Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

A Fluorescent Hydrazone Exchange Probe of Pyridoxal Phosphate for the Assessment of Vitamin B6 Status

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1. Materials and Methods

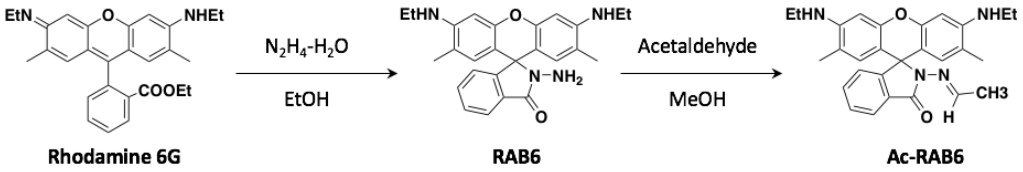
Instrumentation

Fluorescence emission and excitation spectra were recorded on a Jobin Yvon-Spex Fluorolog 3 spectrometer with an external temperature controller or Fluoroskan Ascent microplate fluorometer. ^{1}H-/^{13}C-NMR spectra were recorded on Varian Mercury 400 MHz NMR or Varian Inova 300 MHz spectrometer and internally referenced to the residual solvent signal. Coupling constants (*J* value) were reported in Hertz. The chemical shifts (δ) were reported in ppm. Multiplicities of peaks were indiated by s (singlet), d (doublet), t (triplet), dd (doublet of doublets), and m (multiplet). High-resolution mass spectrometry analysis was performed by the Vincent Coates foundation mass spectrometry laboratory at Stanford University and mass spectra were analyzed with MestReNova software. Epifluorescence microscopy for cell bioimaging was conducted on a Nikon Eclipse 80i microscope equipped with Nikon Plan Fluor 40× objective, and QIClick digital CCD camera with a high pressure 100W mercury lamp as the excitation source.

Chemicals

All chemicals were purchased from Sigma Aldrich, Oakwood chemical, and Alfa Aesar and used without further purification.

Synthesis of RAB6 and Ac-RAB6



Scheme S1. Synthetic scheme of **RAB6** and **Ac-RAB6**.

2-Amino-3',6'-bis(ethylamino)-2',7'-dimethylspiro[isoindoline-1,9'-xanthen]-3one (**RAB6**)

Rhodamine 6G (100 mg, 0.21 mmol) and hydrazine monohydrate (104 mg) were suspended in ethanol and heated at reflux until the color of solution was changed into dim transparent yellow). After the reaction mixture cooled down to rt, the mixture was subjected to extraction with saturated sodium bicarbonate and ethyl acetate. The organic layer was separated and washed with brine and dried with sodium sulfate. The product was purified with column chromatography (ethyl acetate:hexane = 3:7) to give a pure compound as white solid in 85% yield. ESI-MS [M+H] = Calculated: 428.22; Observed: 429.4. ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.96 – 7.98 (m, 1H), 7.45 – 7.47 (m, 2H), 7.06 – 7.08 (m, 1H), 6.41 (s, 2H), 6.28 (s, 2H), 3.21 – 3.25 (q, *J* = 3 Hz, 4H), 1.93 (s, 6 H), and 1.32 – 1.35 (t, *J* = 3 Hz, 6H). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.2, 152.2, 151.7, 147.5, 147.2, 132.6, 130.0, 128.2, 127.7 (two carbon), 126.8, 126.7, 123.8, 123.1, 118.0, 104.9, 96.85 (two carbon), 76.0, 66.3, 38.4 (two carbon), 16.74 (two carbon), and 14.8 (two carbon).

3',6'-bis(ethylamino)-2-(ethylideneamino)-2',7'-dimethylspiro[isoindoline-1,9'-xanthen]-3-one (**Ac-RAB6**)

RAB6 (100 mg, 0.23 mmol) and acetaldehyde (14 µL) were dissolved in methanol and heated at reflux for 3 h. The reaction mixture was concentrated *in vacuo* and the crude was purified with flash chromatography (ethyl

acetate:hexane = 50:50) to give a pure compound as white solid in 45% yield. ESI-MS [M+H] = Calculated: 454.24; Observed: 454.6. ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.99 – 8.02 (m, 1H), 7.40 –7.46 (m, 3H), 6.96 – 7.01 (m, 1H), 6.38 (s, 2H), 6.36 (s, 2H), 3.18 – 3.25 (q, *J* = 6 Hz, 4H), 1.9 (s, 6H), 1.31 – 1.35 (t, *J* = 6 Hz, 6H), and 1.24 – 1.29 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.4, 153.0, 150.8, 147.5 (two carbon), 157.4 (two carbon), 133.4, 128.1, 127.7, 127.4 (two carbon), 123.5, 123.3, 118.1 (two carbon), 106.0, 96.9 (two carbon), 65.0, 38.4 (two carbon), 19.9, 16.7 (two carbon), and 14.8 (two carbon).

DFT Calculation Details

For the DFT calculations, the Gaussian 16 package (Revision B.01, Inc., Wallingford CT, **2016**.) was used, where the Kohn-Sham molecular orbitals were calculated using the hybrid functionals B3LYP[1] as well as M06[2] utilizing the 6-31G(d)[3] basis set in both cases. In addition, Grimme dispersion correction (GD3)[4] was used with the M06 functional. The geometry optimized ground states showed no imaginary frequencies in the vibrational frequency analysis. Hirshfeld population analysis[6] was performed on the Hirshfeld and CM5[5] charges. These theory levels were chosen based on previous results for hydrogen-bond based systems.[5, 6] Beside the gas phase simulation, solvent effects were additionally taken into account utilizing the polarizable continuum model (PCM), where the cavity was estimated by UFF radii and the solvent was water (ε = 78.3553).[7]

Cellular Imaging and Protein Knock-Down

HeLa human cervical cancer cells were cultured in DMEM supplemented with FBS (10%), penicillin (100 U/mL), streptomycin (100 U/mL), and L-Glutamine (4 mM) in a humidified incubator at 37 °C with 5% CO_2. The cells were passaged when they reached approximately 80% of confluency. The cells were seeded onto a 8-well cell culture slide at a density of 2.5 × 10^4 cells and incubated for 16 h at 37 °C with 5% CO_2. The cells were washed with PBS and filled with 350 µL of DMEM and 150 µL Opti-MEM containing 4.5 µL of Lipofectamine RNAiMAX and 1.5 µL siPDXK (Santa Cruz Biotech.). For control cells, the cells were incubated with 350 µL of DMEM and 150 µL Opti-MEM containing 4.5 µL of Lipofectamine RNAiMAX. And the cells were incubated for 24 h at 37 °C with 5% CO_2. Then, 10 µM of Ac-RAB6 and/or 0, 30, 50 µM of PL were added to the cells, and incubated for 12 h. After the cells were washed with PBS for three times, the racks are detached and the cells were covered with a cover glass. The prepared slide glass was mounted on an epifluorescence microscope and imaged. The imaging data was processed and calculated by using the software ImageJ (version 1.52).

In Vitro Fluorescence Measurement of PDXK Activity

All the stock solutions of the probes, aldehydes, $MgCl_2$, and ATP were prepared as 10 mM concentration in DMSO (the fluorescent probes) or D.I. water (the others). To a solution of Tris buffer (25 mM, pH 7) with **RAB6** (10 µM), pyridoxal (100 µM), $MgCl_2$ (250 µM), and ATP (1.5 mM), 0.37 ng/µL of recombinant human PDXK (Novus biotech #8658-PK-050) was added and the solution was incubated at 37 °C.

Western Blot Analysis

Cells were trypsinized for 5 min at 37 °C, and transferred into e-tube (1.5 mL) using DMEM supplemented with 10% FBS to neutralize the trypsin. The cells in the tube were centrifuged for 3 min at 350 g and the supernatant was removed, then the cells were washed with PBS. The cells were dispensed in 30 µL of PBS with 0.5 µL of 100× protease inhibitors. The cells were placed at -78 °C (dry ice + ethanol) for 20 seconds, then at 37 °C for 60 seconds,

then voltaxed for 20 seconds at rt. This cycle was repeated for 4 times then the tube was sonicated in cold water for 10 min. After the centrifuging the debris down for 30 min at 13000 g, 6 µL of supernatant was mixed with 2.5 µL of Laemmeli (4.5×). The mixture was placed on the heat block (87 °C) for 5 min to denaturate the proteins isolated from cells. After cooling it down in the ice, it is loaded to 4–12% NuPage Gel (Invitrogen). After the electrophoresis was done in NuPage Running buffer (1×), the gel was transferred to membrane by electroblotting in transfer buffer (1×). The membrane was blocked with 5% non-fat dry milk in PBST buffer for 30 min then filled with new blocking solution (1 mL) with 0.2 µL GADPH antibody and 10 µL PDXK antibody. After 24 hr incubation in a cold room, the membrane was washed with PBST 3 times, 10 min each. The membrane was further incubated with PBST solution with the secondary antibodies (PDXK and GADPH) for 1 h. The membrane was imaged with LI-COR Odyssey after washing it with PBST 3 times, 10 min each.

2. Supporting Figures

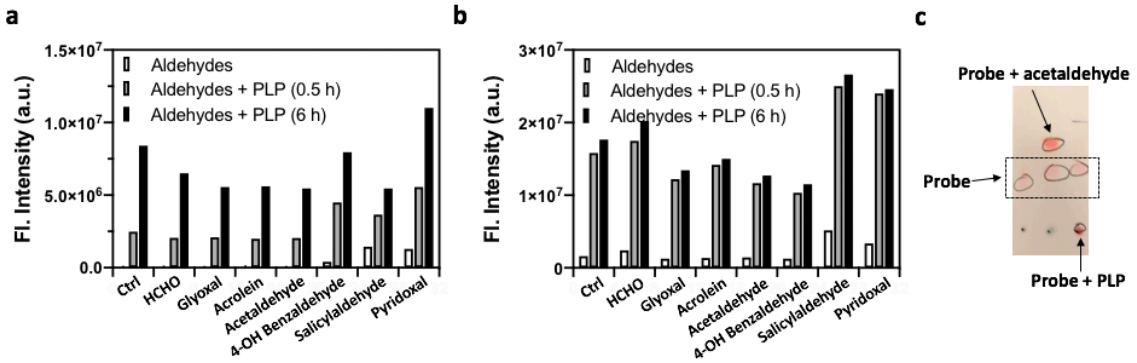


Figure S1. Exchangeability tests of the rhodamine hydrazone. **RAB6** (10 µM) was incubated with different kinds of aldehydes (100 µM) for 30 min to form the corresponding hydrazone (blank bars). Then, PLP (200 µM) was added to the mixture to evaluate the exchangeability of hydrazone occupied with different aldehydes for PLP. (a, b) Exchangeability tests in (a) Tris buffer (pH 7, 25 mM), and (b) acetate buffer (pH 5, 25 mM). (c) The hydrazone formation of **RAB6** with acetaldehyde or PLP was observed on a TLC plate (ethyl acetate:hexane = 30:70). Emission was collected at 550 nm under the excitation of 525 nm.

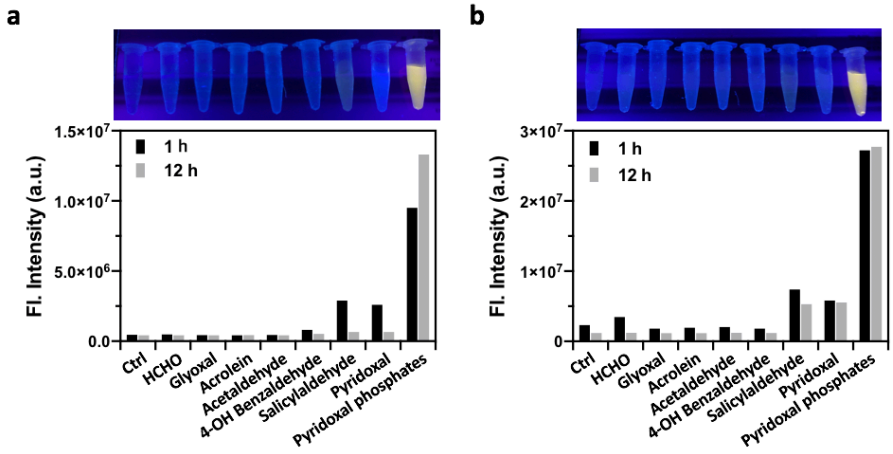


Figure S2. Selectivity test of **RAB6** (10 µM) with different kinds of aldehydes (100 µM) after 1 h or 12 h of incubation at 37 °C in (a) pH 7 (25 mM Tris buffer) or (b) pH 5 (25 mM Acetate buffer). Emission was collected at 550 nm with 525 nm excitation. Images above were taken after 1 h incubation under UV-light irradiation (365 nm).

