

Supporting Information

for

DFT/TD-DFT calculations on the sensing mechanism of a dual response near-infrared fluorescent chemosensor for superoxide anion and hydrogen polysulfides: Photoinduced electron transfer

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Table S1 The test results of TD-DFT calculation for Keto-Cy

No.	Functional/Basis	Solvation model	Energy ^a (nm/eV)	<i>f</i>
1	PBE1PBE/TZVP	PCM	489/2.54	1.9621
2	PBE1PBE/TZVP	CPCM	499/2.49	2.0069
3	B3LYP/TZVP	PCM	504/2.46	1.8974
4	B3LYP/TZVP	CPCM	514/2.41	1.9475
5	BP86/TZVP	CPCM	596/2.08	1.7347
6	BP86/6-311G*	CPCM	588/2.11	1.6683
7	BP86/6-311++G**	CPCM	600/2.07	1.7727
8	B3LYP/6-311++G**	CPCM	520/2.38	1.9568
9	B3LYP-D3/TZVP	CPCM	513/2.42	1.9433
10	B3LYP-D3/6-311+G*	CPCM	518/2.39	1.9557
11	B3LYP-D3/6-311++G**	CPCM	519/2.39	1.9524

^a The value of experimental absorption is 535 nm.

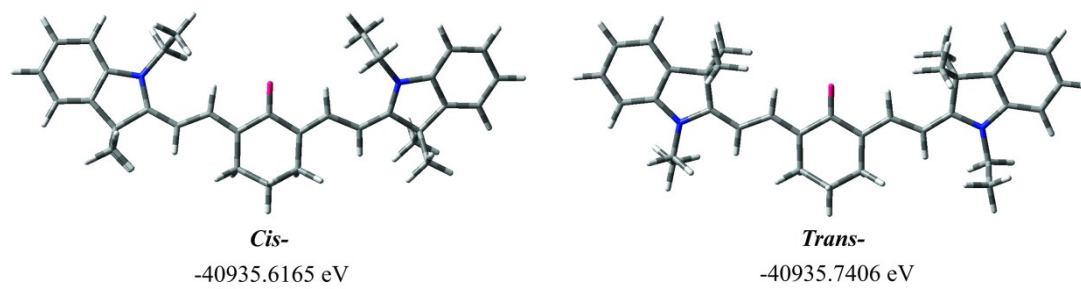


Fig. S1 The calculated *cis*- and *trans*-configurations and the corresponding absolute free energies of Keto-Cy.

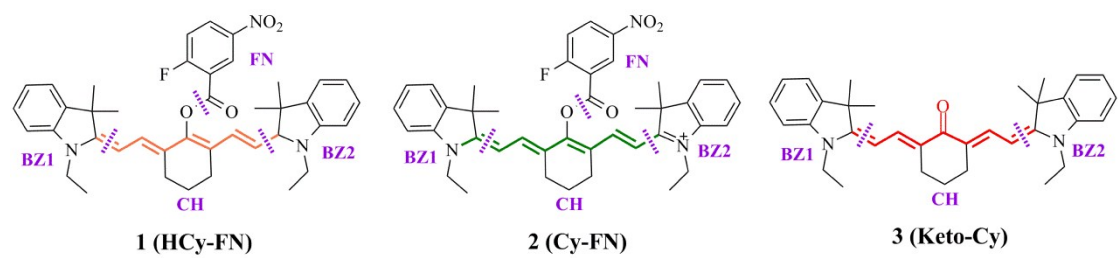


Fig. S2 The partitioning scheme for the research on MO compositions.

