A metal-mediated base pair that discriminates between the canonical pyrimidine nucleobases

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Electronic Supplementary Information

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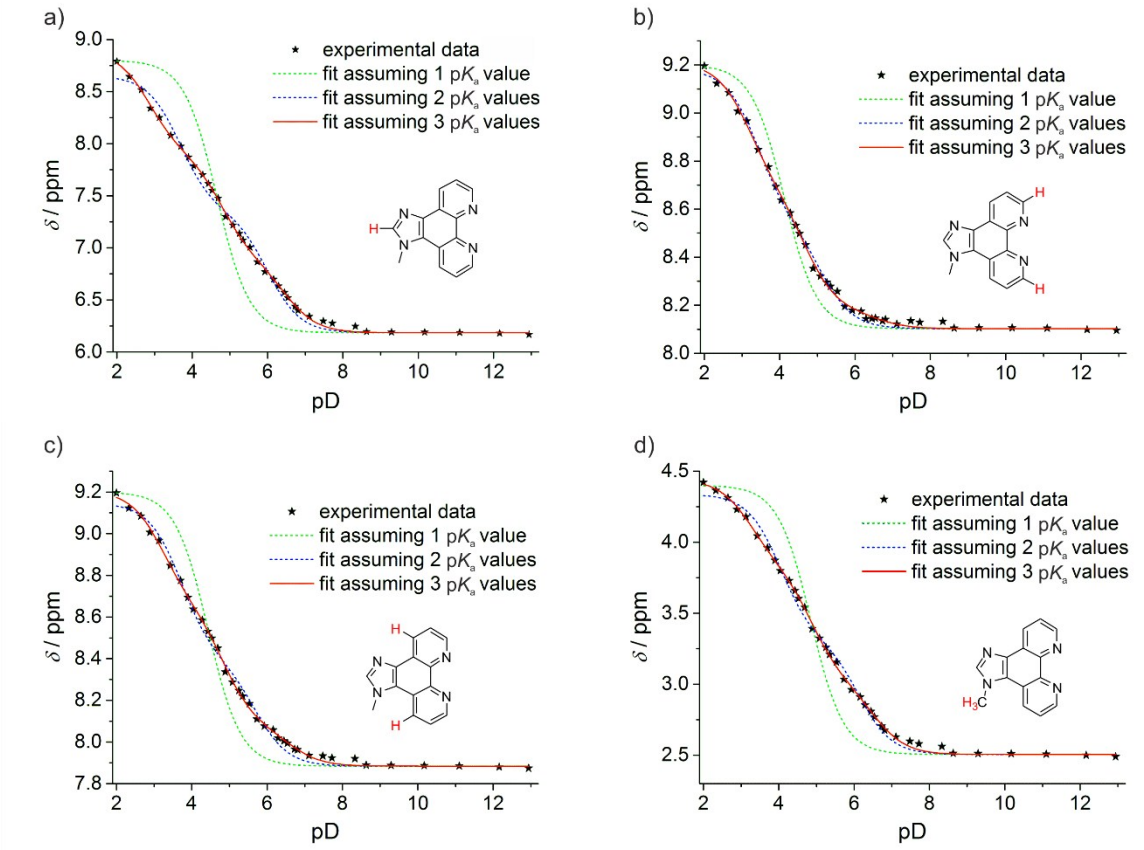


Figure S1. Determination of the pK_a values of compound **1** based on chemical shift changes. a) Plot for the imidazole hydrogen atom; b) plot for H2/H9; c) plot for H4/H7; d) plot for CH_3.