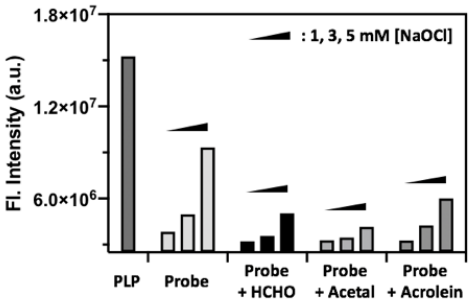


Figure S3. Comparison of false-positive signals from the oxidation by hypochlorous acid. **RAB6** (10 μM) was incubated with formaldehyde, acetaldehyde or acrolein (100 μM) for 30 min, then different concentrations of sodium hypochlorite (1, 3, or 5 mM) were added. The leftmost bar indicates the intensity of the signal from **RAB6** (10 μM) + PLP (0.1 mM) when incubated for 30 min. Emission was collected at 550 nm (excitation 525 nm).

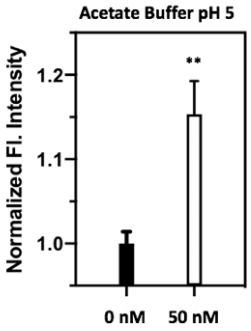


Figure S4. Detection limit of RAB6. Experiments were measured with 10 μM of **RAB6** and 50 nM of PLP in acetate buffer (pH5, 25 mM) after 12 h of incubation. Emission was collected at 550 nm (excitation 525 nm).

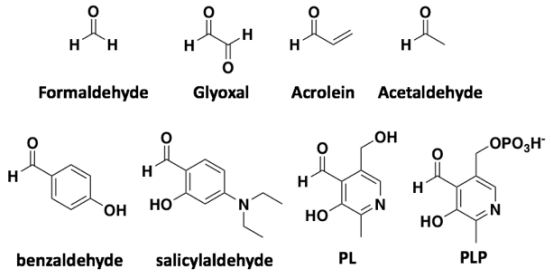


Figure S5. Chemical structures of aldehydes used in the selectivity tests.

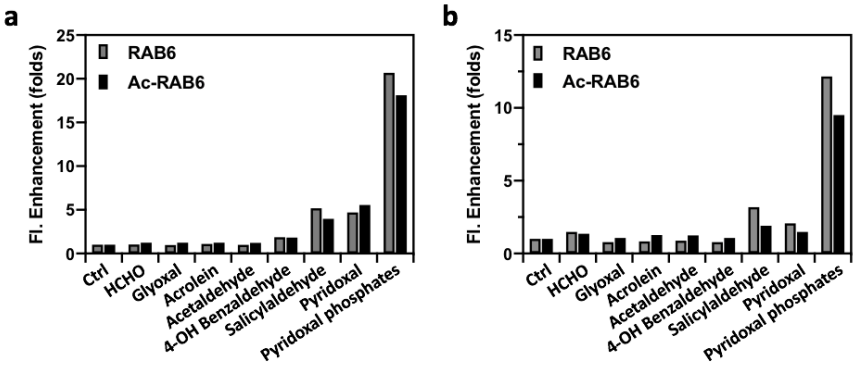


Figure S6. Selectivity comparison between **RAB6** (10 μM) and **Ac-RAB6** with different kinds of aldehydes (100 μM) after 1h of incubation at 37 °C in (a) pH 7 (25 mM of Tris buffer) or (b) pH 5 (25 mM of Acetate buffer). Emission was collected at 550 nm (excitation of 525 nm).

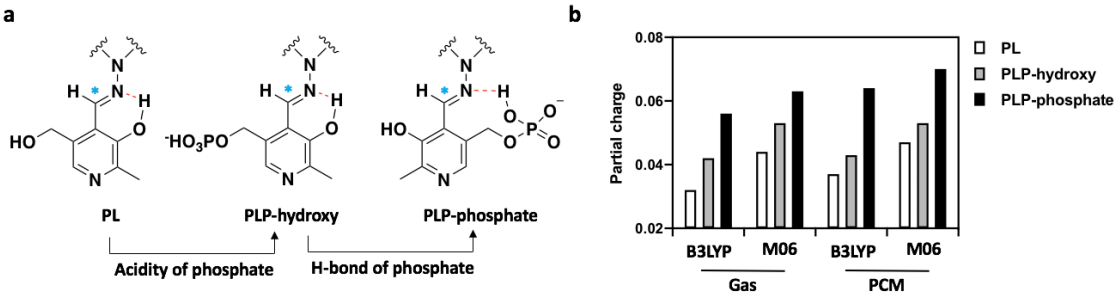


Figure S7. Calculation of partial charges at the carbons marked with blue stars. (a) Structures of PL and two different conformations of PLP adducted probes, and (b) calculated results.

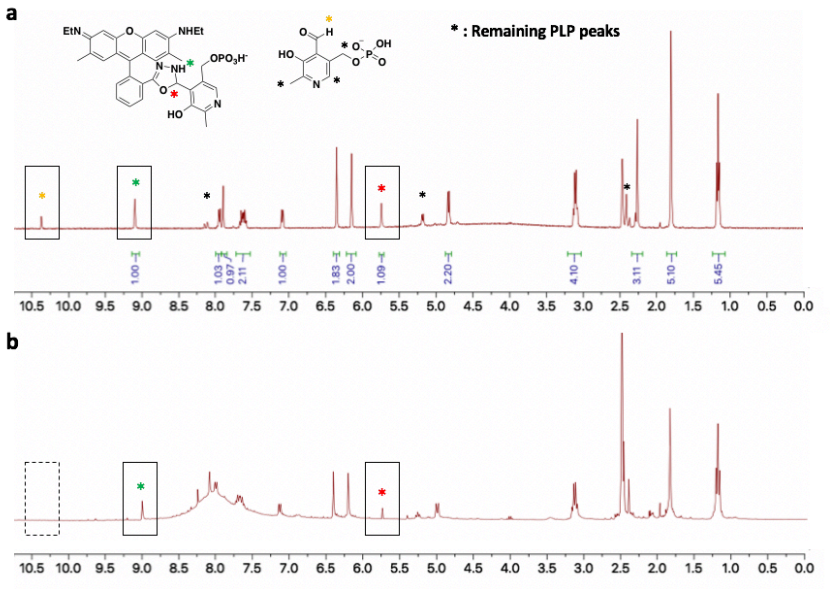


Figure S8. Crude ^{1}H-NMR data of the probe after reaction with PLP. (a) **RAB6** (0.01 mmol) and PLP (2 equiv.; 0.02 mmol) were dissolved in DMSO-d6 (0.75 mL) and incubated for 6 hours at 37 °C. The spectrum shows clean conversion, with resonance (*, ~5.75ppm) consistent with proposed cyclized product. (b) To solution shown in fig. S8a, one drop of TFA was added to acidify the solution and the solution was heated for 12 h at 95 °C. The data provide evidence of the robustness of the adduct.

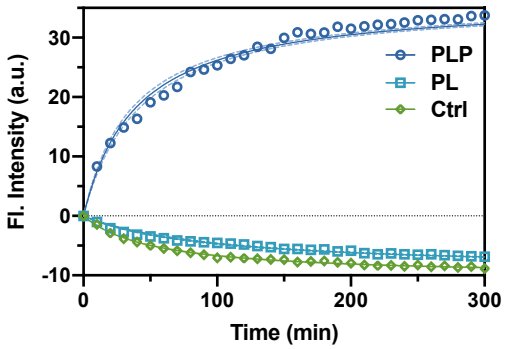


Figure S9. Comparison of kinetics of **RAB6** (10 µM) for the detection of PL (100 µM) and PLP (100 µM) at pH 7 (25 mM Tris buffer). Emission was collected at 555 nm under the excitation of 485 nm.

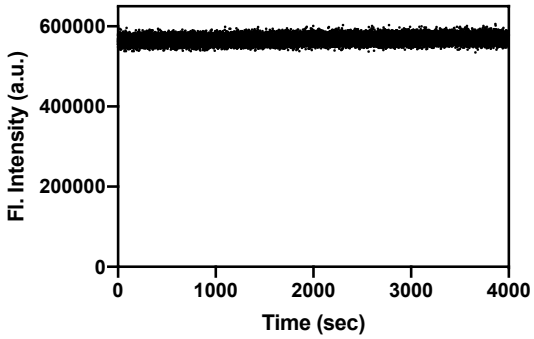
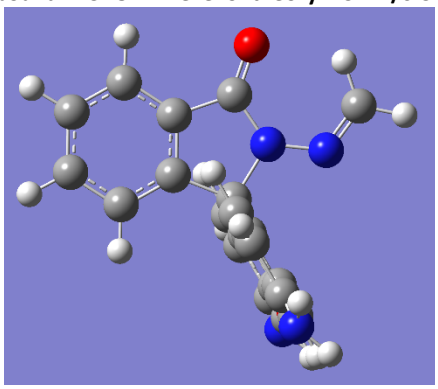


Figure S10. Photostability test of **RAB6** after detecting PLP. Fluorescence intensity of **RAB6** (10 μM) incubated with PLP (100 μM) for 12 hr at 37 °C was measured at 550 nm under the irradiation of 525 nm laser every 0.1 sec.

3. XYZ Coordinates

Gas Phase

Compound: HCHO Level of theory: B3LYP/6-31G(d)



xyz-coordinates

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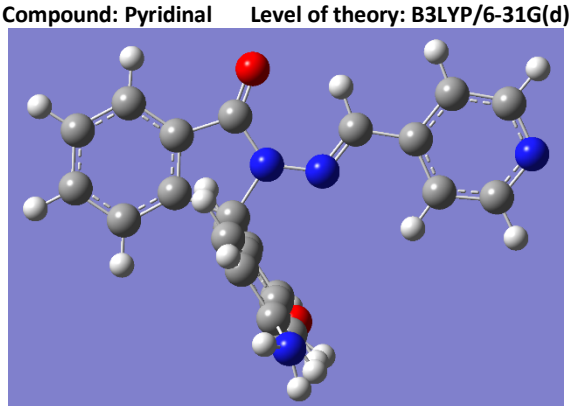
Compound: Pyridinal **Level of theory: B3LYP/6-31G(d)**



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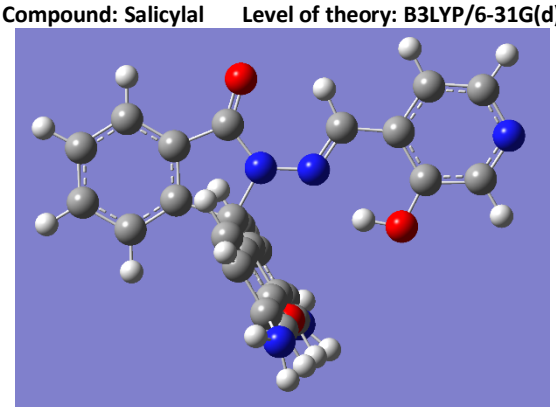
Compound: Salicylal Level of theory: B3LYP/6-31G(d)