Appendix: List of coordinates

Coordinates for HCy-FN (ground state)

Coordinates for Cy-FN (ground state)

Coordinates for Keto-Cy (ground state)

Coordinates for HCy-FN (excited state)

Coordinates for Cy-FN (excited state)

Coordinates for Keto-Cy (excited state)

Coordinates for HCy-FN (ground state)

C	-7.17757300	-1.24136400	0.35552300
C	-6.67933900	0.01887400	0.69503800
C	-7.54219600	1.03010200	1.07334200
C	-8.91970200	0.77633900	1.10676400
C	-9.40548900	-0.48243400	0.76064700
C	-8.54299900	-1.51288600	0.37706200
C	-4.90002500	-1.43264400	0.09804500
C	-5.16462400	0.01271800	0.57085700
H	-7.16235500	2.00978100	1.34017200
H	-9.60678100	1.56055000	1.39952000
H	-10.47218400	-0.67163900	0.78396000
H	-8.93692800	-2.48267300	0.10379500
N	-6.11871400	-2.09074500	0.02675500
C	-6.30647800	-3.47951400	-0.37908200
C	-6.44733100	-3.65987300	-1.89101000
H	-7.19621200	-3.85131500	0.12931400
H	-5.46691800	-4.06188100	0.00094800
H	-6.58518800	-4.71771800	-2.12427100

H	-7.31141900	-3.11137400	-2.27008700
H	-5.55744800	-3.30785400	-2.41501300
C	-4.51982700	0.29345900	1.94557300
C	-4.71656400	1.05895800	-0.47160700
C	7.15322000	-1.05448900	0.78108900
C	7.22449200	-0.36560200	-0.44125500
C	8.42430500	0.16345400	-0.87960900
C	9.57314900	0.02308800	-0.08822800
C	9.49569800	-0.65537200	1.12550300
C	8.29041500	-1.19903500	1.57890300
C	4.94581700	-0.83048800	0.08093800
C	5.86964800	-0.42076900	-1.13021300
H	8.47939100	0.68891700	-1.82687000
H	10.51507100	0.44404600	-0.41801400
H	10.38286100	-0.75942000	1.73988600
H	8.24967700	-1.71541000	2.52940200
N	5.87000900	-1.54306500	0.99793700
C	5.40963900	-1.90447200	2.33594400
C	5.19732300	-0.72988300	3.29759800
H	6.13282800	-2.60472500	2.75943800
H	4.47597400	-2.45777800	2.22008200
H	4.87450700	-1.10521500	4.27150600
H	6.11845800	-0.16226100	3.44268300
H	4.42878200	-0.04693700	2.93058400
C	5.90865600	-1.49511400	-2.23562400
C	5.42302200	0.91604400	-1.72869000
C	-0.12100200	2.57937200	1.32587700
C	-0.16603000	2.30006200	-0.04616300
C	-0.30583700	3.38432900	-0.91356900
C	-0.39796000	4.66990200	-0.41197100

C	-0.35363500	4.93342300	0.95445600
C	-0.21257500	3.87086800	1.82707100
H	-0.34134800	3.20524600	-1.97741900
H	-0.42611600	5.94556000	1.32413000
H	-0.17019100	4.02537400	2.89674400
F	0.01964300	1.59562200	2.22436400
N	-0.54674100	5.78928500	-1.35216200
O	-0.63169700	6.92303900	-0.89087300
O	-0.57907700	5.54099300	-2.55313500
C	0.10263000	-3.82093500	-1.64959000
C	1.37163500	-3.36368400	-0.93358200
C	1.27252900	-1.93849100	-0.43783800
C	0.03684700	-1.39413700	-0.26852500
C	-1.22937700	-2.07210900	-0.41337900
C	-1.14262500	-3.53106800	-0.81281100
H	0.02255300	-3.29817800	-2.60800300
H	1.58664500	-4.02787500	-0.08725600
H	-1.12190700	-4.15283400	0.09147900
C	-0.07227300	0.94784200	-0.68007300
O	-0.03559900	0.79365300	-1.87962800
O	-0.03817400	-0.05563100	0.21140400
C	2.48193400	-1.19857300	-0.12711500
C	3.74217100	-1.64950500	-0.25907700
C	-3.71191600	-2.03557300	-0.20741700
C	-2.41234900	-1.44332100	-0.13961200
H	-3.63314700	1.07807700	-0.58422000
H	-5.16092600	0.85069600	-1.44635000
H	-5.04075600	2.05154500	-0.15284300
H	-3.43172800	0.28273900	1.88849200
H	-4.83091200	1.27815400	2.30016800

