Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Photoluminescence study of optically active Diaminopyridine intercalated Graphene oxide

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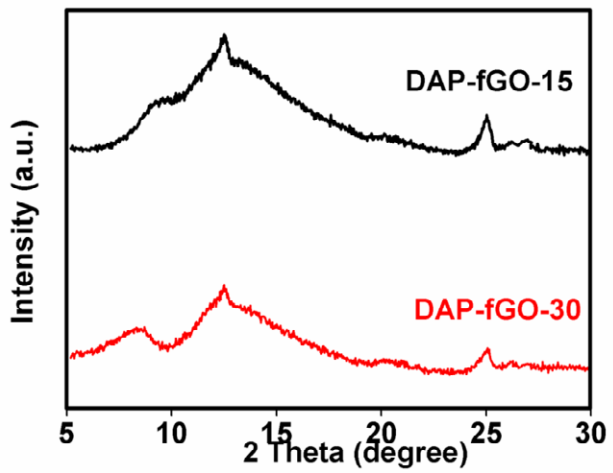

Figure S1 XRD pattern of DAP-fGO 15 and 30 shows the rise of intercalation peak with increasing in DAP content

Calculation of mean crystallite thickness of Graphene oxide:

The mean crystallite thickness of the Graphene oxide has been calculated applying the following Debye-Scherrer equation:

$$t = K\lambda/FWHM \cos\theta \ldots (1)$$

where t is the mean crystallite thickness, K is a constant (value of 0.9), λ is the wavelength of the X-ray used (λ= 1.5418 Å), θ is the angular position of the first diffraction peak and FWHM is the broadening of the [001] diffraction line (calculated as full width at half maximum of the peak height and expressed in radians).

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The value of the average crystallite thickness for GO is found to be ~73 Å.

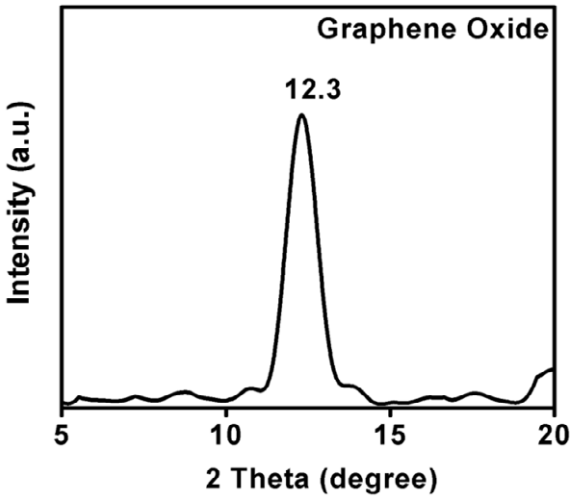

Figure S2 XRD pattern of graphene oxide

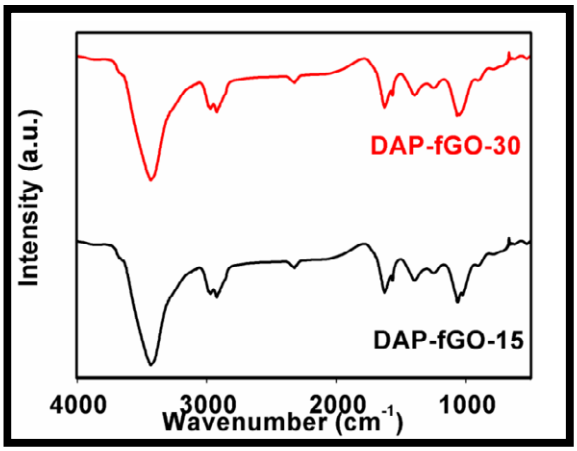

Figure S3 FTIR spectra of DAP-fGO 15 and 30 shows the diminish of the C-O-C peak at 1067 cm-1 and rise of C-O peak of C-OH at 1047 cm-1 with increasing in DAP content

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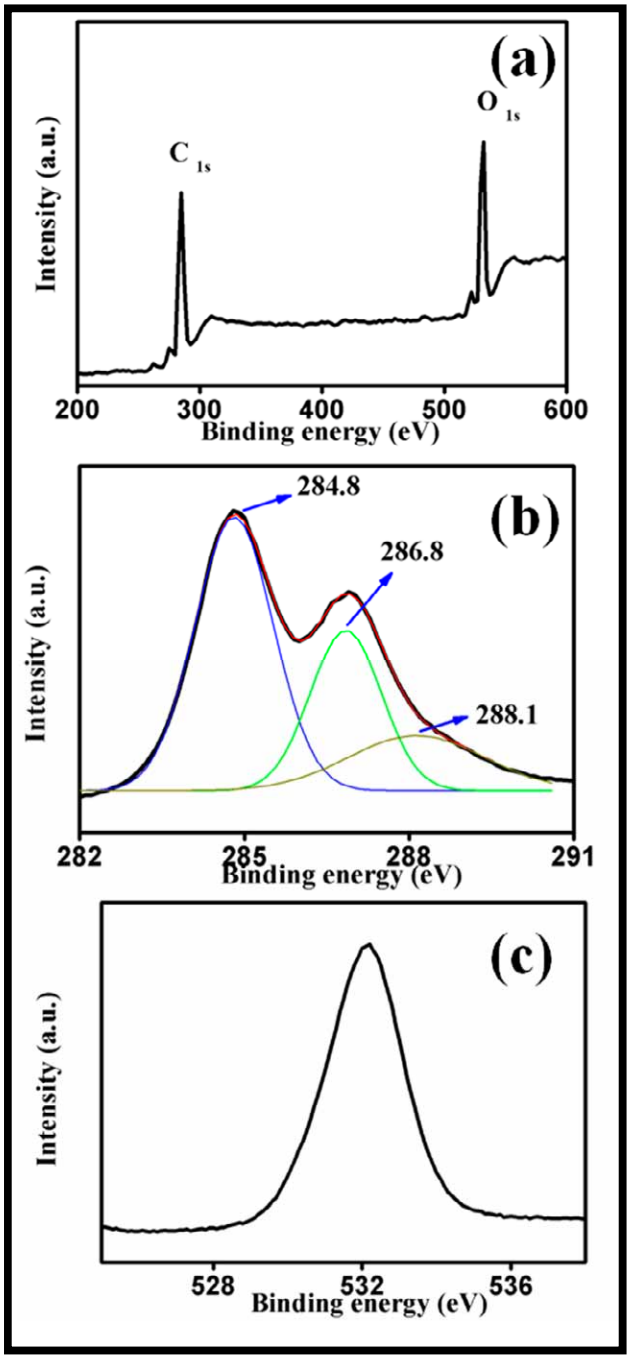