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H	4.67555700	4.75724400	5.69051900
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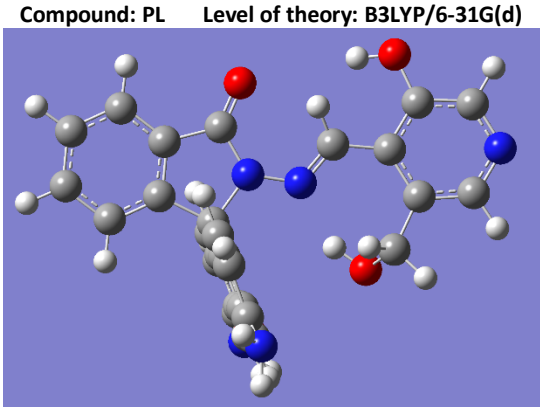
H	-4.39273200	1.86934200	5.28300400
H	-1.86112600	0.12261000	7.20657700
H	0.70565000	0.70542600	-2.41890000
H	3.46795500	-0.52164100	-0.40457700
H	0.33609200	-0.50528100	6.30621500
H	-3.03118700	1.48223400	3.27747400
H	3.33345100	-0.87058000	2.02247500
H	-0.50586800	1.17002700	-0.33482900
H	2.23635600	0.01350500	-2.43647000
H	-3.91943700	1.35494000	6.80622800
H	3.93582000	2.46786200	5.35552700
H	0.33549900	-2.94609300	3.30662900
H	1.43499200	-4.97197800	4.24372100
H	3.46476100	-4.77992300	5.64356400
H	4.44221800	-2.51793100	6.13687700
H	0.95056000	6.61295100	3.11421600
H	1.08415400	3.09793000	3.41094900

Compound: PL **Level of theory: B3LYP/6-31G(d)**

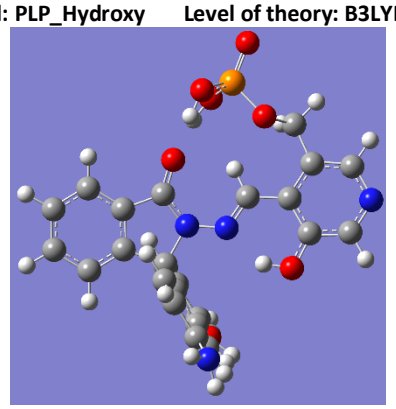


xyz-coordinates

C	-0.30518300	0.19670600	-0.21647000
C	-0.21665000	0.02655000	1.18845400
C	1.07516200	-0.05674200	1.75140900
C	2.19673700	-0.00680700	0.91389000
N	2.11234700	0.13356500	-0.40558100
C	0.88680200	0.24088400	-0.93956200
C	-1.34997500	-0.13361700	2.10154900
N	-2.52411600	0.34985500	1.85832800
N	-3.51740100	0.18094400	2.77533300
C	-3.38956000	-0.06566400	4.14196500
C	-4.76082800	0.03843800	4.68792000
C	-5.65149200	0.36989900	3.66889300
C	-4.92036000	0.53424300	2.33931000
C	-5.18113900	-0.15562900	6.00291300

C	-6.53974700	-0.00924300	6.27944000
C	-7.44151000	0.32176300	5.25633500
C	-7.00793000	0.51376700	3.94146300
C	-5.39853900	-0.44571700	1.28155300
C	-5.74103000	-0.02825800	-0.00821000
O	-5.72370200	1.28342200	-0.39830300
C	-5.34700700	2.24707900	0.49936100
C	-4.98033000	1.96043300	1.81853300
C	-5.36765900	3.55144000	0.00476700
C	-5.01042500	4.62240700	0.82773400
C	-4.64575800	4.35386900	2.16442200
C	-4.63480200	3.05154200	2.63288000
C	-5.48266700	-1.82197000	1.54726100
C	-5.88324100	-2.73614500	0.58786600
C	-6.22387000	-2.29674100	-0.70943900
C	-6.15145400	-0.92999900	-0.99219100
O	-2.34972400	-0.30731100	4.74628900
N	-6.57016200	-3.21369700	-1.69769700
N	-5.06761200	5.93267200	0.35924500
O	1.32021200	-0.19046100	3.08721400
C	-1.62674200	0.31422400	-0.95293500
O	-2.28809000	1.54853000	-0.72618000
H	-2.60611400	1.49932700	0.19537000
H	3.18724700	-0.08060000	1.35825900
H	-4.98781900	6.03425700	-0.64490300
H	-4.37244100	5.17334800	2.82397000
H	-7.10182100	-2.84167600	-2.47410200
H	-5.92816700	-3.79528200	0.82780600
H	-4.34334900	2.86615500	3.66317600
H	-5.65237900	3.70604700	-1.03126200
H	-5.22187300	-2.18050300	2.53944100
H	-6.39996500	-0.54294800	-1.97577600
H	-6.94579800	-4.09225900	-1.36482900
H	-4.47292400	6.58929600	0.84907100
H	-1.17324700	-0.68578400	3.01983000
H	-7.71124300	0.77195500	3.15507600
H	-8.49676500	0.43221300	5.49098200
H	-6.90612200	-0.15242800	7.29200800
H	-4.46131300	-0.41252700	6.77421100
H	0.84895500	0.36495500	-2.02052500
H	0.52608700	0.01576400	3.60556300
H	-2.27412600	-0.53652800	-0.69105000
H	-1.43413900	0.26132000	-2.02908500

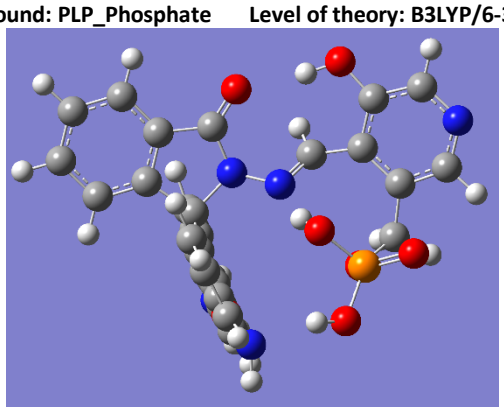
Compound: PLP_Hydroxy Level of theory: B3LYP/6-31G(d)



xyz-coordinates

C	0.37624100	0.10585200	0.35092600
C	0.21229000	0.22003800	1.75607900
C	1.35554200	0.54331800	2.52343000
C	2.58898200	0.69730600	1.86173500
N	2.73700100	0.57685000	0.54944600
C	1.64510100	0.29772800	-0.18356500
C	-1.09586300	0.02172400	2.36315100
N	-1.27318700	0.21812000	3.63194500
N	-2.52012400	0.07933300	4.17705100
C	-3.74643200	0.19124000	3.57032200
C	-4.74841600	0.12627300	4.64956800
C	-4.10280900	0.00305600	5.87933200
C	-2.59090800	0.00009900	5.69520700
C	-6.13834800	0.16443500	4.54203400
C	-6.88104000	0.07320500	5.71829100
C	-6.23673800	-0.05455600	6.95843800
C	-4.84208500	-0.09196000	7.05282100
C	-1.92165400	1.21294400	6.31470600
C	-0.72689000	1.09846500	7.03327300
O	-0.11533800	-0.10453300	7.27671500
C	-0.73708300	-1.26417000	6.89299400
C	-1.93428500	-1.28197800	6.17054500
C	-0.08967400	-2.43706800	7.28210100
C	-0.63144100	-3.68292700	6.95091500
C	-1.84199500	-3.72066600	6.22525600
C	-2.46497200	-2.54278800	5.85126900
C	-2.44192700	2.50774700	6.15109500
C	-1.81210500	3.62584400	6.66845700
C	-0.60464100	3.49103600	7.38821100
C	-0.07474500	2.20932000	7.56863000
O	-3.96649700	0.32473500	2.35422400
N	0.06322500	4.61174300	7.86045600
N	-0.02716100	-4.85946100	7.37752900
O	1.33923900	0.70436900	3.85730600
C	-0.76934900	-0.23309200	-0.57271600
O	-1.83421600	0.72352100	-0.38693600
P	-3.33018900	0.35311300	-0.92314000
O	-3.47259200	0.19996900	-2.37869500
O	-3.72264100	-0.98250700	-0.09361900
O	-4.17008400	1.54782400	-0.25510700
H	3.46918100	0.93500200	2.45596100
H	0.96042000	-4.79614600	7.58867100
H	-2.28446300	-4.67836300	5.96436400
H	0.72842100	4.45732700	8.60632100
H	-2.23992900	4.61273500	6.51380000
H	-3.39225700	-2.59519200	5.28718500
H	0.83469600	-2.35556500	7.84574700
H	-3.36838900	2.63696100	5.59848800
H	0.85089200	2.05290300	8.11396500
H	-0.49945200	5.43975300	8.00311200
H	-0.25070500	-5.68671100	6.83952700
H	-1.91011300	-0.27365400	1.71985800
H	-4.35072800	-0.19094300	8.01614700
H	-6.83355500	-0.12562100	7.86353400
H	-7.96598100	0.09893100	5.67731600
H	-6.61237200	0.26101200	3.57006900
H	1.79694900	0.22695900	-1.25877300
H	0.40703700	0.61403500	4.16992800
H	-1.15068400	-1.24297300	-0.37286400
H	-0.43440400	-0.19984800	-1.61377800
H	-3.92992800	-0.76834200	0.84115500
H	-4.12019100	1.52116700	0.72133800

Compound: PLP_Phosphate **Level of theory: B3LYP/6-31G(d)**

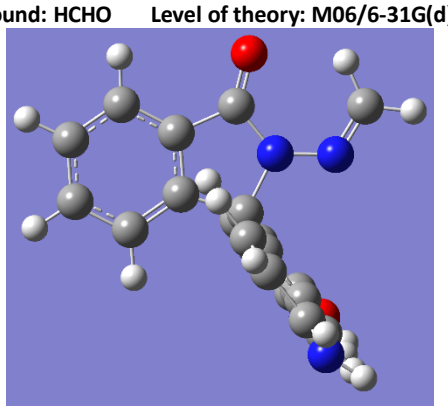


xyz-coordinates

C	3.30229500	-1.62639600	0.82304400
C	2.34352400	-2.18415800	-0.04685300
C	2.77063000	-3.14125400	-0.99191300
C	4.11619200	-3.53566000	-0.98579400
N	5.01961000	-3.02671000	-0.15355700
C	4.61748800	-2.08478100	0.70853000
C	0.89569600	-1.92522900	-0.08978100
N	0.35728400	-0.77035300	-0.27856400
N	-0.97751700	-0.87808800	-0.66419300
C	-1.31366200	-1.57886600	-1.81605400
C	-2.65688800	-1.09699900	-2.19795200
C	-3.05665700	-0.08777500	-1.32227300
C	-1.98453800	0.17600100	-0.26873700
C	-3.46269100	-1.52335300	-3.25260700
C	-4.70227500	-0.90526900	-3.41319300
C	-5.11210100	0.10675600	-2.53202500
C	-4.29671100	0.52324100	-1.47533100
C	-1.35710700	1.55284100	-0.36917100
C	-1.01422800	2.26827700	0.78280700
O	-1.39244200	1.89061800	2.04188600
C	-2.14263500	0.75566000	2.20561100
C	-2.47903000	-0.08895200	1.14417500
C	-2.54738500	0.49939400	3.51608900
C	-3.31088400	-0.63547400	3.80619000
C	-3.65656800	-1.50358900	2.74819500
C	-3.24328400	-1.22513600	1.45643000
C	-0.94156700	2.07805200	-1.60173700
C	-0.15886600	3.21868000	-1.68431200
C	0.24999700	3.86488400	-0.50545400
C	-0.22919800	3.41864600	0.72413400
O	-0.61540500	-2.41272300	-2.39126900
N	1.25808700	4.85045800	-0.54043400
N	-3.77091800	-0.87549800	5.09647200
O	1.94652300	-3.72032100	-1.89989700
C	2.97799700	-0.63567900	1.92127500
O	2.50163000	0.65671000	1.49311700
P	3.33472500	1.50899900	0.38518300
O	4.76483400	1.15784800	0.27294500
O	2.44381800	1.29717600	-0.94495300
O	3.03005700	3.01524900	0.85011500
H	4.44464400	-4.29022600	-1.69778700
H	-3.24440000	-0.43507600	5.83996700
H	-4.25352700	-2.38894700	2.95078100
H	1.19323900	5.54472100	0.19762500
H	0.19486500	3.56976400	-2.64961200
H	-3.51663500	-1.90932600	0.65797300

H	-2.25715500	1.19893900	4.29413800
H	-1.20700000	1.55297200	-2.51489000
H	0.07316000	3.88824600	1.65449800
H	1.37354400	5.29882500	-1.44343000
H	-3.99644900	-1.83897800	5.30781400
H	0.26445700	-2.81597700	-0.09763400
H	-4.62165700	1.30571100	-0.79587600
H	-6.08144300	0.57668200	-2.67399500
H	-5.35795700	-1.20827900	-4.22435700
H	-3.12197100	-2.31000100	-3.91874800
H	5.38688700	-1.65872900	1.34741000
H	1.12657200	-3.20072200	-2.05363200
H	2.17159800	-1.01419800	2.55692000
H	3.86915600	-0.49488700	2.53981600
H	1.64436800	0.75412200	-0.74683900
H	2.59139800	3.57728000	0.16934300