H	-4.83345900	-0.45011700	2.68025500
H	-3.75878800	-3.06728500	-0.52888600
H	-2.35583600	-0.41151700	0.17435500
H	-2.03456600	-3.82363700	-1.36796900
H	0.16419800	-4.88869100	-1.87125800
H	2.22466400	-3.45111200	-1.60999900
H	2.35074600	-0.19763800	0.27083200
H	3.93708400	-2.64999800	-0.62852800
H	6.18113700	-2.47389000	-1.83565900
H	4.93925900	-1.58391700	-2.73097000
H	6.64977100	-1.21783300	-2.98801000
H	6.08216000	1.21203600	-2.54790300
H	4.40927800	0.83612200	-2.12996400
H	5.43328200	1.70900800	-0.97815600
H	4.61207800	0.10252900	0.55564800

Coordinates for Cy-FN (ground state)

C	-7.17822800	-0.90279200	-0.16271400
C	-6.62183800	0.31618900	-0.54162000
C	-7.44251200	1.39121100	-0.83293800
C	-8.82796600	1.22727900	-0.73520500
C	-9.36966500	0.00151100	-0.35027900
C	-8.55078300	-1.08950000	-0.05523500
C	-4.92181100	-1.26896800	-0.12121100
C	-5.11037800	0.19426400	-0.55783000
H	-7.02391600	2.34505700	-1.13130300

H	-9.48469200	2.05881700	-0.95847000
H	-10.44426600	-0.11090800	-0.27549700
H	-8.98158900	-2.03375200	0.24872600
N	-6.14139400	-1.82999500	0.06582600
C	-6.40159700	-3.21206900	0.48499500
H	-7.35171900	-3.50524700	0.04125900
H	-5.63901600	-3.84985400	0.04216900
C	-6.44277100	-3.37612400	2.00287900
H	-7.22611300	-2.75740200	2.44293500
H	-6.65267100	-4.41913800	2.24620700
H	-5.48821100	-3.10361000	2.45505900
C	-4.48715700	1.18707200	0.44824100
H	-3.39942600	1.13493800	0.44771900
H	-4.77657300	2.20196600	0.17184800
H	-4.84339700	0.99136900	1.46068000
C	-4.57304900	0.43424200	-1.98672600
H	-4.84228700	1.44258800	-2.30486300
H	-3.48856100	0.34298600	-2.02865300
H	-5.00843600	-0.27677400	-2.69045700
C	7.13776800	-0.87715900	0.07389200
C	6.59187800	0.32750900	-0.36209000
C	7.41984600	1.39370400	-0.66488100

C	8.80244900	1.23302100	-0.52880200
C	9.33409000	0.01914400	-0.09523500
C	8.50765600	-1.06207600	0.21435900
C	4.88158200	-1.24655300	0.05693200
C	5.08134100	0.20482100	-0.41247200
H	7.00927100	2.33767700	-1.00312000
H	9.46493400	2.05693900	-0.76306900
H	10.40685900	-0.09263600	0.00303200
H	8.93110200	-2.00066700	0.54510000
N	6.09354500	-1.78965400	0.32710300
C	6.34309700	-3.16033500	0.78877800
H	7.23414500	-3.12834100	1.41395200
H	5.51827700	-3.45635700	1.43376700
C	6.52583300	-4.15085000	-0.35930900
H	7.37219300	-3.87129800	-0.98830200
H	6.71724400	-5.14416000	0.05033000
H	5.63124100	-4.20258400	-0.98140400
C	4.57991300	0.41002600	-1.85920500
H	4.85591900	1.41103000	-2.19430200
H	5.03404800	-0.31638800	-2.53476800
H	3.49700200	0.31560800	-1.92674500
C	4.43346400	1.22107300	0.55460800