Figure S4 Low range XPS spectra for Graphene oxide (GO) showing the presence of only carbon and oxygen functionalities (b) Deconvoluted XPS peaks for C-1s in GO (c) High resolution XPS peak of O-1s of GO

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Optical Property of GO:

Graphene does not possess any fluorescence property due to lack of band gap however graphene oxide (GO) possesses very weak fluorescence property[1]. GO exhibits very weak photoluminescence (PL) property in the visible and near-infrared region[2] due to the presence of finite band gap[3]. The weak PL in GO arises due to recombination of electron–hole (e–h) pairs in localized electronic states of plausible configuration arising from the heterogeneous atomic and electronic structures of GO[4]. Another reason for the poor emissive property of GO is the presence of oxygen functionalities e.g. hydroxyl, and epoxy groups which usually induce non-radiative recombination as a result of transfer of their electrons to the holes present in sp2 clusters producing non-radiative localized electron–hole (e–h) pairs[5,6].

Fig S5 shows the UV-Vis absorption and PL spectra of pristine GO. GO dispersions show a maximum absorption at 230 nm and a shoulder at ~290 - 300 nm, which is assigned to the π- π* transition of aromatic C=C bonds and n– π * transition of the C=O bonds respectively. The PL spectrum of the GO solution displays a broad emission band exhibiting maximum intensity at ~519 nm with an excitation at 340 nm.

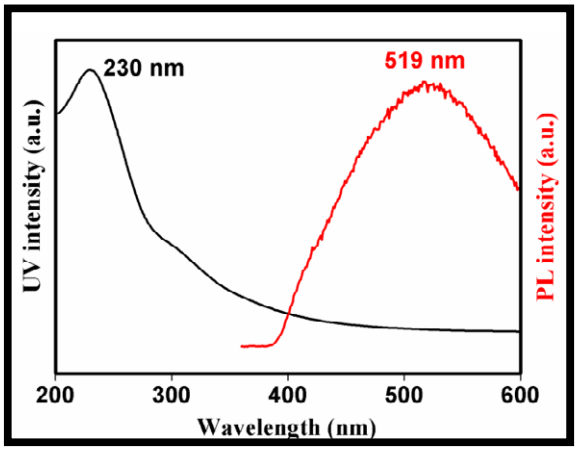

Figure S5 UV- VIS absorption and PLspectra of GO

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Optical Property of DAP-fGO composite:

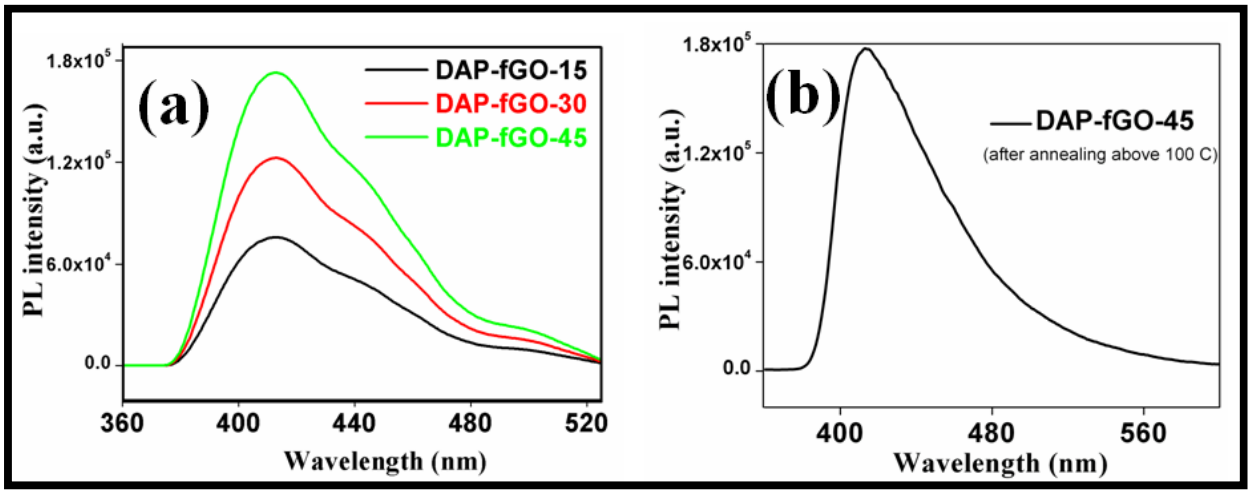


Figure S6 (a) PLspectra of different DAP-fGO composites and (b) PLspectra of DAP-fGO-45 after annealing

Effect of pH and concentration on optical Property of DAP-fGO composite:

The fluorescence of the aqueous solution of DAP-fGO composites can also be tuned by controlling the pH value of the solution using diluted HCl and NaOH as well as buffer solution. As observed in Fig. S7 (a), the PL intensity of DAP-fGO-45 gradually increases with decrease in pH (from pH 10 to pH 1). The other two DAP-fGO composites (DAP-fGO-15 and DAP-fGO-30) show similar behaviour. This aspect of the pH dependent fluorescence is related to the passivation of radiative defects embedded in the DAP-fGO-45 composite. As a result of changes in pH, the protonation - deprotonation of the hydroxyl, carboxylic and amine groups of DAP-fGO-45 composite may cause electrostatic doping or charging to the DAP-fGO-45 composite, which in turn results in the shifting of the Fermi level. With decrease in pH, the –OH, COOH, -NH groups as well as =N- atoms of pyridine rings of the composite are get protonated. It

destabilizes n-π* state but stabilizes the π-π* state of the composite, which inturn reduces the energy gap between the states resulting in the decrease of the vibronic interaction. As a result the symmetry of the π-π* state increases and the Franck-Condon factor decreases. This results in a decrease in radiationless decay which explains the bright fluorescence intensity of the DAP-fGO-45 composite with decrease in pH.

Figure S7 (b) shows the concentration-dependent PL spectra of DAP-fGO-45 composite. It has been observed that at lower concentration (1 − 40 mg/L) the PL intensity gradually increases with concentration, but at higher concentrations (>40 mg/L) PL intensity gradually decreases. The concentration-dependent PL behavior of DAP-fGO-15 and DAP-fGO-30 composites follow the same manner.