Compound: HCHO Level of theory: M06/6-31G(d)+GD3

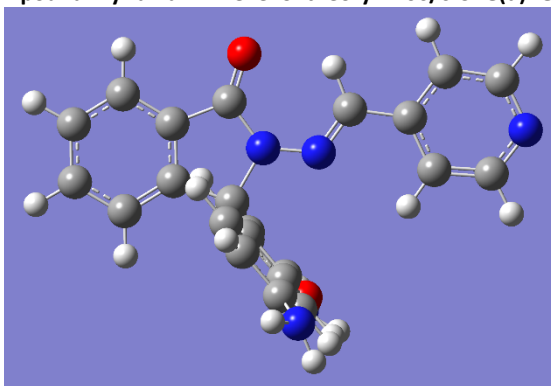


xyz-coordinates

C	0.00641500	-0.05007700	0.02053700
C	0.00291400	-0.03633700	1.41110300
C	1.18173800	0.02347300	2.15038100
C	2.38090300	0.06375200	1.43341700
C	2.41205500	0.05166700	0.05336000
C	1.21214000	-0.00901700	-0.67548000
C	1.16711100	-0.05560800	3.65576900
C	-0.22986700	0.15751100	4.18053700
C	-1.33659500	0.09188700	3.33764600
O	-1.23125700	-0.07088100	1.98857500
C	-2.63626200	0.20328100	3.81948700
C	-2.86330400	0.38004600	5.18213000
C	-1.75900600	0.44800800	6.04854600
C	-0.47881200	0.33464100	5.54460600
C	2.17751000	0.86557300	4.29607400
C	3.12756100	0.13915800	4.99904900
C	2.83548200	-1.30617200	4.89156800
N	1.69190000	-1.38261000	4.10783400
C	2.23906200	2.24921000	4.24854400
C	3.27966200	2.88067300	4.92506900
C	4.23648600	2.14523700	5.63258000
C	4.16935300	0.75766900	5.67703000
N	-4.15070900	0.54251700	5.67139400
N	0.98964300	-2.46708900	3.69151100
C	1.35746500	-3.64411400	4.02390600
O	3.45590400	-2.23348700	5.37970100
N	1.22943000	0.02828300	-2.06163400
H	0.40770900	-0.34506500	-2.51863400
H	3.36292100	0.09147600	-0.47737800
H	-4.88865800	0.16268700	5.09294700
H	-1.92065400	0.59308400	7.11637100

H	3.31993100	0.09800200	1.98690800
H	-0.94866100	-0.08632100	-0.50162100
H	0.36899700	0.37640500	6.22931900
H	-3.46025200	0.15535700	3.10895600
H	-4.27460600	0.31728500	6.64981700
H	2.08739200	-0.28882000	-2.49374300
H	0.73323800	-4.45325300	3.64386700
H	2.22406100	-3.87870900	4.64076500
H	1.49229700	2.81908100	3.69595700
H	3.35105600	3.96691700	4.90338600
H	5.03829900	2.66797100	6.15093500
H	4.89854800	0.15764500	6.21890200

Compound: Pyridinal **Level of theory: M06/6-31G(d)+GD3**

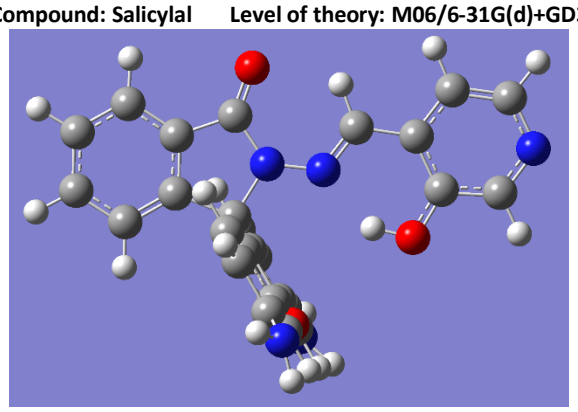


xyz-coordinates

C	-3.83776200	-0.03633400	-0.25938400
C	-2.63501500	-0.08469900	-0.94600000
C	-2.61574400	-0.16465400	-2.33186000
C	-3.78418900	-0.19888800	-3.08106600
C	-4.99302300	-0.15032600	-2.39716400
C	-5.01648000	-0.07007400	-1.00088200
C	-1.22114800	-0.20607800	-2.81734600
N	-0.44299300	-0.14602300	-1.66685800
C	-1.23196300	-0.06587100	-0.39222900
C	-0.91836100	-1.25866900	0.47312800
C	-0.05428200	-1.14372000	1.56023900
O	0.45382900	0.05189100	1.97525900
C	-0.03164600	1.20252900	1.42718400
C	-0.89474400	1.21062400	0.33335000
C	0.38092500	2.37525800	2.04854600
C	-0.06131000	3.60902300	1.57484000
C	-0.93313700	3.63727900	0.47287400
C	-1.32747100	2.45770400	-0.12652900
C	-1.37229700	-2.54143600	0.15347200
C	-0.99547000	-3.65410300	0.87883600
C	-0.12089400	-3.51867700	1.97041300
C	0.34290600	-2.24793300	2.30486800
N	0.89347900	-0.15357300	-1.52101600
C	1.68243400	-0.22188400	-2.53201200
C	3.12404000	-0.22660300	-2.28796300
C	4.00895400	-0.31669600	-3.36270700
C	5.37612200	-0.32179800	-3.10984500
N	5.90557000	-0.24421000	-1.88992300
C	5.04850300	-0.15657100	-0.86651600
C	3.66977700	-0.14392300	-1.00285300
H	3.63233400	-0.38229100	-4.38314200
H	3.01285400	-0.07016200	-0.13845300

H	6.08381000	-0.39235800	-3.93833900
O	-0.82343200	-0.27820300	-3.96559300
N	0.22720300	-4.62239800	2.73264400
H	1.08208500	-4.53394200	3.26633300
H	-1.37187200	-4.64074800	0.61025800
N	0.38115200	4.78820500	2.14983700
H	0.73035100	4.71769300	3.09623500
H	-1.28287300	4.59485600	0.08813200
H	-2.03735100	-2.66376100	-0.70204100
H	1.01179000	-2.09314600	3.15027800
H	-1.99300200	2.49565500	-0.98958200
H	1.05347000	2.30373400	2.90214300
H	-0.20902800	5.59713200	2.00911900
H	0.15704800	-5.51555200	2.26284000
H	1.32973100	-0.27781900	-3.56431500
H	-3.85287800	0.02497900	0.82860200
H	-5.97451900	-0.03395200	-0.48486700
H	-5.93128400	-0.17509900	-2.94825500
H	-3.73290700	-0.26222100	-4.16669000
H	5.49755500	-0.09186600	0.12650800

Compound: Salicylal Level of theory: M06/6-31G(d)+GD3

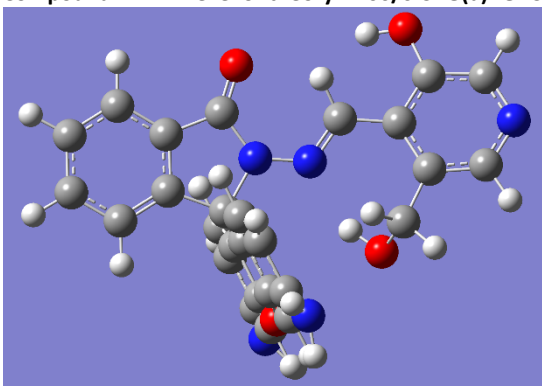


xyz-coordinates

C	0.40760900	0.78322800	0.19088100
C	0.33809000	0.55765600	1.56115900
C	1.36196100	-0.08148600	2.25682500
C	2.47800100	-0.48543500	1.51624800
C	2.57277400	-0.27202400	0.15687200
C	1.52897700	0.37578200	-0.52813400
O	-0.80519300	0.99516000	2.16202400
C	-1.00612600	0.72879300	3.48429800
C	-0.05506200	0.09685100	4.28247400
C	1.31135300	-0.25448900	3.75310600
C	1.78046100	-1.61868700	4.20015300
C	2.91856800	-1.51712300	4.98789800
C	3.30300300	-0.09917500	5.13657000
N	2.35255100	0.60432000	4.40666500
C	1.22466200	-2.85594000	3.91832500
C	1.84212500	-3.98581200	4.44924200
C	2.98918500	-3.88026600	5.24281300
C	3.54282300	-2.63643400	5.52213600
C	-0.39112600	-0.11815400	5.62322200
C	-1.60677400	0.27137000	6.14585200
C	-2.55205800	0.91299800	5.32572800
C	-2.23785600	1.13310400	3.98686900
N	2.21816700	1.93595300	4.23267100
C	3.05368900	2.78011100	4.73729600
C	2.84982500	4.20264500	4.52401600
C	1.76649300	4.73240800	3.79519000

C	1.67920000	6.12549700	3.66582500
N	2.55125100	6.97636100	4.18505800
C	3.58091800	6.47281000	4.87708000
C	3.76335800	5.11489400	5.06703100
O	0.81422600	3.98975300	3.22042500
O	4.23928400	0.36897000	5.75861800
N	-3.79077000	1.26997800	5.83053000
N	1.63822100	0.64062100	-1.88098200
H	4.61410800	4.74227600	5.63763100
H	4.28535200	7.19291700	5.29430200
H	-4.28131000	1.99316700	5.32084300
H	-1.84164000	0.08552800	7.19343600
H	0.77419900	0.82214800	-2.37366200
H	3.45874400	-0.59147500	-0.39098100
H	0.33800800	-0.60253600	6.27369300
H	-2.93871900	1.62207400	3.31213200
H	3.29872800	-0.98116700	2.03587300
H	-0.42411500	1.29159300	-0.29433600
H	2.27474200	0.05200700	-2.40102400
H	-3.83254000	1.40601900	6.83200300
H	3.91557900	2.46351200	5.32821000
H	0.33058400	-2.93474600	3.30020400
H	1.42475900	-4.97013700	4.24373200
H	3.44860100	-4.78207500	5.64309200
H	4.43422200	-2.52218600	6.13656700
H	0.83856600	6.53320700	3.10053000
H	1.01930200	3.04338000	3.39509200

Compound: PL **Level of theory: M06/6-31G(d)+GD3**

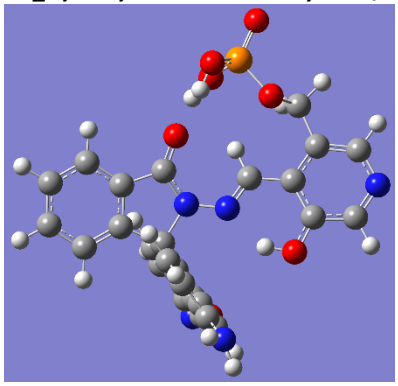


xyz-coordinates

C	-0.56553200	-0.06361700	-0.22187300
C	-0.31975300	-0.02731500	1.16920400
C	1.01923700	-0.04472900	1.59047800
C	2.03728500	-0.12021200	0.63798300
N	1.80734900	-0.16678600	-0.66488400
C	0.53521800	-0.13155100	-1.06869800
C	-1.36004000	-0.05584700	2.19288900
N	-2.54134400	0.39357800	1.95062200
N	-3.52109900	0.30862000	2.87373000
C	-3.43696900	-0.01000300	4.22397100
C	-4.82551600	0.06442100	4.71606600
C	-5.67629500	0.41583700	3.67614900
C	-4.90495400	0.62382000	2.39284600
C	-5.29581100	-0.17378000	6.00072300
C	-6.66218300	-0.04988700	6.22150600