H	4.72942600	2.22927600	0.26129900
H	3.34606800	1.16796200	0.52900500
H	4.76519300	1.04943500	1.57968300
C	-0.01528300	-4.39141100	-0.01986700
C	1.23880800	-3.67502000	0.47669100
C	1.22860700	-2.20214100	0.12468100
C	-0.01905700	-1.58375300	-0.03711100
C	-1.26932400	-2.20644200	0.08374000
C	-1.28386300	-3.67763400	0.44267200
H	-0.00065700	-4.42765100	-1.11350800
H	1.32162100	-3.78624600	1.56452000
C	-3.73946800	-1.97940000	0.07090100
H	-3.83882200	-3.00409600	0.39897100
C	-2.44936200	-1.48019700	-0.10133200
H	-2.33943100	-0.44927900	-0.40049900
H	-2.15515700	-4.15857100	-0.00405800
H	-1.39266100	-3.78451000	1.52856000
H	-0.01887000	-5.42367900	0.33567800
H	2.12233800	-4.15106200	0.04917100
C	2.41110900	-1.46897100	-0.01368200
H	2.30694600	-0.43566500	-0.30689200
C	3.69646600	-1.96453500	0.19842600

H	3.79014700	-2.99480400	0.50986300
C	-0.01090700	2.11463800	0.03500400
C	0.07440000	3.13629200	0.98238100
C	0.10705500	4.45793600	0.57737900
C	0.05624200	4.81894100	-0.76632500
C	-0.03140100	3.81901700	-1.71668500
C	-0.06367900	2.49128800	-1.31363000
H	0.11494200	2.88102200	2.03046900
H	0.08301400	5.85804300	-1.05947900
H	-0.07606800	4.05087500	-2.77218700
F	-0.15632700	1.57077200	-2.28173800
N	0.19572100	5.51102200	1.59888200
O	0.24872600	5.17550000	2.77752700
O	0.21192100	6.67861700	1.22310000
C	-0.04001300	0.71972200	0.56541700
O	-0.07486600	0.46216400	1.74465500
O	-0.01284400	-0.21944100	-0.40591100

Coordinates for Keto-Cy (ground state)

C	7.17417100	-0.20407700	0.19977000
C	6.60542200	-1.47622300	0.11924300
C	7.41330000	-2.59804800	0.09629600

C	8.80348700	-2.43765400	0.15085300
C	9.35864200	-1.16210800	0.22679100
C	8.55239900	-0.02130400	0.25106300
C	4.91165800	0.18278300	0.12491600
C	5.09223100	-1.34831700	0.07353500
H	6.98150000	-3.59043400	0.03566200
H	9.44821400	-3.30757400	0.13141000
H	10.43522200	-1.04616200	0.26463700
H	8.99649100	0.96369500	0.30320500
N	6.15922700	0.76020100	0.22058100
C	6.42747200	2.19487400	0.28611600
C	6.54215900	2.85356900	-1.08865300
H	7.35219300	2.32680400	0.84737400
H	5.63696000	2.66200000	0.87310800
H	6.74451200	3.91974600	-0.96838000
H	7.35783400	2.41375900	-1.66500000
H	5.61758200	2.74294500	-1.65695400
C	4.46341200	-2.04188400	1.30177400
C	4.54873100	-1.95200600	-1.23920300
C	-7.18066300	-0.19144600	-0.06468000
C	-6.61148200	-1.46482900	-0.11750900
C	-7.41997200	-2.58566800	-0.15970100

C	-8.81090000	-2.42324500	-0.14357700
C	-9.36627300	-1.14685300	-0.08475700
C	-8.55946800	-0.00699000	-0.04247800
C	-4.91621800	0.19186500	-0.06036200
C	-5.09745400	-1.33876300	-0.12233000
H	-6.98804300	-3.57885400	-0.20412500
H	-9.45603800	-3.29250400	-0.17525400
H	-10.44329000	-1.02986200	-0.06884800
H	-9.00293700	0.97827500	0.01010900
N	-6.16579600	0.77284900	-0.04803400
C	-6.43432300	2.20782400	0.00430800
C	-6.49391300	2.76424400	1.42681200
H	-7.38059000	2.37935200	-0.50843800
H	-5.66719800	2.71820100	-0.57782000
H	-6.70333400	3.83528300	1.39200900
H	-7.28481700	2.28056500	2.00263400
H	-5.54696200	2.61833400	1.94863800
C	-4.51868200	-1.93411000	-1.42426800
C	-4.50342200	-2.04125400	1.11751100
C	0.00495500	3.21017800	-0.66287400
C	-1.24781600	2.63158400	-0.01196600
C	-1.26812300	1.11971600	-0.05966600