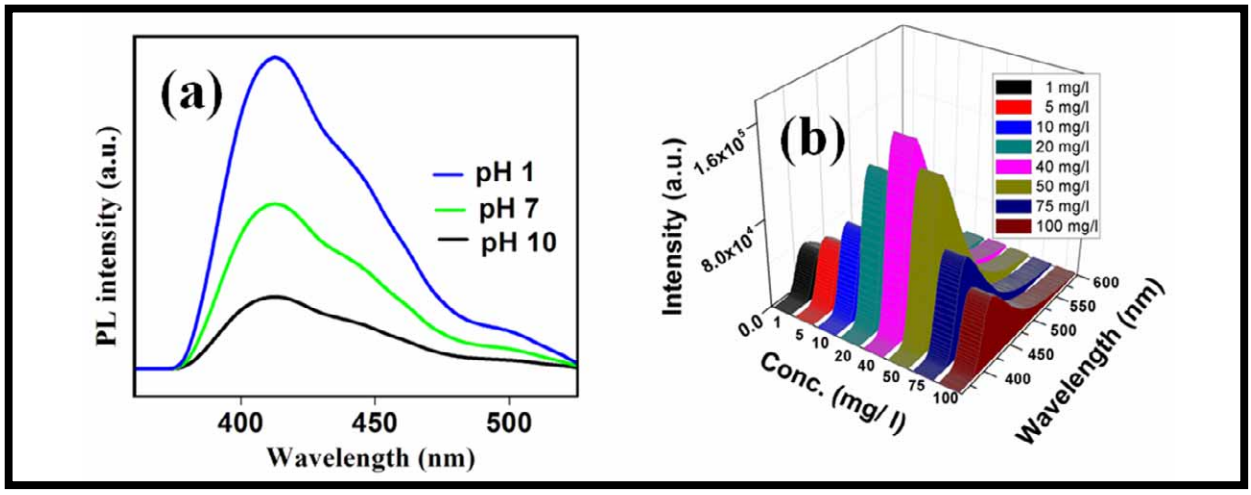


Figure S7 (a) pH and (b) Concentration dependent PLspectra of DAP-fGO-45

Photo-stability:

To investigate the photo-stability of the composite, the time-dependent fluorescence intensity of DAP-fGO-45 composite (Figure S8) was measured at an interval of 120 s over the total period of

1200 s under constant irradiation. During the experiment no such significant change in PL intensity was observed.

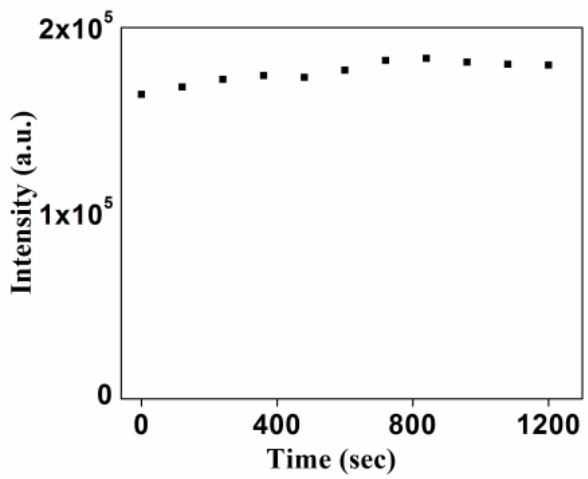
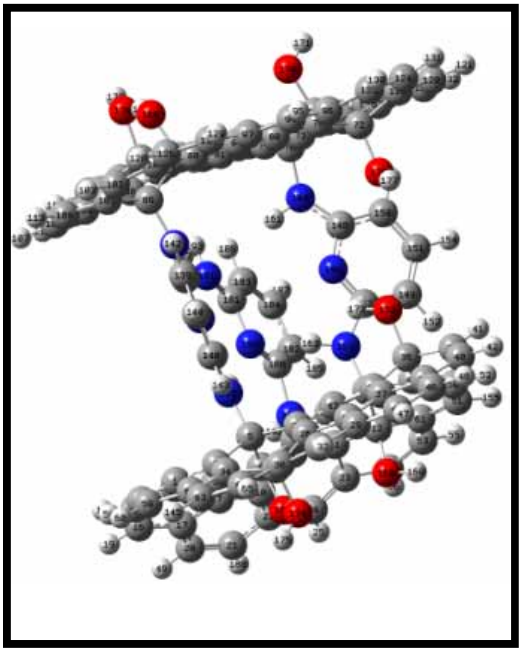


Figure S8 Variation of PL intensities with increase in time of DAP-fGO-45.

Atomic coordinates of all calculated structures:



Parent structure (1)

Bond		**Bond length (Å)**
N^{156}-C^{89}, N^{5}-C^{158}	:	~ 1.448
C^{22}-C^{93}	:	10.505
C^{20}-C^{115}	:	10.556
C^{24}-C^{90}	:	10.613
		Bond angle (deg)
C^{137}-N^{156}-C^{89}	:	132.73
C^{147}-N^{162}-C^{13}	:	134.24