C	-7.52188400	0.30320300	5.17594700
C	-7.03904300	0.54033200	3.89148600
C	-5.29252300	-0.34335200	1.30320500
C	-5.57995800	0.08416300	0.00816000
O	-5.63177200	1.39598400	-0.34555800
C	-5.30287300	2.34451200	0.57210500
C	-4.97886100	2.04459100	1.89463600
C	-5.31638500	3.65199300	0.09904500
C	-5.00354700	4.70815500	0.95029300
C	-4.68486900	4.42547300	2.29108000
C	-4.67457300	3.12038800	2.73614000
C	-5.29474500	-1.72310800	1.53427100
C	-5.56732500	-2.63436600	0.53520300
C	-5.85183900	-2.18454800	-0.76724700
C	-5.86115700	-0.81431700	-1.01564900
O	-2.42300200	-0.28122100	4.84421800
N	-6.06974200	-3.09199000	-1.78847300
N	-5.05119300	6.01715100	0.50224900
O	1.40822300	0.00435100	2.88719100
C	-1.94985100	-0.04587300	-0.82000400
O	-2.56048100	1.21907300	-0.76372900
H	-2.73967900	1.36902800	0.18205900
H	3.07263200	-0.13796400	0.98310600
H	-4.95697700	6.14165300	-0.49735600
H	-4.44592600	5.24236900	2.97129200
H	-6.55573700	-2.73998000	-2.60229600
H	-5.55186600	-3.70357100	0.74415900
H	-4.41441500	2.91466600	3.77512500
H	-5.56390900	3.81963100	-0.94773100
H	-5.06650400	-2.08578500	2.53734600
H	-6.06577600	-0.41785800	-2.00881200
H	-6.38466900	-4.01074900	-1.50746800
H	-4.49646500	6.67978300	1.02803500
H	-1.12532500	-0.50132000	3.16298600
H	-7.70663400	0.81771600	3.07597000
H	-8.58891100	0.39502400	5.37172300
H	-7.07092900	-0.22841700	7.21421900
H	-4.60239400	-0.44805800	6.79389400
H	0.37100600	-0.16592200	-2.14805900
H	0.66862600	0.25232300	3.45970800
H	-2.57692900	-0.81911500	-0.33872800
H	-1.87617600	-0.30825900	-1.88345800

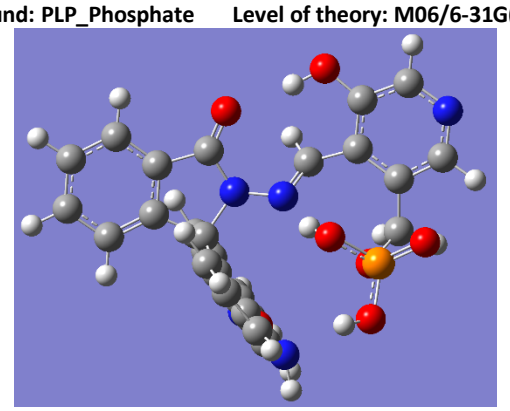
Compound: PLP_Hydroxy Level of theory: M06/6-31G(d)+GD3



xyz-coordinates

C	0.39663500	0.07901400	0.45258200
C	0.20966800	0.23878100	1.84347300
C	1.32397300	0.62869400	2.61097200
C	2.55935900	0.78137400	1.96042200
N	2.73094000	0.61015500	0.66301600
C	1.66196500	0.28038500	-0.07249200
C	-1.09266500	0.00596700	2.44117300
N	-1.30294100	0.29949800	3.67914700
N	-2.54783500	0.11488900	4.19995700
C	-3.75965000	0.24996100	3.58054900
C	-4.76573000	0.16926800	4.64841900
C	-4.13081600	0.02568600	5.87589200
C	-2.63243600	0.02050200	5.70363000
C	-6.14933700	0.21109600	4.53419800
C	-6.89391400	0.10212600	5.70245500
C	-6.25859300	-0.04557900	6.93982000
C	-4.86953100	-0.08681100	7.04149900
C	-1.95893800	1.21236800	6.32861700
C	-0.70739500	1.09526300	6.93227300
O	-0.07157800	-0.10081800	7.08983400
C	-0.72820500	-1.25063900	6.76750500
C	-1.98019900	-1.25834800	6.15525700
C	-0.06373600	-2.42559200	7.09719200
C	-0.64449000	-3.66020800	6.81239700
C	-1.90924300	-3.68755900	6.19654000
C	-2.54742500	-2.50704700	5.87822100
C	-2.50226000	2.49843900	6.23379900
C	-1.84184000	3.60921000	6.71508400
C	-0.57601400	3.47250800	7.31466000
C	-0.01999100	2.19859900	7.42260900
O	-3.96185300	0.40935100	2.37230500
N	0.11512900	4.58427100	7.74795700
N	-0.01714100	-4.83663100	7.17485300
O	1.29512200	0.85081600	3.92718800
C	-0.73217000	-0.29484000	-0.46020500
O	-1.80636300	0.62569000	-0.27213000
P	-3.26325500	0.19673600	-0.83617700
O	-3.32654700	-0.06246800	-2.27462700
O	-3.65980500	-1.07839400	0.05967900
O	-4.14134300	1.40548000	-0.28602700
H	3.42286500	1.06633400	2.56447100
H	0.98300900	-4.78545900	7.31565600
H	-2.37884500	-4.64522800	5.97482100
H	0.86403900	4.43024400	8.40875900
H	-2.28767500	4.59864600	6.62059400
H	-3.52129000	-2.54383500	5.38854900
H	0.90943100	-2.35425600	7.58026800
H	-3.47671400	2.62382600	5.76069500
H	0.95694300	2.04206500	7.87683800
H	-0.42849600	5.41485800	7.93698500
H	-0.30254200	-5.66685400	6.67302700
H	-1.87764500	-0.41539300	1.81912500
H	-4.37316300	-0.20212600	8.00449100
H	-6.86284800	-0.12979900	7.84132100
H	-7.98068200	0.12958200	5.65787000
H	-6.61723100	0.32434900	3.55792800
H	1.82495200	0.17569400	-1.14688900
H	0.36497900	0.78188100	4.24049600
H	-1.08375100	-1.32024600	-0.25538600
H	-0.40235900	-0.26519400	-1.50767100
H	-3.92104000	-0.80202400	0.96149900
H	-4.08485100	1.47867300	0.68578400

Compound: PLP_Phosphate Level of theory: M06/6-31G(d)+GD3



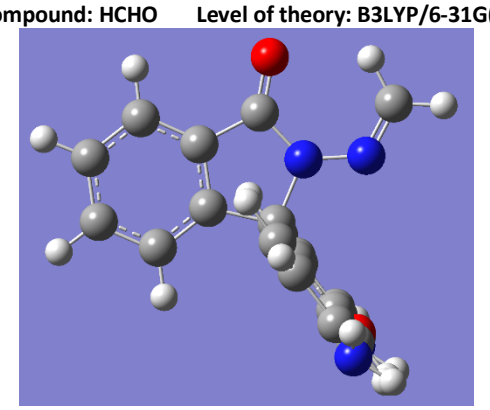
xyz-coordinates

C	3.19602900	-1.58023500	0.91472600
C	2.29266600	-2.15300700	0.00787000
C	2.76961400	-3.09027800	-0.92205500
C	4.11483400	-3.46102800	-0.85706200
N	4.96691000	-2.94522400	0.01634800
C	4.51736200	-2.01630300	0.85939500
C	0.85325900	-1.91434300	-0.08101200
N	0.31957200	-0.76221600	-0.27149200
N	-0.99522000	-0.87244300	-0.68264400
C	-1.30934100	-1.55665600	-1.84498200
C	-2.64620700	-1.07148300	-2.22720000
C	-3.04851900	-0.07547900	-1.34519300
C	-1.99025800	0.17713600	-0.29650400
C	-3.44376200	-1.48001300	-3.28785800
C	-4.67656800	-0.85745600	-3.44451400
C	-5.08731600	0.14114300	-2.55584700
C	-4.27978900	0.54141400	-1.49343300
C	-1.34920200	1.53507400	-0.39640300
C	-0.93278400	2.20505200	0.75299500
O	-1.24647600	1.79414200	2.01051300
C	-2.04142600	0.70062700	2.17481400
C	-2.47194700	-0.08395800	1.10751600
C	-2.39876900	0.41898100	3.48824900
C	-3.20731800	-0.68012000	3.77098100
C	-3.64888700	-1.48683700	2.70633300
C	-3.27845800	-1.18578100	1.41189700
C	-0.96467100	2.06496800	-1.63104900
C	-0.16129500	3.18476800	-1.72271100
C	0.29627800	3.80057400	-0.55165700
C	-0.13176300	3.33707500	0.68497300
O	-0.60100400	-2.37256600	-2.41861600
N	1.29586100	4.78413300	-0.60416800
N	-3.61237000	-0.94638900	5.06571500
O	1.99605300	-3.67042200	-1.86039400
C	2.79427100	-0.59151000	1.97542300
O	2.34024400	0.67707000	1.50287700
P	3.23549000	1.48611100	0.42720200
O	4.64320500	1.06924000	0.37220800
O	2.37871300	1.30967700	-0.91561300
O	2.98912500	2.99936000	0.85902100
H	4.48442600	-4.20861500	-1.56128400
H	-3.04199700	-0.55301000	5.80236000
H	-4.28601400	-2.34650800	2.91156400
H	1.23601200	5.48396800	0.12888300
H	0.16877700	3.54959200	-2.69425000
H	-3.61735600	-1.82720500	0.59757400
H	-2.03613600	1.07545300	4.27768500

H	-1.27795000	1.55578000	-2.54281800
H	0.23238100	3.77352200	1.61338600
H	1.40827700	5.22037700	-1.51297300
H	-3.89969400	-1.89720200	5.25531100
H	0.22465400	-2.81249200	-0.11172200
H	-4.59863600	1.31859300	-0.79942600
H	-6.05670400	0.61544500	-2.69863600
H	-5.33097600	-1.14755800	-4.26406300
H	-3.09855100	-2.26035500	-3.96357800
H	5.25106800	-1.57323300	1.53438300
H	1.17881900	-3.16230500	-2.04968500
H	1.95189600	-0.97739900	2.56483300
H	3.64517300	-0.43868500	2.65305900
H	1.58010000	0.75895900	-0.74466400
H	2.58981800	3.55922600	0.15503700

PCM Model

Compound: HCHO Level of theory: B3LYP/6-31G(d)

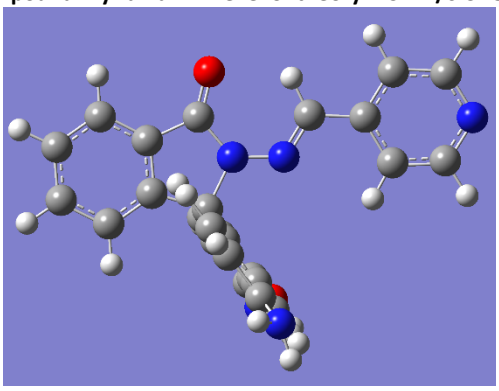


xyz-coordinates

C	-0.00444100	0.01033700	-0.00364200
C	-0.00361000	0.00682400	1.40132400
C	1.24530000	0.00284500	2.02920600
C	2.44087100	0.00554000	1.30797700
C	2.41950400	0.00927500	-0.09191000
C	1.16642900	0.01156800	-0.74430700
O	1.39417400	0.00156400	3.39460500
C	0.28076500	0.10167800	4.19259400
C	-1.02084000	0.11076000	3.68276900
C	-1.29679800	-0.05323700	2.19734300
N	-2.00868000	-1.36041000	1.93916000
C	-3.26705600	-1.21716200	1.37014000
C	-3.46844300	0.24205600	1.21423000
C	-2.34776300	0.92479600	1.68396700
C	-2.30180300	2.31498900	1.64170900
C	-3.40469400	2.99708200	1.11819600
C	-4.53127800	2.30515900	0.64621600
C	-4.57385500	0.91169500	0.69017500
C	-2.06444800	0.22126700	4.61695500
C	-1.83107600	0.31931300	5.97909200
C	-0.50841800	0.31062700	6.47543200
C	0.54515500	0.20032000	5.56003200
O	-4.04032800	-2.12215700	1.06514300
N	-1.33096400	-2.49193900	2.29152600
C	-1.84540000	-3.65403700	2.11472400
N	-0.26103600	0.47627000	7.83401900
H	0.63081200	0.12144700	8.15865700
H	-2.66444400	0.40485800	6.67103200
N	3.59945300	0.07776200	-0.82528800
H	4.42454900	-0.27214800	-0.35246100