C	0.00024700	0.36666500	-0.07927000
C	1.26921000	1.11723500	-0.03434900
C	1.25662500	2.63023800	-0.01162700
H	0.00422700	2.97409400	-1.73257000
H	-1.29375900	2.97557600	1.03049400
H	1.31239500	2.98906600	1.02544000
O	-0.00037700	-0.88972400	-0.12413200
C	-2.43341600	0.40150400	-0.06724300
C	-3.75560600	0.92264500	-0.02305200
C	3.75299500	0.91662400	0.08525300
C	2.43198100	0.39612900	0.01119200
H	3.46414800	-1.86998100	-1.29965200
H	4.98179300	-1.45090000	-2.10657200
H	4.81253100	-3.01012600	-1.28751700
H	3.37815400	-1.94611800	1.30230100
H	4.71172800	-3.10477700	1.28520100
H	4.84836800	-1.61399700	2.22898100
H	3.85814400	1.99303500	0.11401500
H	2.30471900	-0.67756800	-0.00717200
H	2.14601000	3.01859800	-0.51295200
H	0.00621000	4.29971300	-0.57402500
H	-2.13731700	3.03381000	-0.50192300

H	-2.30743300	-0.67173400	-0.10948600
H	-3.86033600	1.99711700	0.04707200
H	-4.92959200	-1.42829800	-2.29967400
H	-3.43305200	-1.84892300	-1.45510700
H	-4.77889200	-2.99242200	-1.48576300
H	-4.75553700	-3.10300500	1.08871200
H	-3.41822200	-1.95059900	1.14748000
H	-4.91079500	-1.61709000	2.03677500

Coordinates for HCy-FN (excited state)

C	-7.01527900	-1.42952300	0.41469700
C	-6.55457600	-0.18947500	0.84892100
C	-7.45451300	0.76323500	1.29401300
C	-8.81606200	0.45074600	1.29147000
C	-9.26128200	-0.79636400	0.84929100
C	-8.36396900	-1.76329800	0.40054800
C	-4.75210800	-1.54027100	0.16378400
C	-5.04533700	-0.14596800	0.73192000
H	-7.11532800	1.73304300	1.63699300
H	-9.53467100	1.18410800	1.63517800
H	-10.32074700	-1.01955100	0.85188300
H	-8.71625300	-2.72510800	0.05435700

N	-5.91041300	-2.21577200	0.02447400
C	-6.06772000	-3.57877300	-0.50801100
C	-6.23734300	-3.59981300	-2.02509800
H	-6.93564700	-4.01068200	-0.01393300
H	-5.20519100	-4.16462200	-0.19986700
H	-6.36664600	-4.63249300	-2.35253100
H	-7.11559100	-3.03027000	-2.33141800
H	-5.36021900	-3.18715400	-2.52499600
C	-4.40507700	0.04489600	2.12635900
C	-4.61901300	0.97798200	-0.23998200
C	7.27180900	-0.85520300	0.71392500
C	7.27361800	-0.13085800	-0.48816400
C	8.44184600	0.43440900	-0.96572900
C	9.62823700	0.28988500	-0.23366900
C	9.61966100	-0.42626800	0.96075100
C	8.44661000	-1.00499100	1.45287600
C	5.03350900	-0.65996500	0.12353700
C	5.89094300	-0.18963000	-1.11934100
H	8.44280900	0.98898400	-1.89768100
H	10.54659500	0.73685500	-0.59406200
H	10.53657300	-0.53326000	1.52905400
H	8.45875400	-1.55035100	2.38782600