Energy: -5522.33 hartree unit

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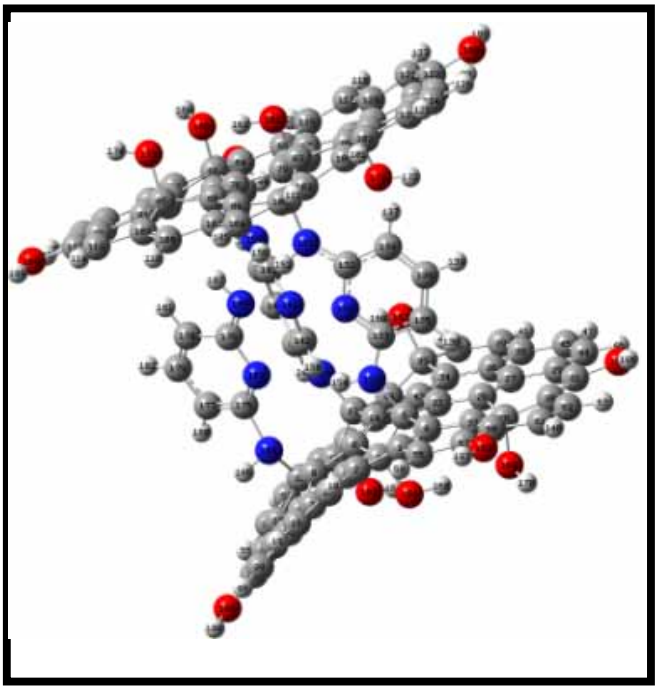
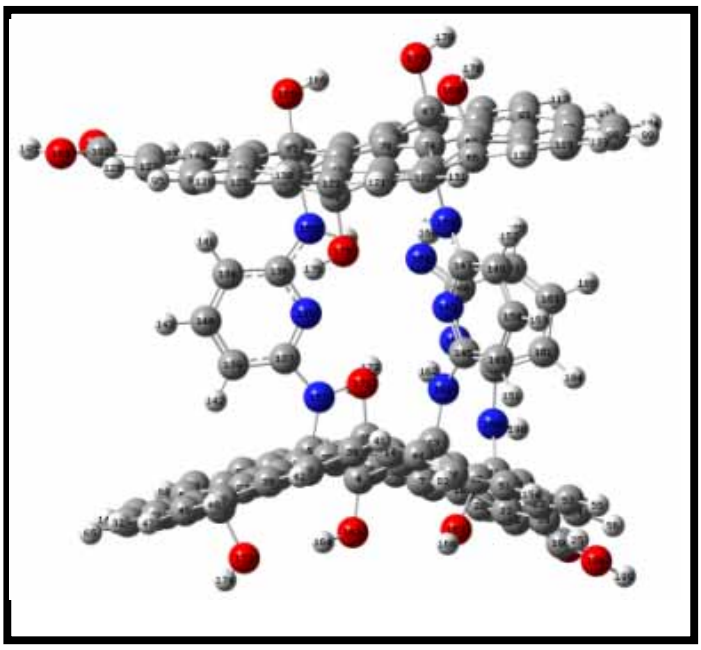


Hydroxyl group enriched (2)

Bond	**Bond length (Å)**
N^{151}-C^{87}, N^{153}-C^{5} :	~ 1.446
C^{53}-C^{99} :	10.12
C^{88}-C^{24} :	10.68
C^{20}-C^{113} :	10.57
Bond angle (deg)	
C^{133}-N^{153}-C^{5} :	127.18
C^{68}-N^{155}-C^{143} :	136.90

Energy: -5969.19 hartree unit



Carboxylic group enriched (3)

Bond	**Bond length (Å)**
N^{161}-C^{13}, N^{159}-C^{70} :	~ 1.4712
C^{20}-C^{115} :	10.51
C^{101}-C^{54} :	10.18
C^{24}-C^{90} :	10.66
Bond angle (deg)	
C^{70}-N^{159}-C^{147} :	135.76
C^{137}-N^{157}-C^{5} :	127.26

Energy: -5895.67 hartree unit

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List of atoms with their cartesian coordinates in Angstrom unit:

Parent structure (1):	**X**	**Y**	**Z**
C	5.45308800	0.68673000	3.03629200
C	5.19426300	-0.77268300	3.18176700
C	4.89035200	-1.51519800	2.07598200
C	4.75554200	-0.87143100	0.70683200
C	4.26710100	0.56378900	0.84584300
C	5.21197600	1.28051200	1.79652100
C	4.99486800	-2.92601000	2.11496000
C	3.80294900	-1.62140100	-0.22924600
C	3.77567000	-3.09583000	-0.04115700
C	4.67214800	-3.69576800	0.97918200
C	3.36596400	-3.94455500	-1.17610800
C	3.21845500	-3.18232100	-2.47362000
C	2.47541300	-1.82231700	-2.34108400
C	3.27455400	-1.02058500	-1.29370900
C	5.49862600	-1.45439900	4.39594000
C	5.66099400	-2.79797900	4.43071800
C	5.47261000	-3.57538100	3.26188300
H	5.64569100	-0.88985600	5.29192000
H	5.94937000	-3.28609800	5.34081800
C	5.76061700	-4.96010700	3.18948900
C	5.57334300	-5.65238500	2.03648400
C	4.98588900	-5.02799400	0.90696300
C	3.95418700	-5.30741300	-1.30786700
C	4.66955500	-5.80434200	-0.30105500
H	5.04616000	-6.80782400	-0.34978600
C	4.84922600	2.30981400	-0.87220100
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C	5.96116300	2.82346300	0.00090500
C	5.25508300	4.14433200	-2.45687400
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C	4.24184100	1.14947700	-0.55801700
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C	3.25881700	0.99224400	-2.75860700
C	2.24881900	0.35379900	-3.70340500
C	3.83767600	2.25253300	-3.07704100
C	2.27456100	0.96644100	-5.08049800
C	3.68390300	2.82100900	-4.37006800
C	2.89000200	2.09658900	-5.36188600
H	1.62787100	0.50534200	-5.79702400
H	2.80070500	2.53824900	-6.33552600
C	3.52186200	0.41841500	-1.54677900
C	2.47586200	-1.14917800	-3.71491800
C	5.05540800	4.68551300	-3.69687600
C	4.28866600	4.01224400	-4.65893600
H	5.49329500	5.63325100	-3.94288400
H	4.17288100	4.44337100	-5.63381200
H	6.14891400	-5.45336200	4.05881300
C	2.49034600	-1.90019300	-4.80856800
C	2.53560900	-3.36885600	-4.77409500
H	2.42309500	-1.45160700	-5.77680600