H	1.12568000	0.01547000	-1.83008700
H	-3.09072200	0.22334800	4.25985500
H	1.57853200	0.19221900	5.89363900
H	-0.95613200	0.00494700	-0.52812900
H	3.37951700	0.00703200	1.85403700
H	3.53746700	-0.27942800	-1.77145700
H	-1.01671200	0.19097100	8.44570300
H	-1.22621000	-4.49186400	2.42773900
H	-2.82425300	-3.84380700	1.68742200
H	-1.43439700	2.85869800	2.00462300
H	-3.38929500	4.08245100	1.07603400
H	-5.37332700	2.86132400	0.24500800
H	-5.43514000	0.35664300	0.33059100

Compound: Pyridinal **Level of theory: B3LYP/6-31G(d)**

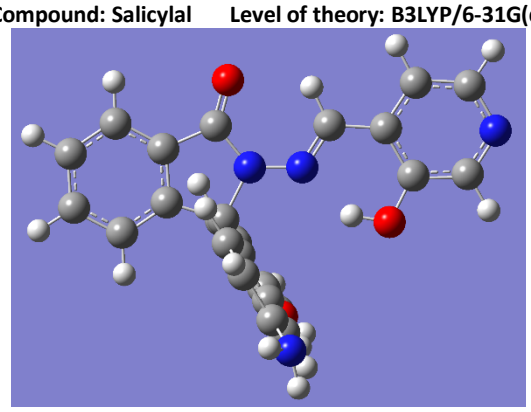


xyz-coordinates

C	-3.81621500	-0.03326400	-0.24968000
C	-2.60869000	-0.08596800	-0.93909100
C	-2.59495600	-0.16507500	-2.33101200
C	-3.77164100	-0.19436400	-3.07973000
C	-4.98340400	-0.14169300	-2.39165200
C	-5.00213900	-0.06196000	-0.99016600
C	-1.19919200	-0.20854600	-2.81835900
N	-0.40363600	-0.15301800	-1.67652600
C	-1.19033200	-0.07019600	-0.38304700
C	-0.88526500	-1.27497900	0.48984800
C	-0.15183400	-1.15110800	1.67377000
O	0.27945000	0.05894800	2.15996200
C	-0.12550000	1.21499000	1.53849700
C	-0.85704700	1.21928100	0.34695300
C	0.23656600	2.39319900	2.19366700
C	-0.12321000	3.63608300	1.65850200
C	-0.86262800	3.66049000	0.45493400
C	-1.21253800	2.47565200	-0.17205500
C	-1.26483700	-2.57463900	0.11435100
C	-0.93692300	-3.68836400	0.87051200
C	-0.19493900	-3.54324100	2.06397600
C	0.19190600	-2.25557700	2.45497400
N	0.94320700	-0.16227400	-1.55566400
C	1.71709100	-0.22593300	-2.58677400
C	3.17199000	-0.23178500	-2.39001200
C	4.01861700	-0.29699500	-3.50602900
C	5.39941900	-0.30196900	-3.31245300
N	5.98455500	-0.24758600	-2.10761800
C	5.16600700	-0.18517200	-1.04183100
C	3.77841700	-0.17450900	-1.12372800
H	3.60860100	-0.34287600	-4.51094200
H	3.17067300	-0.12282700	-0.22716900

H	6.06755900	-0.35222300	-4.17046100
O	-0.80295900	-0.27872800	-3.97867300
N	0.08319300	-4.64563900	2.86451200
H	0.87653500	-4.54023200	3.48599400
H	-1.25065500	-4.67765900	0.54885100
N	0.28549700	4.81991500	2.26241400
H	0.49145000	4.75392500	3.25229300
H	-1.15427100	4.61354400	0.02230300
H	-1.82922500	-2.71280400	-0.80377500
H	0.75819200	-2.09441700	3.36735400
H	-1.77996700	2.52084300	-1.09754900
H	0.79793800	2.32403100	3.12063400
H	-0.28989100	5.62835800	2.05766000
H	0.10986200	-5.53451900	2.37892100
H	1.34236000	-0.27547700	-3.60517300
H	-3.84030900	0.02842500	0.83431600
H	-5.95557700	-0.02180900	-0.47123900
H	-5.92019300	-0.16231400	-2.94047000
H	-3.73423500	-0.25631200	-4.16312600
H	5.65196800	-0.14133200	-0.06869200

Compound: Salicylal **Level of theory: B3LYP/6-31G(d)**

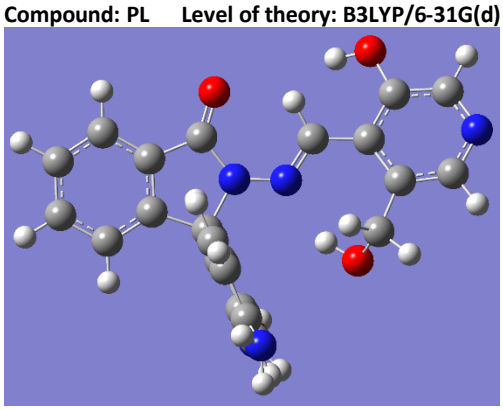


xyz-coordinates

C	0.35025300	0.74565400	0.17015000
C	0.29842100	0.53943900	1.54989900
C	1.35685600	-0.03945600	2.25714300
C	2.49091700	-0.40509600	1.51124800
C	2.57095300	-0.20689400	0.14322200
C	1.49032900	0.37847500	-0.55479500
O	-0.87095700	0.93841600	2.15054200
C	-1.05916500	0.69071400	3.48871000
C	-0.07487800	0.11970400	4.30137500
C	1.30253600	-0.22721900	3.76333600
C	1.77581100	-1.60858500	4.20310000
C	2.91722500	-1.51468500	4.99827400
C	3.30264300	-0.09635100	5.15816900
N	2.35734600	0.62730000	4.43643100
C	1.22238400	-2.85102600	3.91072500
C	1.84197100	-3.98987400	4.43491500
C	2.99112000	-3.89060300	5.23518000
C	3.54339500	-2.64371500	5.52642300
C	-0.40642800	-0.07709100	5.65315400
C	-1.64291000	0.27248800	6.16903300
C	-2.62562900	0.84796500	5.33196300
C	-2.31430100	1.05118200	3.98216000
N	2.25889000	1.96588400	4.26101100
C	3.09525200	2.80369500	4.78947600
C	2.92023300	4.23256700	4.55224300
C	1.87339800	4.76536200	3.76192200
C	1.80045000	6.15825900	3.60070000

N	2.66161900	7.01662200	4.14934900
C	3.65683300	6.51112300	4.90034400
C	3.81904800	5.14973600	5.12277200
O	0.94154100	4.00115900	3.15532800
O	4.24867900	0.37005900	5.78655600
N	-3.89061700	1.14151600	5.82570200
N	1.58464600	0.63583900	-1.91672400
H	4.63917200	4.78883300	5.73726900
H	4.34733500	7.22823600	5.33786600
H	-4.41033100	1.83864000	5.30570700
H	-1.86344000	0.10403700	7.21948100
H	0.70162900	0.72760300	-2.40480200
H	3.46536400	-0.50049000	-0.39918300
H	0.33432600	-0.51304400	6.31786500
H	-3.03760300	1.48761300	3.29999800
H	3.33445700	-0.85817000	2.02481700
H	-0.50684700	1.19394200	-0.32332300
H	2.23064800	0.04364500	-2.42503500
H	-3.93547200	1.31204800	6.82334200
H	3.92778100	2.48036500	5.40674100
H	0.33366300	-2.93752300	3.29255700
H	1.42601500	-4.96971400	4.21872300
H	3.45072900	-4.79238200	5.62841600
H	4.43149800	-2.54401300	6.14301800
H	0.99552400	6.56832200	2.99310800
H	1.14667200	3.05723100	3.37571700

Compound: PL Level of theory: B3LYP/6-31G(d)

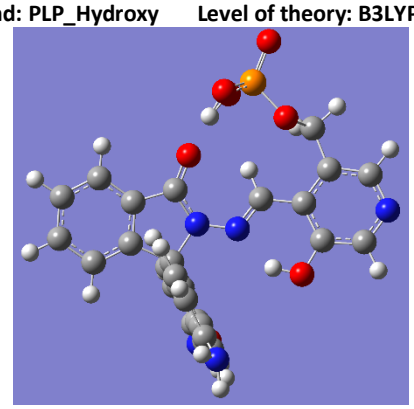


xyz-coordinates

C	-0.35034900	-0.05101900	-0.18620900
C	-0.19207600	0.05240700	1.22028500
C	1.12969600	0.14463100	1.70935200
C	2.20551700	0.10101900	0.81372900
N	2.05441300	-0.01227100	-0.50429600
C	0.79953900	-0.07594700	-0.97608900
C	-1.27885800	-0.01093600	2.20435500
N	-2.49241300	0.32539600	1.90795400
N	-3.49139700	0.23162400	2.81947600
C	-3.42202300	-0.10336900	4.17185800
C	-4.80599700	-0.00113500	4.67668200
C	-5.65740500	0.38786300	3.64383600
C	-4.88348800	0.58029600	2.34208000
C	-5.27337500	-0.24001900	5.96932300
C	-6.63741300	-0.07798800	6.20783300
C	-7.49902000	0.31271100	5.17026300
C	-7.01928300	0.54919000	3.87832600
C	-5.32859300	-0.38512800	1.25625700
C	-5.73861800	0.05960200	-0.00434000
O	-5.78680500	1.38710200	-0.34976800

C	-5.37150400	2.33293700	0.55377900
C	-4.93453900	2.01468800	1.84390500
C	-5.42361100	3.64966300	0.09211400
C	-5.03129400	4.70564900	0.92338500
C	-4.58502900	4.40206900	2.22993800
C	-4.54576300	3.08810200	2.66410700
C	-5.34651800	-1.77325900	1.47532400
C	-5.74545100	-2.67074800	0.49898300
C	-6.15924900	-2.20301600	-0.76890900
C	-6.15273000	-0.82289300	-1.00380400
O	-2.40720500	-0.41126100	4.79125900
N	-6.50344800	-3.09740700	-1.77517700
N	-5.13658500	6.02481000	0.50063100
O	1.45471000	0.26528300	3.02796800
C	-1.70312100	-0.15325200	-0.86321900
O	-2.44424300	1.06198100	-0.81403000
H	-2.72024300	1.13568800	0.12178000
H	3.21735200	0.16684700	1.20864200
H	-5.12590000	6.16309600	-0.50296400
H	-4.27523800	5.20491900	2.89316100
H	-7.09544300	-2.72237900	-2.50687700
H	-5.74223100	-3.73763400	0.70439900
H	-4.19765000	2.87987100	3.67224500
H	-5.77086100	3.83275200	-0.92028400
H	-5.03705400	-2.15659500	2.44395300
H	-6.46276100	-0.41668900	-1.96186000
H	-6.83456700	-4.00013300	-1.45604700
H	-4.52519100	6.68067900	0.97221200
H	-1.03983400	-0.37115100	3.20080400
H	-7.69419900	0.85098200	3.08274400
H	-8.55882600	0.43387600	5.37517700
H	-7.03912700	-0.25455300	7.20104400
H	-4.58916100	-0.54192100	6.75642800
H	0.69971800	-0.16221000	-2.05657500
H	0.69100800	0.55804800	3.54999400
H	-2.27884200	-0.97941000	-0.42209000
H	-1.55218400	-0.38312000	-1.92205500

Compound: PLP_Hydroxy **Level of theory: B3LYP/6-31G(d)**

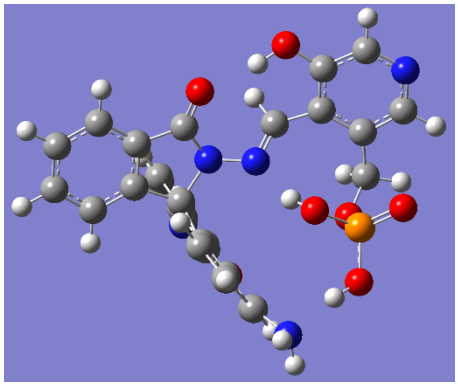


xyz-coordinates

C	0.37350900	0.08937900	0.33150500
C	0.21600000	0.19745200	1.73571000
C	1.35698900	0.53935400	2.49642100
C	2.58350000	0.71410700	1.83031000
N	2.72709200	0.59601100	0.51401800
C	1.63555200	0.30063700	-0.21406700
C	-1.08659200	-0.02349900	2.34907300
N	-1.26407800	0.18891100	3.61367500
N	-2.50277100	0.04145500	4.16436200