N	6.00657900	-1.37210000	0.97868400
C	5.61171600	-1.76257200	2.33144100
C	5.42256800	-0.60622200	3.31884900
H	6.36585200	-2.45547500	2.70979600
H	4.68479500	-2.33326800	2.24958100
H	5.15188800	-1.00231500	4.30025300
H	6.33913100	-0.02396300	3.43038200
H	4.62546500	0.06740100	2.99871000
C	5.89795200	-1.22757600	-2.25963700
C	5.39098000	1.15681900	-1.64918900
C	0.11362700	2.67149500	1.15909600
C	-0.25008900	2.30647500	-0.14123000
C	-0.85746400	3.26774700	-0.95112800
C	-1.11418500	4.55690000	-0.47426600
C	-0.73574200	4.89262700	0.83948800
C	-0.11796200	3.95052200	1.64195600
H	-1.14791000	3.00597600	-1.95578700
H	-0.92800000	5.88723000	1.21111400
H	0.19044400	4.19649200	2.64980400
F	0.74471000	1.79492200	1.98335000
N	-1.74983000	5.49648100	-1.29571000
O	-1.98221500	6.68623600	-0.83858200

O	-2.09476000	5.16377800	-2.49941000
C	0.32198400	-3.79217200	-1.63175400
C	1.54980600	-3.31195400	-0.86440500
C	1.41652700	-1.88071200	-0.41313300
C	0.14836500	-1.35445600	-0.26077400
C	-1.05862800	-2.08283000	-0.40360000
C	-0.95607900	-3.52188000	-0.84359400
H	0.27147700	-3.27428100	-2.59381900
H	1.70940000	-3.94027800	0.02060200
H	-0.98110400	-4.15777300	0.04993800
C	-0.05895600	0.96239000	-0.74152700
O	-0.02573500	0.74527100	-1.93033600
O	0.03300400	-0.02553800	0.18969100
C	2.57992400	-1.09247900	-0.10125500
C	3.85636800	-1.51588900	-0.20629300
C	-3.51864600	-2.10878600	-0.17826100
C	-2.28210500	-1.48305200	-0.08256500
H	-3.53622700	1.04358600	-0.32982000
H	-5.04333700	0.81786900	-1.23203700
H	-4.98473100	1.93145500	0.14261600
H	-3.31773600	0.06231500	2.06884700
H	-4.73968900	0.99622600	2.54168200

H	-4.70532600	-0.75391800	2.80580700
H	-3.54327600	-3.12184200	-0.55080000
H	-2.24272000	-0.46741100	0.27738900
H	-1.82620700	-3.79412800	-1.44118200
H	0.40883500	-4.85915700	-1.84206700
H	2.44195000	-3.41935300	-1.48138400
H	2.40938500	-0.08845600	0.26831400
H	4.08176400	-2.51981700	-0.54633100
H	6.20952000	-2.21220600	-1.90566400
H	4.90845200	-1.32035200	-2.71324400
H	6.59694700	-0.90941600	-3.03548900
H	6.00743600	1.49133100	-2.48640300
H	4.36205300	1.07026600	-2.00760000
H	5.42158300	1.92384500	-0.87299700
H	4.68289500	0.24648800	0.63387000

Coordinates for Cy-FN (excited state)

C	-7.17928600	-0.85946200	-0.06949600
C	-6.63601600	0.34328900	-0.51115700
C	-7.46879400	1.41155400	-0.79566900
C	-8.84466100	1.24721600	-0.62386900
C	-9.37198200	0.03375800	-0.17525800

C	-8.54393100	-1.04811700	0.11133100
C	-4.93725400	-1.23252600	-0.12531300
C	-5.13153100	0.21217600	-0.59474700
H	-7.06712000	2.35519400	-1.14351800
H	-9.51275500	2.07135700	-0.84005800
H	-10.44172000	-0.07074600	-0.04635800
H	-8.95797600	-1.98292700	0.46262500
N	-6.12701700	-1.78139300	0.13778500
C	-6.37943000	-3.15415900	0.61730700
H	-7.34616500	-3.44854800	0.21490200
H	-5.63771500	-3.81084100	0.17049100
C	-6.36883100	-3.25035400	2.14033900
H	-7.12802700	-2.60402000	2.58171700
H	-6.58531900	-4.28037900	2.42697900
H	-5.39449800	-2.97655700	2.54641800
C	-4.45424800	1.22936500	0.35338100
H	-3.36869900	1.17571500	0.29680700
H	-4.75834800	2.23436800	0.05995500
H	-4.75960800	1.06326400	1.38715400
C	-4.65769300	0.39690200	-2.05617000
H	-4.93261500	1.39811300	-2.38926800
H	-3.57744400	0.29305500	-2.14333400