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C	2.99931100	-5.46450700	-3.55991200
C	3.58192200	-6.04399800	-2.51253200
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H	3.79530600	-7.09497800	-2.52593900
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C	6.63761200	2.67857700	3.69688000
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H	7.15863100	3.23480900	4.45136300
C	2.78916800	-4.02472500	-3.64741600
C	6.52505200	3.19641700	2.41690800
C	7.12589000	4.47998400	2.04342600
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C	-5.66432000	-0.76342200	-2.87984600
C	-5.23959100	0.44234900	-3.31478900
C	-5.62030500	-1.05154500	-1.38820200
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C	-4.43501300	-0.40288700	-0.68783400
C	-5.71645000	-2.51032100	-1.01119600
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C	-4.33047700	1.04505700	-1.12563900
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C	-3.85272700	3.73779400	-1.85569200
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C	-3.65907200	3.39286700	-0.57944000
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C	-6.43624600	-4.76281600	-1.45041700
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C	-2.26261300	3.13908200	4.30909600
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H	-1.97196700	1.09712700	6.98701700
C	-2.05317200	2.74222100	5.56730200
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C	-3.20204000	-0.87058400	5.60779000
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C	-4.96481400	-3.84750100	4.46183400
C	-4.39319500	-2.98834900	5.29909900
H	-4.17014800	-3.27726100	6.30819000
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C	-5.48037800	0.92964000	-4.67650100
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C	-4.73720100	4.50918500	-4.41369200
C	-4.17909500	5.48675600	-3.50299400
C	-2.52496000	6.36465600	2.29310600
C	-2.71035100	6.72704700	1.02511800
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H	-5.16561600	4.86531100	-5.33174100
H	-5.87518600	0.24591900	-5.39704400
H	-6.51313500	-1.55383600	-4.72824000
H	-6.95812200	-3.75392500	-3.90768800
H	-6.40539100	-6.11863900	0.16684900
N	0.89162800	1.27394300	2.01888900
C	-0.05335200	2.16668000	2.30049500
C	2.11714200	1.62461800	1.67913600
C	0.24170200	3.52985500	2.24454600
C	2.50078900	2.96045700	1.62076600
C	1.52652500	3.89505700	1.90876800
H	-0.49752100	4.26215100	2.42457700
H	3.48839300	3.25811700	1.37262000
H	1.77325800	4.93810600	1.85835600
H	7.65062100	5.02007400	2.80705400
N	-1.05995200	-1.45877400	-1.61777100
C	-0.13877700	-1.99461800	-2.39922200
C	-2.35711000	-1.51129300	-1.89168700
C	-0.48473600	-2.61229700	-3.58888000
C	-2.79244900	-2.08445000	-3.08430900
C	-1.83221600	-2.62359300	-3.91220600
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H	-3.81969600	-2.12323000	-3.34210700
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N	-1.26276500	1.58009800	2.59610800
H	-1.20371000	0.57153600	2.44961600
N	2.92939500	0.54001200	1.40095700
H	2.42941300	-0.33015500	1.45323100
N	-3.11447000	-1.03404000	-0.84228700
H	-2.50572700	-0.84366700	-0.06211300
N	1.12551800	-1.85296800	-1.82126600
H	1.02288400	-1.60780500	-0.84934400
O	6.07920700	-0.90871700	0.14843700
H	6.35435300	-0.05957400	-0.24218900
O	-4.73754100	2.97368400	2.93649300

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H	-5.15696000	2.16075100	3.25732900
O	4.63260600	-2.92161800	-2.67841800
H	4.78373700	-2.53128100	-3.55024400
O	-6.74282000	-0.36866500	-0.76143600
H	-7.56498400	-0.63637400	-1.19379500
O	0.91373000	0.69195500	-3.27113900
H	0.71426600	0.37884200	-2.37636400
O	7.07485200	1.98407300	-0.48645900
H	7.89673200	2.23408100	-0.03576300
O	-2.70022500	2.24853100	-3.38617900
H	-2.20537500	3.01029800	-3.72380000
O	-5.96506600	-0.51232400	3.99380500
H	-6.59134000	-1.21123300	4.23467600
C	0.94404900	-3.64409200	0.29452500
C	-0.72157200	-2.47503100	1.38624600
C	0.19914000	-4.73444800	-0.05253200
C	-1.56559200	-3.64186400	1.14214600
C	-1.13090500	-4.69541300	0.42764000
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H	-2.56866400	-3.61097300	1.51096000
H	-1.78933600	-5.51720500	0.22227600
H	5.82703200	-6.69251500	1.98130100
N	0.60613500	-2.57616600	0.94541700
N	2.41930000	-3.87001200	0.02334500
N	-1.15756500	-1.40928000	1.97029500
H	2.60920400	-4.69422600	0.57242000
H	-2.10915200	-1.54594200	2.28147200

Hydroxyl group enriched structure (2):

C	5.60115000	0.13043100	2.79038800
C	5.32700900	-1.33198300	2.72492700
C	4.95274900	-1.88987300	1.53516300
C	4.75285300	-1.03941500	0.29230000
C	4.29233000	0.35765500	0.68279900
C	5.29392500	0.91096700	1.67928200
C	5.03236500	-3.28891900	1.34957300
C	3.74201100	-1.62831600	-0.69518500
C	3.69812000	-3.11321000	-0.73931200
C	4.63491800	-3.87187900	0.12987600
C	3.22484100	-3.77095700	-1.97259400
C	3.02384300	-2.81237500	-3.12440400
C	2.31054700	-1.48400500	-2.74158300
C	3.17392700	-0.86358600	-1.62532600
C	5.68631400	-2.20085400	3.79406600
C	5.82549100	-3.53610800	3.61108400
C	5.56022500	-4.11781500	2.34780300
H	5.89165600	-1.78839300	4.75926000
H	6.15241900	-4.16277600	4.41710800
C	5.81476900	-5.47678700	2.04563400
C	5.55308600	-5.97748300	0.81293100
C	4.91473600	-5.17618200	-0.17069300
C	3.78361900	-5.10115400	-2.34261500
C	4.53309400	-5.75961400	-1.46101700

