -5.53997606350873 3.03119129490962 -2.64162437092418

H -7.17900301738458 1.25415931952162 -3.21906285625497

C -1.59110551889643 -1.08150929660004 2.07515834144682

H -2.43976166685105 -0.74505247879247 2.68349820374231

H -1.91246017549155 -1.99376090256931 1.54954044939621

H -0.79773885372036 -1.37655802209796 2.76760836544240

1 imaginary frequency: -300.45 cm-1

SP = -956.294841736569

U = -956.05152226

H = -956.05057805

G = -956.10628782

**29 carbanion**

N -2.94505931253304 -0.64261155783391 -0.90871531730190

C -1.64857335708894 -0.01987393616915 -0.80439194738088

C -0.99997830304880 -0.10187473845097 0.39873682596154

C 0.41882390974544 0.36264766213818 0.50484793221219

O -1.19893642716769 0.52488945035643 -1.89636832214284

S 1.59093421925197 -1.05238141327639 0.41399932767663

C 3.14145876803871 -0.17215930552163 0.72430437430929

H 0.68072199427311 1.05407749650636 -0.29810596347262

H 0.60571343821525 0.85790273466093 1.46432759898094

H 3.32671907563644 0.57436831347413 -0.05240412040814

H 3.12050075927043 0.31608685436833 1.70205907781447

H 3.95556693881323 -0.90054603835035 0.71277306907187

C -4.10611772740736 0.08563179634734 -1.19897132025138

C -5.35022615548287 -0.54866726758528 -1.03262722796739

C -6.53359622424665 0.12053898802285 -1.31720241341553

C -6.51332863358383 1.43713855031750 -1.78218874558981

C -5.28367586446861 2.07142976582359 -1.93979482547950

C -4.08922482814756 1.41382114056280 -1.64805815008130

H -5.37529869229283 -1.57453975505698 -0.67314820627993

H -7.48102250032283 -0.39237028492323 -1.17501905923192

H -3.14370517259851 1.92631709451642 -1.77465805829363

H -3.11339613511982 -1.35213978047167 -0.20958437711537

H -5.24477736398731 3.09919527971091 -2.29104893178337

H -7.43844676970630 1.95712283776033 -2.01093957902821

C -1.59146359562321 -0.76473736640734 1.62603544782350

H -2.66885587453711 -0.59100659720200 1.72143003210637

H -1.43365528014164 -1.85324662697817 1.65657086461654

H -1.12410088573962 -0.35901329633903 2.53114201465039

0 imaginary frequencies

SP = -956.313588742604

U = -956.06979541

H = -956.0688512

G = -956.12608902

**29 anti-adduct**

N -3.01170625190715 0.22298599167539 0.19577432482091

C -1.92816511581046 0.95936762700399 0.54547743501281

C -1.03053730960201 0.31977698679758 1.59868103385923

C 0.40558302183645 0.24811774775537 1.08153542857647

O -1.67565965969034 2.07472166353255 0.08369857118362

S 0.51873241852751 -0.85125502517571 -0.36128609519685

C 2.22040863396505 -0.48866982298463 -0.85299349835321

H -3.06953843959621 -0.69756776543066 0.61026832776822

H 0.74610063946474 1.24536052200005 0.79009383119225

H 1.05919986716637 -0.12743476371771 1.87258502786264

H 2.32743489432967 0.56507694199104 -1.12024832501786

H 2.91667081947382 -0.73932847526476 -0.04956139008431

H 2.45162044208972 -1.10226507614435 -1.72618403474551

C -4.02881960693133 0.51588157806313 -0.74550750885797

C -4.87356299118461 -0.54253040651747 -1.09945828304752

C -5.91097676846965 -0.34102234525803 -2.00024719455390

C -6.11874165887924 0.91839567294617 -2.56325407444100

C -5.27790077799568 1.96798150175873 -2.20701018813635

C -4.23482673712481 1.78112018128629 -1.29968082195802

H -4.70999533969881 -1.52357653000062 -0.66105517403274

H -6.55782244854384 -1.17233965378033 -2.26389592645227

H -3.59772337907281 2.60992607140328 -1.02821816005860

H -5.43098947924264 2.95518248137428 -2.63317561128056

H -6.92781113909232 1.07734804022578 -3.26921493593246

H -1.38818341959816 -0.69266723075174 1.81425633374415

C -1.09451056101915 1.15540064653505 2.88253666571882

H -0.47666150117632 0.69475701659933 3.65820502062155

H -0.72321736149241 2.16814847655631 2.70018813108199

H -2.12140079072534 1.22310794752168 3.25369109070648