H	-5.13341800	-0.33069400	-2.71489500
C	7.09863400	-0.88234400	0.14343800
C	6.57483100	0.31602700	-0.33321000
C	7.42200700	1.37253400	-0.61893300
C	8.79312400	1.19894300	-0.42032200
C	9.30154900	-0.01200800	0.05617300
C	8.45861900	-1.08068600	0.34866400
C	4.85567200	-1.23905900	0.04382300
C	5.07110600	0.19631700	-0.44370000
H	7.03499600	2.31368400	-0.98940100
H	9.47240200	2.01335500	-0.63855500
H	10.36831200	-0.12517000	0.20141700
H	8.85883700	-2.01622000	0.71403500
N	6.03299800	-1.78491800	0.36409500
C	6.26386900	-3.15891100	0.85093000
H	7.12827800	-3.11294600	1.50940600
H	5.41365800	-3.44809700	1.46285600
C	6.49481300	-4.14697800	-0.28935600
H	7.36025100	-3.86321200	-0.88899700
H	6.67972300	-5.13445200	0.13559500
H	5.62122000	-4.20845900	-0.93930700
C	4.62815400	0.36380700	-1.91663300

H	4.91684100	1.35835600	-2.25805100
H	5.11176100	-0.37609900	-2.55557100
H	3.54918200	0.26611200	-2.02404100
C	4.38156300	1.23110800	0.47634800
H	4.69616000	2.23028300	0.17415000
H	3.29698600	1.18146000	0.39932800
H	4.66619500	1.07843500	1.51808600
C	-0.04235600	-4.40091800	-0.12271600
C	1.20972100	-3.68343900	0.37356600
C	1.19875100	-2.21787000	0.02304100
C	-0.03934900	-1.58284600	-0.14855900
C	-1.28251200	-2.21531100	-0.01889400
C	-1.30735400	-3.68013900	0.33445800
H	-0.02548600	-4.44601100	-1.21525100
H	1.28374900	-3.77557200	1.46422400
C	-3.73486100	-1.95977000	0.03290700
H	-3.82989900	-2.97757900	0.38082600
C	-2.47096400	-1.46709900	-0.19159900
H	-2.35502700	-0.44477500	-0.51334300
H	-2.18398400	-4.15520600	-0.10568300
H	-1.41434500	-3.77037900	1.42249800
H	-0.04935900	-5.42795600	0.24428100

H	2.09815700	-4.15972500	-0.04085200
C	2.39228300	-1.46990900	-0.10474900
H	2.28835700	-0.44470800	-0.42165300
C	3.64836200	-1.96567200	0.15689000
H	3.73315500	-2.98971700	0.48814900
C	-0.00704900	2.09980600	-0.01552800
C	0.13459400	3.09751500	0.95325700
C	0.19785500	4.44788600	0.60169800
C	0.10973300	4.80882200	-0.75636800
C	-0.03567700	3.83021700	-1.72181500
C	-0.09004100	2.49308800	-1.35772400
H	0.20169400	2.81596300	1.99152700
H	0.15530600	5.85042200	-1.03452100
H	-0.10827200	4.09150900	-2.76954400
F	-0.24147300	1.58625500	-2.35593700
N	0.35357400	5.42690900	1.59105800
O	0.43576800	5.07200900	2.83404600
O	0.41032400	6.67415800	1.24588800
C	-0.05244300	0.70710400	0.48803900
O	-0.09315400	0.39809700	1.65497100
O	-0.02855100	-0.23042300	-0.50880500

Coordinates for Keto-Cy (excited state)