SUPPORTING INFORMATION

H	4.89177700	-6.74588000	-1.66637200
C	4.81318100	2.34761900	-0.76417600
C	4.55906500	3.13046500	-1.91288500
C	5.97611400	2.71912100	0.11356100
C	5.13844900	4.41519700	-2.04664500
C	6.30675900	4.19072500	0.10047000
C	5.95452600	4.93508800	-0.95119700
C	4.20740800	1.15624500	-0.60778100
C	5.90692800	2.13048100	1.50589200
C	3.11336600	1.35484700	-2.75138000
C	2.04867000	0.88062400	-3.73159200
C	3.68794900	2.64855300	-2.89269300
C	2.01425000	1.70509200	-4.99331600
C	3.47029400	3.42189600	-4.06346900
C	2.62393400	2.86609800	-5.11918700
H	1.33208100	1.36492600	-5.74374800
H	2.49201800	3.45839100	-6.00384200
C	3.42907000	0.59481700	-1.66133700
C	2.25046500	-0.60347300	-3.99107000
C	4.87507400	5.16079100	-3.16024300
C	4.06104800	4.64905700	-4.18050900
H	5.29803200	6.13798500	-3.25030100
H	3.89504600	5.23642600	-5.06190300
H	6.23806500	-6.10484700	2.80553300
C	2.19522800	-1.17425000	-5.18751300
C	2.22241400	-2.63036200	-5.38670600
H	2.08530900	-0.57877300	-6.06881500
C	2.72158200	-4.89430400	-4.54272400
C	3.34622800	-5.63440200	-3.62914900
H	2.40061700	-5.33662600	-5.46565800
H	3.54643400	-6.67090100	-3.81825400
C	6.37067000	0.69169900	3.80111200
C	6.86149600	1.97444900	3.68791400
H	6.63115800	0.11990000	4.66715100
C	2.52501100	-3.45740500	-4.39233700
C	6.68552700	2.69001300	2.51195800
C	7.31990700	3.98881400	2.31331300
C	7.13167700	4.68607300	1.19674900
H	7.61635400	5.63781500	1.09277700
C	-5.82831000	-0.25852100	-2.70858900
C	-5.53018800	1.04727000	-2.90251100
C	-5.70615700	-0.79766100	-1.28266100
C	-4.81577200	1.81466800	-1.86063100
C	-4.49585100	-0.25309100	-0.53316000
C	-5.79677900	-2.29512200	-1.13038200
C	-4.29658800	3.19903400	-2.20737600
C	-4.43561700	1.25472700	-0.71579900
C	-4.61660800	-0.66543000	0.92653900
C	-5.50850800	-2.85102200	0.13862200
C	-4.00325600	4.04335900	-0.98535000
C	-3.87761600	2.03885100	0.37818500
C	-4.09535500	0.11286200	1.87237000
C	-4.99772400	-2.04500300	1.19613500
C	-3.70266400	3.47511900	0.18536100
C	-3.72148200	1.49336600	1.58448300
C	-3.79705000	-0.41416200	3.20737800
C	-4.84414400	-2.56957800	2.44984200

SUPPORTING INFORMATION

C	-3.22450100	4.27033600	1.31686600
C	-3.37782700	2.29457600	2.80414500
C	-2.96452400	0.21128000	4.03571000
C	-4.53011300	-1.66003600	3.62929600
C	-2.96957900	3.70236800	2.50045100
C	-2.30794800	1.53265200	3.62096100
C	-5.55717400	-4.73800800	1.66465700
H	-5.74293000	-5.77404000	1.85390300
C	-5.78321400	-4.20816200	0.37940900
C	-5.11349100	-3.93985600	2.67872300
C	-3.36997800	6.26878500	-0.05970200
H	-3.28438600	7.32582800	-0.20578600
C	-3.91666900	5.48933700	-1.14627100
C	-3.03361900	5.70533000	1.10998900
C	-6.56688900	-4.44634100	-1.88885900
H	-6.97050900	-5.04255100	-2.68355300
C	-6.33089900	-3.06358400	-2.12109000
C	-6.30638900	-4.99684200	-0.68171100
C	-2.01330100	3.82492600	4.72870700
H	-1.63486900	4.39356200	5.55788600
C	-2.44037000	4.45974100	3.62276000
C	-1.99572100	2.38127200	4.86226300
C	-1.91160200	0.34836200	6.20684000
H	-1.60361500	-0.08636100	7.13816800
C	-1.71969700	1.77288900	6.01964600
C	-2.56539700	-0.39406800	5.30333000
C	-2.95034500	-1.77919600	5.52598200
C	-3.81139100	-2.40960200	4.73292300
H	-2.51437900	-2.28776400	6.36552100
H	-1.42969800	2.35279300	6.87498200
C	-4.83699800	-4.49754300	4.00652800
C	-4.21890400	-3.79308500	4.94742600
H	-3.96507300	-4.24590900	5.88742300
C	-6.38176600	-1.18319700	-3.69167800
C	-6.62074000	-2.46394900	-3.41402100
C	-5.88248100	3.13814700	-4.15758900
H	-6.34735800	3.65285500	-4.97726600
C	-6.00703300	1.81744600	-4.06081600
C	-5.17221300	3.94189900	-3.19018900
C	-5.14763800	5.27527500	-3.23330100
C	-4.45291000	6.06183500	-2.24018700
C	-2.29954300	5.89822000	3.42935700
C	-2.56049000	6.47264600	2.25648300
H	-1.95484500	6.48258000	4.26065100
H	-2.43459200	7.53017200	2.12587200
H	-5.68328600	5.79635300	-4.00573700
H	-6.57643000	1.29003600	-4.78823400
H	-6.99549200	-3.08829900	-4.19870400
H	-6.50282500	-6.03572100	-0.50204300
N	0.99014400	0.89664900	2.12499400
C	0.07485400	1.74123000	2.59272400
C	2.20333900	1.28684300	1.78297900
C	0.38902700	3.09385800	2.73632700
C	2.60598200	2.61099700	1.91796900
C	1.66146000	3.49657100	2.39855500
H	-0.32890600	3.79343500	3.06794100
H	3.58490500	2.93673600	1.67030000