0 imaginary frequencies

SP = -956.835711030770

U = -956.57709941

H = -956.5761552

G = -956.63268513

**29 syn-adduct**

N -3.01511145021916 0.17152985092758 0.19629049999601

C -1.94967556622001 0.89354220675280 0.61672395869339

C -1.02490239412506 0.22429744014990 1.63385887477874

C 0.39575392545048 0.19129446753279 1.05792511348083

O -1.70564483294090 2.03909024709693 0.22603805276243

S 0.49333694784842 -0.87069411175916 -0.41806294486093

C 2.10115813172482 -0.32124460073418 -1.03586114825753

H -3.10159159120075 -0.76067194522896 0.57622847774103

H 0.70265101769584 1.19774558656382 0.76678548656518

H 1.08756605149070 -0.17848998896885 1.81863321183976

H 2.07616948336417 0.74281463394751 -1.28141458159368

H 2.88498025553279 -0.51290136029518 -0.29962620875899

H 2.32006063042765 -0.89088066127160 -1.94140913891691

C -4.00452589395992 0.50391923596675 -0.76053257967420

C -4.91955430862400 -0.50699651137528 -1.07966878303052

C -5.92804197279360 -0.27494940285687 -2.00513963882274

C -6.03830935540880 0.96870248204908 -2.62840969538174

C -5.12780628174002 1.97021004541126 -2.30870676717076

C -4.11073717853351 1.75214961701977 -1.37792034975930

H -4.83218933032195 -1.47689801141808 -0.59685216636465

H -6.62883283194019 -1.07028008865931 -2.24042989382129

H -3.41459766157497 2.54207571049834 -1.13883608666792

H -0.99760917027892 0.92596955620712 2.47522173792850

C -1.47225404845626 -1.14076925011628 2.15795078656975

H -0.75063984929319 -1.49349657024847 2.89965478398466

H -2.44957870836091 -1.08245114891861 2.64614462730459

H -1.52082664969084 -1.89706207487131 1.36705858373025

H -5.20279855035902 2.94411976395073 -2.78362842627055

H -6.82544881749287 1.15232488264777 -3.35301578602340

0 imaginary frequencies

SP = -956.833446240724

U = -956.57477351

H = -956.57382930

G = -956.62958611

**30**

N -3.20524462744164 0.28399292984156 0.00416131276543

C -1.89120474790809 0.35812305763925 -0.34331158832558

C -0.92769025831239 -0.19037515851788 0.67510516899407

C 0.37340022855491 0.00479501744910 0.45792547034176

O -1.51660894065472 0.84046581550261 -1.41531477876845

H -3.44480273385656 -0.25292693730668 0.82642288509862

H 0.72627537053979 0.53941266798684 -0.41793542316204

H 1.11510212678350 -0.36749025879292 1.15863937233216

C -4.29622614196155 0.65436328693707 -0.82087694498949

C -5.42918103260709 -0.11808562191034 -0.80553079639148

C -4.24932138834915 1.84005392107619 -1.60563421053531

C -6.54060600336973 0.25660371822620 -1.59882500731344

C -5.31422177448089 2.20371549077627 -2.38564140229906

H -3.36358254198124 2.46119428260969 -1.57303489616730

C -7.74290010973782 -0.49003994948607 -1.64841845391882

C -6.48936759706370 1.41213896812378 -2.40334115438694

H -5.27840610025386 3.10798210386891 -2.98415508681988

C -8.60754917380891 0.99691795625004 -3.13241667462305

H -9.45986897018927 1.27685658870338 -3.74481483199774

N -7.55763102602523 1.77509646152939 -3.18068612226182

N -8.76470312825047 -0.14084303308884 -2.39656431021036

H -7.84047569724628 -1.39393627157009 -1.05060218060401

H -5.48174900174882 -1.01826572785455 -0.19980061384220

C -1.45348701378946 -0.92154579593881 1.88302154505687

H -2.07010637005786 -0.26962709289801 2.51181199631156

H -2.06455950496041 -1.78335187881580 1.59274936760246

H -0.62128384182296 -1.28422454034029 2.48906735811405

0 imaginary frequencies

SP = -703.867876260484

U = -703.6404896

H = -703.63954539

G = -703.69262941

**30 TS**

N -3.26168719908973 0.56371439013309 0.32525845111092

C -1.89601380435528 0.82398977987990 0.24180148347115

C -1.05980460238162 0.08001731140424 1.13993286548346

C 0.31538349002764 0.19310119917549 0.99673704583548

O -1.48322886069196 1.67300627889110 -0.59048616627077