C	-3.72961000	0.13915700	3.55508500
C	-4.73261200	0.08664700	4.62788400
C	-4.08941000	-0.01529700	5.86217700
C	-2.57620900	-0.01712600	5.68588900
C	-6.12330600	0.11818100	4.51595800
C	-6.86827600	0.04279600	5.69168800
C	-6.22616000	-0.06311500	6.93582500
C	-4.83123300	-0.09473400	7.03518000
C	-1.91066900	1.20626200	6.28772600
C	-0.73553700	1.10328900	7.04012500
O	-0.13375500	-0.09773900	7.32398700
C	-0.74395500	-1.26501000	6.93618000
C	-1.91947600	-1.29220800	6.17912200
C	-0.10478600	-2.43171200	7.35753700
C	-0.63365700	-3.68482600	7.02414200
C	-1.82124300	-3.73150200	6.25855500
C	-2.43623300	-2.55887000	5.85487900
C	-2.42285500	2.50009300	6.08573900
C	-1.80230400	3.62702700	6.59647000
C	-0.61346100	3.50432300	7.35171000
C	-0.09254600	2.22284000	7.57000700
O	-3.93916000	0.26058300	2.33264100
N	0.04892600	4.63239000	7.81403300
N	-0.04625700	-4.85370700	7.48794100
O	1.33801100	0.70145800	3.83229000
C	-0.77940200	-0.24634300	-0.58220700
O	-1.81670200	0.75870700	-0.41353000
P	-3.34466600	0.46755000	-0.86558800
O	-3.58864800	0.43771100	-2.32407600
O	-3.75933300	-0.91090000	-0.14200900
O	-4.11666200	1.64494000	-0.10015500
H	3.46354900	0.96559000	2.41903900
H	0.93730700	-4.78758200	7.72135800
H	-2.25020500	-4.69278300	5.98992700
H	0.66859000	4.48657100	8.60197500
H	-2.22676900	4.61103100	6.41851200
H	-3.34492700	-2.62112400	5.26243800
H	0.80291200	-2.34570600	7.94704200
H	-3.33603500	2.62203400	5.50991100
H	0.81356500	2.07768300	8.15025800
H	-0.52724600	5.45635900	7.93682600
H	-0.24746400	-5.68568600	6.94624200
H	-1.89540900	-0.35141600	1.71653700
H	-4.34497400	-0.17626000	8.00247500
H	-6.82490500	-0.12110800	7.84007200
H	-7.95279700	0.06422900	5.64800700
H	-6.59860900	0.19767000	3.54338000
H	1.77952900	0.22981500	-1.29000200
H	0.40375400	0.59449800	4.14198200
H	-1.19650700	-1.23391100	-0.35758700
H	-0.44817900	-0.24224200	-1.62374800
H	-3.90725600	-0.78485200	0.82482900
H	-4.09929500	1.51944900	0.87506200

Compound: PLP_Phosphate Level of theory: B3LYP/6-31G(d)

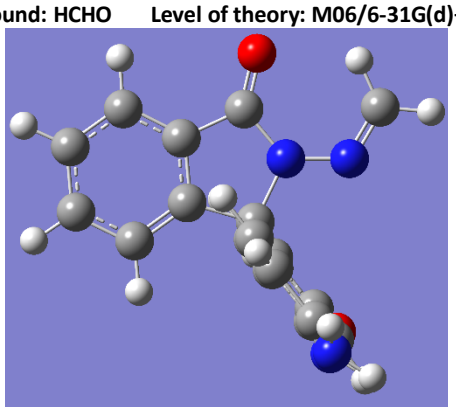


xyz-coordinates

C	3.31005700	-1.61987400	0.79490500
C	2.34098600	-2.15710000	-0.07286700
C	2.75522100	-3.09295800	-1.04457400
C	4.09921000	-3.49040900	-1.06434200
N	5.01300400	-3.00994300	-0.22153600
C	4.62094200	-2.08974000	0.66895600
C	0.88920700	-1.90131200	-0.07914300
N	0.35549800	-0.74762400	-0.28357600
N	-0.98321600	-0.85758200	-0.64980300
C	-1.32517900	-1.56099500	-1.79612800
C	-2.66991000	-1.08888400	-2.17209900
C	-3.07023300	-0.07848200	-1.29631700
C	-2.00022600	0.18847900	-0.24235700
C	-3.47974800	-1.52089000	-3.22250800
C	-4.72181400	-0.90671300	-3.37910300
C	-5.13067300	0.10712700	-2.49879400
C	-4.31265900	0.52856600	-1.44538800
C	-1.37208200	1.56413900	-0.33281600
C	-1.00772100	2.25841200	0.82569300
O	-1.37861900	1.86769300	2.08426100
C	-2.14595000	0.73827200	2.23917300
C	-2.48918300	-0.09220500	1.16881600
C	-2.55164700	0.47594300	3.54788900
C	-3.32488000	-0.65739500	3.82984100
C	-3.67476000	-1.51449600	2.76176500
C	-3.26061600	-1.22751500	1.47199900
C	-0.96566500	2.10194700	-1.56365200
C	-0.15747400	3.22599400	-1.63879800
C	0.28445500	3.83968200	-0.45423800
C	-0.19699700	3.39191800	0.77490700
O	-0.61861000	-2.39068700	-2.37584000
N	1.33972800	4.77817800	-0.48018700
N	-3.79240300	-0.90207200	5.11395300
O	1.91980100	-3.64001100	-1.95996700
C	3.00189900	-0.62304000	1.88943700
O	2.60967100	0.70395200	1.45002200
P	3.36454700	1.49236200	0.25281500
O	4.78577000	1.11866300	0.03906800
O	2.40992500	1.22738100	-1.01511100
O	3.16166200	3.01455300	0.67993500
H	4.42014800	-4.22472900	-1.80041100
H	-3.25637600	-0.48057900	5.86316100
H	-4.27277000	-2.40005700	2.95776800
H	1.28474800	5.48589500	0.24842700
H	0.18442500	3.59150200	-2.60248300
H	-3.53867300	-1.90473100	0.66949300
H	-2.25599600	1.16336800	4.33461100
H	-1.25576600	1.59888700	-2.48149400
H	0.11315100	3.85690000	1.70530700

H	1.47298700	5.22605800	-1.38275500
H	-4.02036100	-1.86834900	5.31558000
H	0.25597100	-2.78915000	-0.04200700
H	-4.63920300	1.31199100	-0.76822800
H	-6.10112700	0.57437300	-2.63848000
H	-5.37981100	-1.21411500	-4.18612900
H	-3.14576300	-2.30855800	-3.89057800
H	5.39182300	-1.69803800	1.32828600
H	1.07728500	-3.13508600	-2.05378200
H	2.15613600	-0.95791300	2.49461000
H	3.87485500	-0.52309000	2.53944800
H	1.59618400	0.71599800	-0.76875000
H	2.59033700	3.60523700	0.10374000

Compound: HCHO Level of theory: M06/6-31G(d)+GD(3)

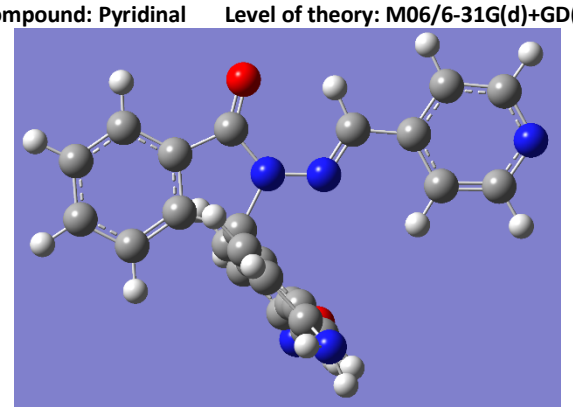


xyz-coordinates

C	0.00636700	-0.03742900	0.01725400
C	0.00374700	-0.02858900	1.40815200
C	1.18189300	0.01537100	2.15043600
C	2.38288500	0.04370000	1.43255900
C	2.41527100	0.03513400	0.05243600
C	1.21421800	-0.00738600	-0.68098100
C	1.16621000	-0.05953000	3.65576300
C	-0.23072400	0.14888300	4.18176500
C	-1.33873000	0.09985400	3.33881400
O	-1.23303800	-0.05773200	1.98649800
C	-2.63884400	0.21640300	3.81905900
C	-2.86839100	0.38241000	5.18536300
C	-1.76078000	0.43125600	6.05323700
C	-0.48100800	0.31389000	5.54889900
C	2.17454800	0.86477700	4.29452800
C	3.12809700	0.14230400	4.99834800
C	2.83881700	-1.30083100	4.89248300
N	1.69759200	-1.38690100	4.11199600
C	2.23107500	2.24858500	4.24417800
C	3.27069300	2.88514300	4.91879200
C	4.23124900	2.15435500	5.62707300
C	4.16909500	0.76642400	5.67447200
N	-4.15000600	0.55839300	5.67353600
N	1.00025100	-2.47744200	3.69792600

C	1.36755300	-3.65506000	4.03256900
O	3.46389500	-2.22962400	5.38263600
N	1.23337200	0.04345500	-2.06254300
H	0.41001000	-0.32040400	-2.52701800
H	3.36665700	0.06107800	-0.47733700
H	-4.89536800	0.18829400	5.09602200
H	-1.92258200	0.56234700	7.12242100
H	3.32330800	0.06588600	1.98451100
H	-0.94687300	-0.06429000	-0.50877000
H	0.36489200	0.34296100	6.23683200
H	-3.46464600	0.17854500	3.11001600
H	-4.27880400	0.32761600	6.65137000
H	2.08841600	-0.28018800	-2.49862000
H	0.74774400	-4.46797200	3.65454100
H	2.23220200	-3.88905100	4.65133900
H	1.48339200	2.81766200	3.69210600
H	3.33835500	3.97112100	4.89493200
H	5.03156200	2.68035700	6.14336600
H	4.90496600	0.17716200	6.21903700

Compound: Pyridinal **Level of theory: M06/6-31G(d)+GD(3)**

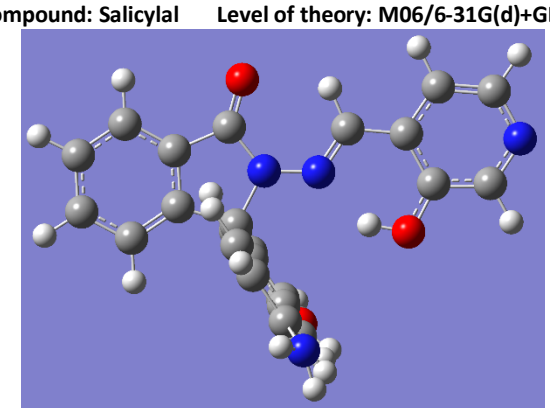


xyz-coordinates

C	-3.83056700	-0.03603800	-0.25425900
C	-2.62994800	-0.08768600	-0.94436800
C	-2.61416000	-0.16891500	-2.33104700
C	-3.78593800	-0.20170700	-3.07724200
C	-4.99264400	-0.15018000	-2.38967700
C	-5.01171400	-0.06819400	-0.99285100
C	-1.22303700	-0.21175300	-2.81636600
N	-0.43912100	-0.15349500	-1.67195200
C	-1.22667500	-0.07067700	-0.39146500
C	-0.91392600	-1.26383100	0.47288200
C	-0.06498900	-1.14967800	1.57236300
O	0.44094500	0.04776200	1.99161900
C	-0.03573800	1.20033700	1.43482200
C	-0.88563100	1.20658800	0.33021300
C	0.37577600	2.37316700	2.05754300
C	-0.05693600	3.60981300	1.57582500
C	-0.91755600	3.63572900	0.46207900
C	-1.31000200	2.45538400	-0.13742000
C	-1.36183200	-2.54885100	0.14684300
C	-0.99532900	-3.66151900	0.87780700
C	-0.13795900	-3.52660800	1.98620700
C	0.32189200	-2.25283600	2.32463900
N	0.89765600	-0.15922300	-1.53301900
C	1.68806200	-0.22308600	-2.54389600