SUPPORTING INFORMATION

H	1.92202400	4.53241800	2.50086000
H	7.93273900	4.36022500	3.10623400
N	-1.17100400	-1.16688000	-1.78842400
C	-0.30378000	-1.61086500	-2.68148600
C	-2.48221500	-1.16186100	-1.99640800
C	-0.72260700	-2.05696900	-3.92431400
C	-2.98756400	-1.56622900	-3.22976000
C	-2.08355900	-2.00622200	-4.17254300
H	-0.04166700	-2.44094900	-4.64059900
H	-4.02744700	-1.57001200	-3.42715800
H	-2.44970600	-2.34849800	-5.12164600
H	2.00062900	-3.00384700	-6.36812000
N	-1.12847000	1.12561800	2.85317900
H	-1.09093400	0.15274900	2.54846200
N	2.98220800	0.25343500	1.29253600
H	2.46857300	-0.60755900	1.22529000
N	-3.17377900	-0.81206200	-0.85828200
H	-2.52669000	-0.74413100	-0.08884800
N	0.98919800	-1.58282600	-2.15865200
H	0.94331600	-1.48794300	-1.15649500
O	6.03866600	-0.99828600	-0.34733300
H	6.34415100	-0.09224600	-0.53849800
O	-4.55645000	2.46374700	3.62369100
H	-4.95625700	1.60855800	3.84395100
O	4.42950000	-2.53243400	-3.35753000
H	4.54415800	-2.01070700	-4.16373200
O	-6.79983300	-0.22592700	-0.51081300
H	-7.64372000	-0.46320900	-0.91869500
O	0.74129300	1.15297100	-3.18129100
H	0.59644400	0.72524800	-2.32417700
O	7.04803500	1.94482800	-0.54773800
H	7.90439500	2.16805000	-0.15058900
O	-3.05817900	2.90339200	-2.91763100
H	-2.51390000	3.70281200	-2.97731400
O	-5.78814700	-1.12408800	4.13937400
H	-6.39314800	-1.84983500	4.35381800
C	0.88243800	-3.68497800	-0.35075800
C	-0.71239300	-2.68460100	0.98710900
C	0.10493400	-4.70126500	-0.82739100
C	-1.58676700	-3.79018400	0.60249300
C	-1.20180900	-4.72425700	-0.28558100
H	0.45608000	-5.41931300	-1.53558500
H	-2.57180400	-3.80723400	1.01796600
H	-1.88218100	-5.49807000	-0.58453900
N	0.59273400	-2.72856300	0.47291300
N	2.33916100	-3.87863200	-0.72868700
N	-1.10133200	-1.72035700	1.75065700
H	2.54006600	-4.78343300	-0.33105300
H	-2.04089700	-1.89063800	2.08053400
O	-4.38684600	7.42912300	-2.38069700
O	-5.23189800	-5.80715300	4.14150100
O	5.81541000	-7.27086800	0.43580900
O	6.28653700	6.25344800	-1.12198100
O	7.61349700	2.57062500	4.67298100
O	-6.61030800	-0.76152300	-5.00809300
H	-5.77284300	-0.59781200	-5.47022000
H	-4.84230000	7.75624100	-3.16381600

H	6.62025800	6.68717300	-0.33031300
H	7.65521300	2.05649500	5.48715900
H	6.26168100	-7.78912000	1.11554300
H	-4.95636200	-6.20002300	4.97826400

Carboxylic group enriched structure (3):

C	-5.06376100	2.07658700	-2.74807400
C	-5.12814500	0.60897000	-2.98914500
C	-5.00868000	-0.25156700	-1.93126700
C	-4.73567300	0.25945200	-0.53053500
C	-3.93248200	1.55100400	-0.59324800
C	-4.69611400	2.52049100	-1.47810200
C	-5.43091200	-1.59305500	-2.05802300
C	-3.97752900	-0.74611900	0.33787200
C	-4.29978600	-2.17476800	0.06500100
C	-5.31973900	-2.49485900	-0.97392100
C	-4.08533000	-3.15036700	1.14753400
C	-3.75397300	-2.52172900	2.48157000
C	-2.71227800	-1.37215200	2.40642700
C	-3.31272000	-0.34831000	1.42218900
C	-5.54889300	0.09343900	-4.24853000
C	-6.00353000	-1.17529000	-4.36973400
C	-6.01641500	-2.03841000	-3.24800400
H	-5.54738000	0.73278500	-5.10515600
H	-6.37669800	-1.53406400	-5.30846800
C	-6.62575500	-3.30379100	-3.25813700
C	-6.65750300	-4.10619700	-2.15474800
C	-5.94580800	-3.71934600	-0.97120800
C	-4.98000600	-4.33286400	1.21570600
C	-5.80678700	-4.59904400	0.20802800
H	-6.40886200	-5.47637100	0.22530300
C	-4.08739900	3.27265700	1.23515000
C	-3.74922500	3.71953600	2.53333500
C	-5.06703000	4.07449700	0.42334600
C	-4.04610900	5.04956100	2.93180100
C	-5.05458900	5.54949600	0.75517200
C	-4.64573000	5.95299600	1.95581900
H	-4.72134700	6.98943000	2.22795000
C	-3.76298300	2.02694400	0.83973900
C	-5.02482500	3.78582600	-1.05772500
C	-2.81288800	1.51508100	2.99870900
C	-1.96387800	0.60629000	3.87802900
C	-3.08470600	2.85209600	3.40360000
C	-1.82571300	1.12552200	5.28640800
C	-2.78657500	3.29087600	4.72165400
C	-2.16246100	2.34666500	5.64797100
H	-1.29027700	0.48658900	5.95681200
H	-1.95920600	2.69676100	6.64151800
C	-3.21742800	1.09121400	1.76420800
C	-2.53797200	-0.79913800	3.81408500
C	-3.71052700	5.45440500	4.19432100
C	-3.10138000	4.56781300	5.09429500
H	-3.91900500	6.45921800	4.50634400

SUPPORTING INFORMATION

H	-2.87633500	4.90107100	6.08824600
H	-7.11228200	-3.64736700	-4.14756200
C	-2.71896800	-1.58747500	4.86560600
C	-3.11599100	-2.99796200	4.75328700
H	-2.53628700	-1.22443500	5.85463200
C	-4.08129700	-4.84769100	3.43800700
C	-4.79317800	-5.20574300	2.37194100
H	-3.95272500	-5.53090500	4.25478100
H	-5.25725200	-6.17154000	2.33023600
C	-5.59398700	3.00131800	-3.63796800
C	-5.79027500	4.31558100	-3.26034300
H	-5.89051400	2.70316600	-4.62087000
H	-6.18170100	5.01957900	-3.96817800
C	-3.52927200	-3.50844600	3.59884900
C	-5.55767100	4.71281700	-1.95340600
C	-5.85467100	6.07150600	-1.49049800
C	-5.60661300	6.45977900	-0.24299500
H	-5.78812100	7.47270000	0.06058200
C	5.43736900	-2.33184100	2.81065000
C	5.29136700	-1.10198000	3.34793100
C	5.32550900	-2.48143800	1.30219500
C	4.87178100	0.03498300	2.50647100
C	4.31487400	-1.52862300	0.68026600
C	5.08516000	-3.88900200	0.81206400
C	4.59322500	1.37360100	3.16226300
C	4.53871600	-0.13506500	1.23159100
C	4.46468000	-1.60677300	-0.82822000
C	4.76367900	-4.06243000	-0.55570300
C	4.67797600	2.52616200	2.18114500
C	4.28807000	0.98902900	0.34400200
C	4.22364000	-0.52997900	-1.57199000
C	4.53918100	-2.94158400	-1.40755700
C	4.41463800	2.33824100	0.88348900
C	4.14722700	0.79515300	-0.96631200
C	3.92886300	-0.65128900	-3.00165300
C	4.36570000	-3.11785300	-2.75174400
C	4.27735000	3.46274600	-0.03952700
C	4.11937600	1.91428500	-1.96229100
C	3.34682000	0.33504300	-3.67726400
C	4.37336400	-1.91689900	-3.68871200
C	4.03084000	3.27885400	-1.34112600
C	2.98415800	1.64867300	-2.97684300
C	4.47604500	-5.50981500	-2.48192500
H	4.42018500	-6.50010500	-2.89206800
C	4.72621300	-5.35610100	-1.10246000
C	4.31509300	-4.42513500	-3.29880400
C	4.72254700	4.98540800	1.80463700
H	4.86830400	5.97498300	2.19437600
C	4.91669500	3.86736100	2.70715400
C	4.41694700	4.80496400	0.51070500
C	5.27292100	-6.27394300	1.06120500
H	5.47043800	-7.11339700	1.69915900
C	5.35991200	-4.96352200	1.60585900
C	4.96916500	-6.46358400	-0.24366800
C	3.38065300	4.12797500	-3.51584000
H	3.25619600	4.93280200	-4.20594400
C	3.83183700	4.38495100	-2.27329900