S 1.32856666299642 -1.35837755296239 -0.51631278536021

C 2.97322980053922 -0.60735744817373 -0.30506480572700

H 0.72068313425466 1.02639526220175 0.43490648089412

H 0.95604008764739 -0.19055428190498 1.78367595146480

H 3.06448856577578 0.32753475863928 -0.86713141149558

H 3.16461434809812 -0.38760890460276 0.75191125465369

H 3.76003050873880 -1.28463006602771 -0.64965683674449

H -3.53471030976913 -0.30653359281500 0.75868629480365

C -1.64577183601025 -0.96816092788781 2.06085434277308

H -2.44338899464377 -0.57496264550976 2.70261565738451

H -2.06347627495203 -1.82729109281011 1.51432508586733

H -0.86433418851852 -1.35909536767493 2.71852327869284

C -4.25617581556459 1.19550069670645 -0.44243297672288

C -5.28572980735106 0.45717831999425 -0.97427022509025

C -4.25645363444483 2.61406320716859 -0.59419518630405

C -6.33753108670454 1.11030308665283 -1.66370547524047

C -5.25681791189095 3.25361533323490 -1.27432756676442

H -3.45788228487343 3.18812086196444 -0.14076080218413

C -7.43806985673618 0.42142242171057 -2.22834534427135

C -6.32844601342593 2.50977131312870 -1.83229334632200

H -5.25380599521555 4.33380901053006 -1.37855078328894

C -8.29819905867101 2.38816485709364 -2.97156904528596

H -9.10550795184481 2.88350103732552 -3.50339242902570

H -5.30941460705260 -0.62327956017269 -0.86153657302497

N -7.33951086602756 3.14519239958409 -2.50278802575858

N -8.40775257381213 1.03346569447173 -2.87147182689432

H -7.50132306405041 -0.66101577934880 -2.13493658065893

1 imaginary frequency: -291.84 cm-1

SP = -1142.131459281030

U = -1141.86135296

H = -1141.86040875

G = -1141.92093629

**30 carbanion**

N -3.21565332916399 -0.03604356822430 -0.09736658976809

C -1.86747665474357 0.47024392333322 -0.13489079466211

C -1.01107733903120 -0.02644430562590 0.81556838613822

C 0.44615322183431 0.29803017624643 0.73900052461813

O -1.58862145799165 1.32167847217029 -1.07176140177286

S 1.39059298004394 -1.05457355846239 -0.08358631824130

C 3.07363968544950 -0.42060198147746 0.11855605238211

H 0.63081774288541 1.21317362897884 0.17341761479535

H 0.88357486687796 0.41359769891820 1.73719013925623

H 3.18963916832590 0.54270933728784 -0.38471379031038

H 3.32207049028793 -0.31064743272375 1.17742450497148

H 3.76441757042675 -1.13751231050178 -0.33126473493550

H -3.29052660944207 -1.02633337985502 0.08744692670930

C -1.43800028890566 -1.04741247545070 1.84742072937155

H -2.42901112103217 -0.83460320524562 2.26331424132154

H -1.47016622168159 -2.07882292311851 1.46204270760149

H -0.73085818656454 -1.05285285497086 2.68527251731418

C -4.27797568573315 0.49652023395335 -0.81566995653111

C -5.23435198993659 -0.32478739752987 -1.37575981677503

C -4.44919932470539 1.91520600816867 -0.90976542335050

C -6.36143505770593 0.23471564167862 -2.02525474437115

C -5.52121122596392 2.46588453753847 -1.55569364581059

H -3.71247109176077 2.55730709410499 -0.44236403006588

C -7.38440814728775 -0.54594405848121 -2.61634910824314

C -6.51567633643255 1.63264631560120 -2.12986813869331

H -5.63859433711959 3.54344192420741 -1.61467971647483

C -8.47163910290212 1.34212563851801 -3.26347436317412

H -9.33514297165854 1.76714570115679 -3.76721749123445

N -8.42414089092966 -0.01893271788637 -3.22605635524481

N -7.59814676658005 2.17967311669191 -2.76469074952225

H -5.13344317930311 -1.40563944099437 -1.32073928161343

H -7.32467840955604 -1.63194783800612 -2.57548789368472

0 imaginary frequencies

SP = -1142.151209205594

U = -1141.88137982

H = -1141.88043561

G = -1141.94280162

**30 anti-adduct**

N -3.26002010919405 -0.25916471321320 0.02773001206670

C -2.22323549668293 0.45907989177041 0.53096230185417

C -1.08542346517560 -0.36353532876437 1.11398315196723