C	3.13034600	-0.22203400	-2.30004500
C	4.01310700	-0.29106800	-3.37881700
C	5.38078800	-0.28798600	-3.13023100
N	5.91357800	-0.22197200	-1.90830200
C	5.05786600	-0.15589400	-0.87949600
C	3.67908900	-0.15273700	-1.01473800
H	3.63718600	-0.34617600	-4.39941600
H	3.02961300	-0.09700900	-0.14361500
H	6.08381300	-0.34154900	-3.96321000
O	-0.82354500	-0.28310200	-3.96829000
N	0.18850500	-4.62495400	2.75919700
H	1.03607700	-4.54015100	3.30738100
H	-1.36423700	-4.64856600	0.60213100
N	0.38785200	4.78768800	2.14561300
H	0.71005900	4.72068100	3.10349600
H	-1.26581800	4.59287200	0.07606000
H	-2.01480900	-2.67372200	-0.71764100
H	0.98058200	-2.10164400	3.17857200
H	-1.96902700	2.49504000	-1.00542700
H	1.03344600	2.30520000	2.92293500
H	-0.20571400	5.59526200	1.99974500
H	0.12649600	-5.52161700	2.29215800
H	1.34027200	-0.27727400	-3.57709600
H	-3.84605400	0.02727100	0.83346400
H	-5.96784500	-0.02910700	-0.47451400
H	-5.93199200	-0.17365600	-2.93796800
H	-3.74650700	-0.26600700	-4.16320400
H	5.50508900	-0.10199300	0.11448800

Compound: Salicylal Level of theory: M06/6-31G(d)+GD(3)

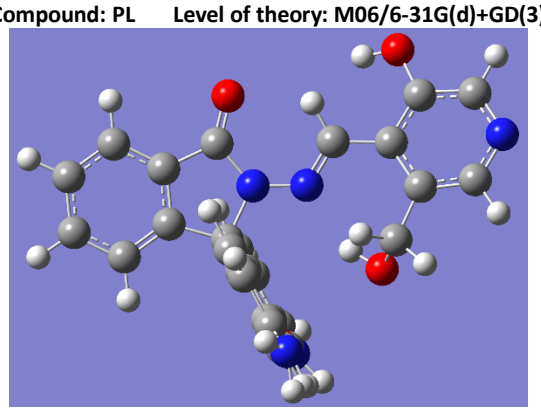


xyz-coordinates

C	0.40325800	0.82143600	0.21561100
C	0.33410200	0.58378200	1.58416800
C	1.35989700	-0.05576900	2.27745000
C	2.47943300	-0.44894600	1.53365300
C	2.57563700	-0.22325800	0.17612700
C	1.52787200	0.42345200	-0.50815200
O	-0.81207200	1.01547300	2.18928400
C	-1.01568700	0.73289000	3.51027200
C	-0.05997300	0.10161500	4.30389200
C	1.30518600	-0.24776800	3.77073600
C	1.77392200	-1.61572200	4.20598600
C	2.91259600	-1.52382300	4.99619200
C	3.29834100	-0.11065600	5.15568000
N	2.34977700	0.60377200	4.43670700
C	1.21549300	-2.84890300	3.91157800
C	1.83095700	-3.98566100	4.43150900
C	2.97804400	-3.89068000	5.22736200
C	3.53423700	-2.65093100	5.51978700
C	-0.39756000	-0.12607900	5.64369900

C	-1.61800700	0.24757200	6.16720500
C	-2.57236200	0.88359400	5.34932700
C	-2.25363100	1.12049000	4.01172300
N	2.23919500	1.93232400	4.24898200
C	3.05991400	2.78126100	4.76860600
C	2.86582000	4.19968700	4.51214800
C	1.82171500	4.70780600	3.71341800
C	1.73785200	6.09418600	3.53926500
N	2.58280000	6.96333400	4.08093300
C	3.57564700	6.48024400	4.84002800
C	3.74903300	5.12716200	5.07617500
O	0.90232200	3.94168400	3.10904800
O	4.23976700	0.35669000	5.77705800
N	-3.81753900	1.20882200	5.84974200
N	1.63889600	0.70297700	-1.85577600
H	4.56979200	4.77497000	5.69970400
H	4.25852400	7.20980700	5.27535600
H	-4.32078000	1.93151800	5.34952300
H	-1.85241700	0.05425600	7.21313100
H	0.76795800	0.85862900	-2.34864800
H	3.46036900	-0.54013800	-0.37443200
H	0.33280200	-0.60913800	6.29380400
H	-2.96167700	1.60614100	3.34194300
H	3.30195600	-0.94770700	2.04754500
H	-0.43254600	1.32020800	-0.27281200
H	2.27217300	0.10915200	-2.37731900
H	-3.86831900	1.33247800	6.85365000
H	3.89948200	2.47855100	5.39615300
H	0.32229900	-2.92299200	3.29180400
H	1.41239400	-4.96664100	4.21517700
H	3.43543000	-4.79689100	5.61856600
H	4.42577600	-2.55306800	6.13662500
H	0.92752400	6.48462400	2.91982500
H	1.10336000	3.00192300	3.33229900

Compound: PL **Level of theory: M06/6-31G(d)+GD(3)**

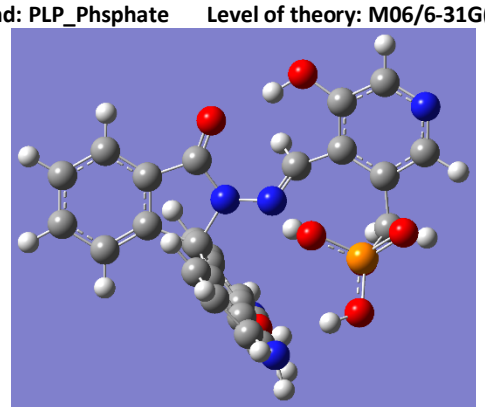


xyz-coordinates

C	-0.53747900	-0.11993000	-0.19004100
C	-0.28271700	-0.00883700	1.19579000
C	1.06233200	0.01368000	1.60018300
C	2.07133400	-0.10083000	0.64158300
N	1.83133800	-0.22128700	-0.65660900
C	0.55300500	-0.22043600	-1.04713100
C	-1.31525800	-0.01007700	2.23028200
N	-2.51446600	0.37392300	1.96302000
N	-3.50060200	0.31065500	2.87765700
C	-3.44560700	-0.04663500	4.22037200
C	-4.83636900	0.03785300	4.69600400

C	-5.66817400	0.42026600	3.65122600
C	-4.87832500	0.63081200	2.37950900
C	-5.32863200	-0.21562100	5.97060800
C	-6.69598700	-0.07407700	6.17477600
C	-7.53610500	0.31049400	5.12346300
C	-7.03207500	0.56220900	3.84934900
C	-5.26413000	-0.33306700	1.28599400
C	-5.61114200	0.10103500	0.00840900
O	-5.68288000	1.41940900	-0.33341300
C	-5.32236200	2.36454800	0.58071100
C	-4.94224100	2.05304100	1.88518100
C	-5.36197700	3.67638500	0.11900200
C	-5.01846500	4.72998600	0.96638900
C	-4.63292600	4.43298200	2.28878700
C	-4.60151400	3.12375900	2.72122600
C	-5.24377300	-1.71606900	1.50387600
C	-5.54908700	-2.62163500	0.50872900
C	-5.89918800	-2.16478400	-0.77714000
C	-5.92980400	-0.78989700	-1.01142200
O	-2.44330900	-0.35576000	4.84558100
N	-6.15134300	-3.06408500	-1.79497300
N	-5.10751200	6.04030100	0.53988300
O	1.47155200	0.12942600	2.88443600
C	-1.92413400	-0.14276700	-0.77970900
O	-2.55160100	1.12027900	-0.75194500
H	-2.77534500	1.25831700	0.18837700
H	3.10972100	-0.08768000	0.97781800
H	-5.06602400	6.18315600	-0.46193200
H	-4.36164800	5.24314600	2.96425900
H	-6.70038700	-2.71161100	-2.56963500
H	-5.52027800	-3.69185300	0.70876500
H	-4.29563100	2.91126200	3.74626900
H	-5.66256200	3.85806400	-0.91177100
H	-4.97395900	-2.08779000	2.49311800
H	-6.19370000	-0.39150900	-1.98992700
H	-6.45421300	-3.98482100	-1.50122700
H	-4.53667500	6.70761600	1.04438100
H	-1.05647600	-0.38256700	3.22354400
H	-7.68687500	0.86146400	3.03121400
H	-8.60385100	0.41467200	5.30626200
H	-7.12084600	-0.26331100	7.15818800
H	-4.65656100	-0.51466200	6.77296800
H	0.37484200	-0.31520200	-2.12052700
H	0.75974900	0.45647000	3.45381000
H	-2.54015200	-0.90291000	-0.26789600
H	-1.85426600	-0.43716700	-1.83470700

Compound: PLP_Phsphate Level of theory: M06/6-31G(d)+GD(3)



xyz-coordinates

C	3.21977000	-1.58548200	0.89937200

C	2.30333100	-2.13195600	-0.00766400
C	2.76856800	-3.04544800	-0.96756500
C	4.11364700	-3.41924400	-0.93180200
N	4.97798400	-2.93535100	-0.04748500
C	4.53730200	-2.03221000	0.82833800
C	0.85808700	-1.89679600	-0.06155600
N	0.32609200	-0.74656200	-0.26538600
N	-0.99089700	-0.86090200	-0.66429800
C	-1.30308000	-1.54650900	-1.82502500
C	-2.63831600	-1.07105000	-2.21093800
C	-3.04675600	-0.07333900	-1.33225000
C	-1.99721000	0.18345400	-0.27634200
C	-3.43252600	-1.48553800	-3.27302100
C	-4.66643400	-0.86655500	-3.43469900
C	-5.08200300	0.13450900	-2.55023000
C	-4.27909400	0.54003000	-1.48565600
C	-1.35731300	1.54159700	-0.36504500
C	-0.93162300	2.19536300	0.79040700
O	-1.23676000	1.76608700	2.04585500
C	-2.05402000	0.68214100	2.19961100
C	-2.48480800	-0.08918900	1.12292700
C	-2.42417100	0.39980500	3.50901800
C	-3.24824900	-0.69367600	3.78089200
C	-3.68724300	-1.49082000	2.70549500
C	-3.30421200	-1.18627900	1.41542500
C	-0.98141600	2.08848900	-1.59597100
C	-0.16703000	3.20172500	-1.67820300
C	0.30886600	3.79475700	-0.50161600
C	-0.12165800	3.32215900	0.73227200
O	-0.58243600	-2.35708500	-2.39884300
N	1.33768700	4.74795800	-0.54338300
N	-3.67426100	-0.95703200	5.06689300
O	1.98494300	-3.59225400	-1.91531000
C	2.84292000	-0.59437200	1.96398500
O	2.43823000	0.69770200	1.48809000
P	3.24921500	1.46454800	0.32963300
O	4.65286200	1.03535200	0.16674200
O	2.32466800	1.25896800	-0.95520700
O	3.08928500	2.98366700	0.74920900
H	4.47485000	-4.14354000	-1.66403100
H	-3.09688400	-0.58561700	5.81141300
H	-4.32937600	-2.34843600	2.90141200
H	1.27939800	5.45724700	0.18319900
H	0.15118100	3.58418500	-2.64642900
H	-3.64355200	-1.82170700	0.59683000
H	-2.06165000	1.04478800	4.30795300
H	-1.30845600	1.59808000	-2.51304600
H	0.23484500	3.76235400	1.66227000
H	1.45969500	5.18976800	-1.45010300
H	-3.96748300	-1.90939600	5.24766100
H	0.22798200	-2.79359100	-0.05306800
H	-4.60462400	1.31893400	-0.79708300
H	-6.05136400	0.60629400	-2.69788100
H	-5.31755300	-1.16131000	-4.25460800
H	-3.09007200	-2.26734100	-3.94818400
H	5.27252700	-1.62511100	1.52467400
H	1.14235000	-3.10028800	-2.04519300
H	1.98381000	-0.95075900	2.54462900
H	3.68913600	-0.46628100	2.65083600
H	1.50998500	0.73697400	-0.74183500
H	2.58683500	3.57324000	0.12354000

4. References

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