SUPPORTING INFORMATION

C	3.01614900	2.80268500	-3.98045600
C	2.56705000	1.22519900	-5.78598600
H	2.24936700	1.10958900	-6.80394200
C	2.72161000	2.56996600	-5.26222600
C	2.92939700	0.15574000	-5.06576500
C	2.98277600	-1.19604700	-5.60313600
C	3.59026100	-2.18776400	-4.95773900
H	2.51243500	-1.37405300	-6.55218000
H	2.67900400	3.38494600	-5.95896200
C	4.01521500	-4.58002200	-4.72715400
C	3.65209700	-3.54902500	-5.48286900
H	3.36267200	-3.69803400	-6.50534600
H	4.04083200	-5.57315000	-5.13133100
C	5.80887800	-3.53068200	3.54609200
C	5.76630700	-4.74528200	2.99424700
C	5.73884800	0.45084300	5.19746300
H	6.07738200	0.62135400	6.20222200
C	5.63087700	-0.79453500	4.74058800
C	5.42916800	1.61886400	4.39602400
C	5.70234200	2.86851700	4.78354400
C	5.38635900	4.01664900	3.96168500
C	4.04968000	5.73190000	-1.72283600
C	4.30472200	5.90852100	-0.42128600
H	4.44315800	6.89909800	-0.04388000
H	5.59069500	4.99512400	4.35001000
H	6.19546200	3.04186100	5.72142800
H	5.86313200	-1.60584100	5.39659900
H	6.09567400	-3.43883100	4.57275700
H	6.02580100	-5.60928300	3.57488600
H	4.92359700	-7.45369400	-0.65369500
N	-0.49041700	1.54922200	-1.78067100
C	0.62605000	2.22198200	-2.04461700
C	-1.60834700	2.14850100	-1.41924200
C	0.63696400	3.61429900	-1.94438500
C	-1.68848700	3.53266500	-1.30947200
C	-0.53431600	4.24046200	-1.58052400
H	1.51678200	4.17235700	-2.11866100
H	-2.58578500	4.03104000	-1.04118300
H	-0.54707800	5.31015400	-1.49736600
H	-6.25490400	6.76099400	-2.20773500
N	0.79926500	-1.82336400	1.61787300
C	-0.21675900	-2.16990900	2.38870800
C	2.04634800	-2.20860500	1.85278500
C	-0.01940400	-2.92980100	3.52879300
C	2.34078500	-2.95214400	2.99318100
C	1.28736400	-3.29333000	3.81294900
H	-0.82542900	-3.23644900	4.14527000
H	3.32939000	-3.26138800	3.21757800
H	1.48328600	-3.88179900	4.68848500
H	-3.07004000	-3.60159700	5.63949100
N	1.67551300	1.39540600	-2.37296900
H	1.39089100	0.41978000	-2.27887800
N	-2.64046800	1.25838200	-1.17876300
H	-2.34316900	0.30258800	-1.27065600
N	2.88736300	-1.86068700	0.81474300
H	2.33398000	-1.47981700	0.06339300
N	-1.41392600	-1.68873500	1.85264900

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H	-1.26529400	-1.41658000	0.89369100
O	-6.03440500	0.49051200	0.03811300
H	-6.09731000	1.33590200	0.51837200
O	5.37777400	1.96967000	-2.66929500
H	5.59288500	1.11340100	-3.06969100
O	-5.06381800	-1.94483000	2.72946600
H	-5.12057600	-1.60634400	3.63356500
O	6.57135400	-2.02100200	0.70725700
H	7.31218800	-2.50971900	1.09057800
O	-0.59366900	0.65148300	3.42654200
H	-0.48336000	0.33444300	2.51782100
O	-6.33396300	3.47700200	0.89127900
H	-7.08502700	3.93247500	0.47951100
O	3.21404400	1.20996200	3.60375200
H	2.89241500	2.03498700	3.99739000
O	5.76008900	-1.61202600	-4.02952700
H	6.20300900	-2.41168600	-4.35067200
C	-1.67646200	-3.33481700	-0.37730800
C	0.20259500	-2.50585900	-1.43410800
C	-1.20419000	-4.59301700	-0.13641100
C	0.74956100	-3.85421700	-1.30693400
C	0.08943000	-4.82965600	-0.65761600
H	-1.76653400	-5.33470900	0.38729800
H	1.72554600	-4.03029600	-1.70682200
H	0.53728100	-5.79691200	-0.53601900
N	-1.10557100	-2.32740700	-0.95931200
N	-3.15918700	-3.23433600	-0.06952100
N	0.87224100	-1.52887800	-1.94837600
H	-3.54095600	-3.96728100	-0.64701900
H	1.75869500	-1.86120800	-2.30234100
C	3.97376300	6.92800000	-2.58680900
O	4.21430600	8.08088300	-1.90423300
O	3.73045300	6.96731600	-3.76977700
H	4.16528600	8.84726900	-2.49278000
C	-7.43419100	-5.35460000	-2.36388000
O	-7.94039800	-5.66503200	-3.41487100
O	-7.57101400	-6.15589200	-1.27965700
H	-8.10545900	-6.93608600	-1.49108800

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