C 0.14912841667816 -0.14087702051537 0.23259290303291

O -2.19412575329033 1.69172301420260 0.51882139587295

S 1.53295303031147 -1.18475474740908 0.77707122762159

C 2.69106744731168 -0.79912930777109 -0.55684615771990

H -0.08165307536686 -0.39723160132775 -0.80567716278318

H 0.45515384438262 0.90797743210232 0.27463512417907

H 2.28385663680496 -1.10258236200934 -1.52401737972659

H 2.92072863961670 0.26876921232153 -0.57144115293049

H 3.61117179058709 -1.35587390169419 -0.36739075030031

H -3.13087779290025 -1.25800721721840 -0.06446606372599

C -0.85827679959970 0.05037192042355 2.57105100841429

H -0.51450405284767 1.08739983607097 2.62592259026030

H -1.78368604038997 -0.04102053916406 3.14745065243874

H -0.10348932124450 -0.58707421625599 3.03774240621911

C -4.38405789500192 0.30571351463094 -0.63082798964819

C -4.81461099928541 -0.22482548056009 -1.81792513101604

C -5.08505752417534 1.38794086599916 -0.02992350746887

C -5.95685888759495 0.32737963509256 -2.44937014440502

C -6.18277214061087 1.93641014072423 -0.63588139610414

H -4.74471123446562 1.76863722860742 0.92569807598047

C -6.46758144310363 -0.15662395730762 -3.67788585912650

C -6.64245643799302 1.41493245131134 -1.87229920108981

H -6.71937905901644 2.76043314812910 -0.17764803314068

C -8.10616862286181 1.41457827399488 -3.61879732280623

H -8.97626132473666 1.83797285940366 -4.11221272505204

N -7.51988626152605 0.36678927881517 -4.26505480363882

N -7.74082253700225 1.95671286470211 -2.48584369430834

H -4.29245201096483 -1.05672577735121 -2.28133267351318

H -5.97979101620190 -0.99537364688962 -4.17042350501862

H -1.36090050445985 -1.42202175085055 1.07460380361543

0 imaginary frequencies

SP = -1142.669452045735

U = -1142.38473602

H = -1142.38379181

G = -1142.4458211

**30 syn-adduct**

N -3.13995738786242 0.32185094974788 0.37874330830459

C -1.97549447429990 0.95164219311151 0.67774804660904

C -1.05123545037698 0.24929677336463 1.67082439011436

C 0.34826228505933 0.14376003691354 1.05651210254359

O -1.66088995723768 2.04433988127773 0.20028518396923

S 0.35806802830661 -0.95785324773274 -0.39334850813774

C 1.95226906411221 -0.46525352169791 -1.08975485063051

H 0.68760396769128 1.12852151321996 0.73042289694929

H 1.04628346606535 -0.23538711729730 1.80673031451912

H 1.94071417535120 0.59050489511744 -1.36973035719942

H 2.75939545400868 -0.65052055730150 -0.37747374637510

H 2.12370726688436 -1.06912769791321 -1.98324344069244

H -3.25457764337521 -0.61915159034668 0.72928381936892

C -1.54817200081313 -1.08736594118216 2.22312865549779

H -2.49673167243922 -0.97531968819679 2.75608456042708

H -1.67499731291792 -1.84124604344606 1.43887919233793

H -0.81268971631008 -1.47580539523823 2.93251298497689

C -4.13048709225209 0.74435152011996 -0.53998521362548

C -4.88158076041959 -0.21680963362373 -1.16999637611408

C -4.40239210076999 2.12344580433361 -0.76271578132364

C -5.91164197701163 0.17506597279885 -2.05769414603992

C -5.38957210746707 2.51009807617063 -1.63046647044657

H -3.82744424279056 2.86990299980919 -0.23227358876303

C -6.72402892987215 -0.75262266822560 -2.75601004027576

C -6.16946076454897 1.53827045293472 -2.30347296896949

H -5.59546762141472 3.56205845089261 -1.79842895730505

C -7.83102660300925 0.96311015876868 -3.75228341324067

H -8.61509857746336 1.25675716965220 -4.44424199051025

N -7.66737258347428 -0.38180900513528 -3.59099103533201

N -7.15689022718700 1.92197299215639 -3.17297502006777

H -4.69373498822780 -1.27289457269642 -0.99662114653105

H -6.57145468946110 -1.82003101923474 -2.60846604017116

H -0.96790482647678 0.95724785887881 2.50401763613333

0 imaginary frequencies

SP = -1142.669068329836

U = -1142.38422880

H = -1142.38328459

G = -1142.44410243