C	7.20104300	-0.14968900	0.23666800
C	6.67657800	-1.44477100	0.12559100
C	7.52460300	-2.53539700	0.10281000
C	8.90691500	-2.32570000	0.18784500
C	9.41758000	-1.03035900	0.29378800
C	8.57620700	0.07992200	0.31883500
C	4.93175800	0.14630500	0.12432400
C	5.16246400	-1.36916600	0.05127900
H	7.13050800	-3.54160700	0.01947100
H	9.58284500	-3.17152200	0.16919200
H	10.48881800	-0.88056100	0.35480400
H	8.98509900	1.07847200	0.39375800
N	6.15999300	0.77050500	0.24946800
C	6.37767300	2.21384300	0.33531300
C	6.48926400	2.88847800	-1.03276000
H	7.28998100	2.36922200	0.90987300
H	5.56343700	2.64704400	0.91496800
H	6.65956600	3.95813600	-0.89605400
H	7.32421900	2.47833400	-1.60293200
H	5.57439100	2.75770600	-1.61204600
C	4.52929200	-2.11164500	1.25160400
C	4.66150700	-1.97149900	-1.28210800
C	-7.21283500	-0.13312200	-0.03208500
C	-6.68512500	-1.43021000	-0.09152600
C	-7.53226900	-2.52164800	-0.11173500
C	-8.91634300	-2.31084700	-0.06842500
C	-9.42979100	-1.01387000	-0.00408500
C	-8.58940300	0.09719600	0.01680500

C	-4.94110500	0.16212700	-0.07799900
C	-5.16960400	-1.35473200	-0.12771300
H	-7.13620100	-3.52936900	-0.15991400
H	-9.59143900	-3.15741900	-0.08320300
H	-10.50210300	-0.86378000	0.03241000
H	-8.99925600	1.09652300	0.07339000
N	-6.17350300	0.78905900	-0.03841700
C	-6.39386200	2.23286600	0.02879700
C	-6.39729300	2.77690200	1.45798500
H	-7.34781700	2.43684700	-0.45613100
H	-5.62653100	2.72248100	-0.56962700
H	-6.57723200	3.85345200	1.43456300
H	-7.18548800	2.31088600	2.05141000
H	-5.43996200	2.59983300	1.95008600
C	-4.63275400	-1.97933800	-1.43710000
C	-4.56913400	-2.07596700	1.10157900
C	0.01292500	3.15320000	-0.68094400
C	-1.24828300	2.55401400	-0.06988200
C	-1.25427000	1.04579800	-0.13168000
C	-0.00097500	0.30575100	-0.16592100
C	1.25299700	1.04060300	-0.08568000
C	1.25218600	2.54929000	-0.03095100
H	0.02916200	2.95116600	-1.75724000
H	-1.32298100	2.87982300	0.97796600
H	1.29824700	2.87873700	1.01746600
O	-0.00228500	-0.97872800	-0.23587400
C	-2.44717100	0.32300700	-0.12866500
C	-3.74803900	0.86423600	-0.07286500
C	3.74113400	0.85077400	0.07458700
C	2.44187900	0.31301300	-0.02986100

H	3.57638800	-1.91580000	-1.36067600
H	5.09849000	-1.44756000	-2.13376000
H	4.95374900	-3.02187400	-1.33737200
H	3.44200900	-2.04716000	1.22856600
H	4.80996200	-3.16606100	1.21475700
H	4.88181300	-1.69427500	2.19619800
H	3.82590300	1.92910900	0.11985200
H	2.32103800	-0.76000000	-0.06571700
H	2.15065400	2.94651900	-0.50865300
H	0.01318100	4.23927700	-0.55544300
H	-2.13027600	2.95791900	-0.57208500
H	-2.32868000	-0.75003900	-0.17100200
H	-3.83186800	1.94213700	-0.01561200
H	-5.05037500	-1.47314400	-2.30897200
H	-3.54626800	-1.91910600	-1.48921700
H	-4.91870800	-3.03200900	-1.48018900
H	-4.85104700	-3.13038400	1.07663600
H	-3.48156000	-2.01413600	1.10616000
H	-4.94529500	-1.64113200	2.02899500