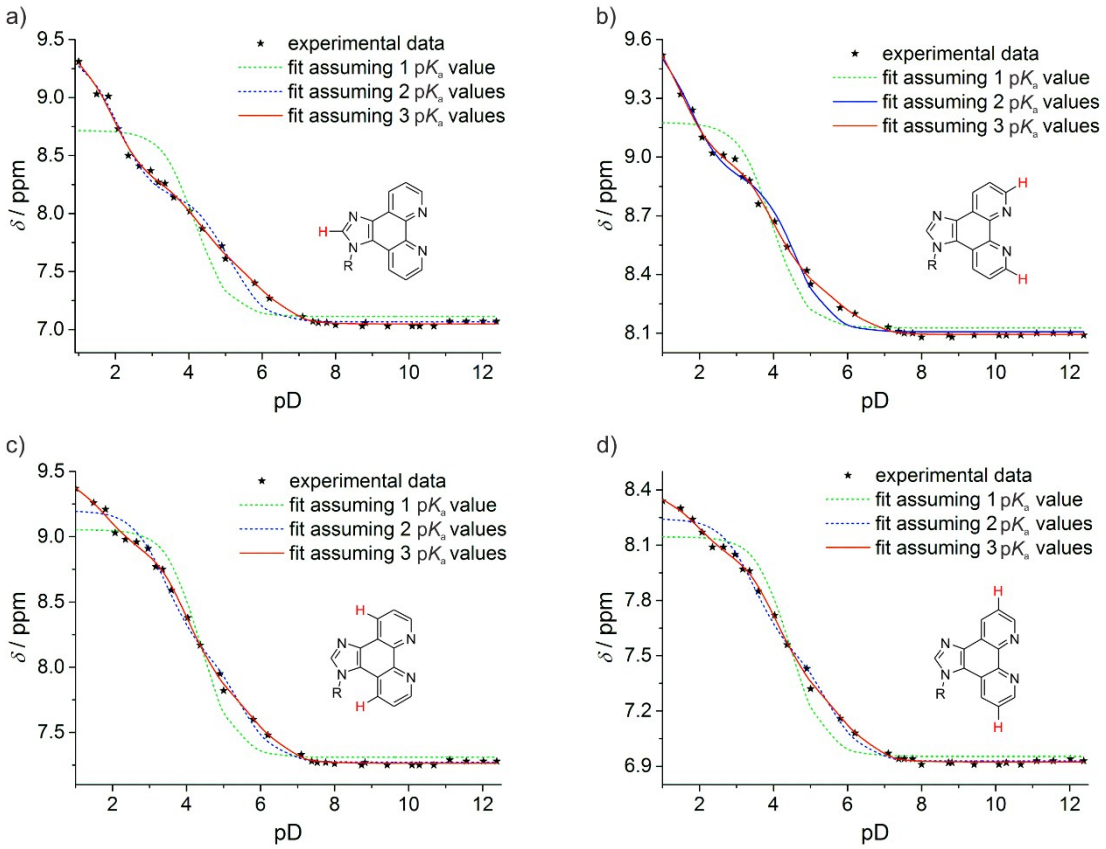


Figure S2. Determination of the pK_a values of compound **P** based on chemical shift changes. a) Plot for the imidazole hydrogen atom; b) plot for H2/H9; c) plot for H4/H7; d) plot for H3/H8.

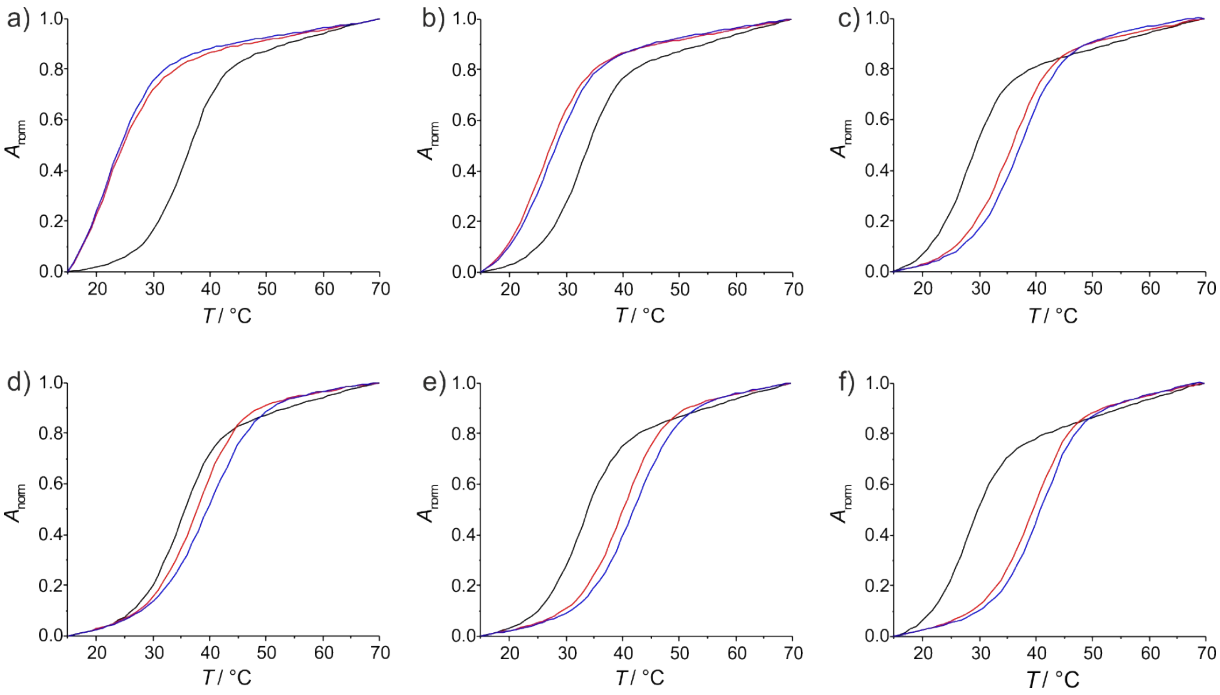


Figure S3. Melting curves of the oligonucleotide duplexes in the presence of increasing amounts of $AgNO_3$ (— 0 equiv. of Ag^+, — 1 equiv. of Ag^+, — 2 equiv. of Ag^+). a) – c) show the melting curves of the duplex containing a central **P**:**T** base pair; d) – f) those of the duplex with a central **P**:**C** base pair. a) and d) were recorded at pH 5.5, b) and e) were recorded at pH 6.8, c) and f) were recorded at pH 9.0.

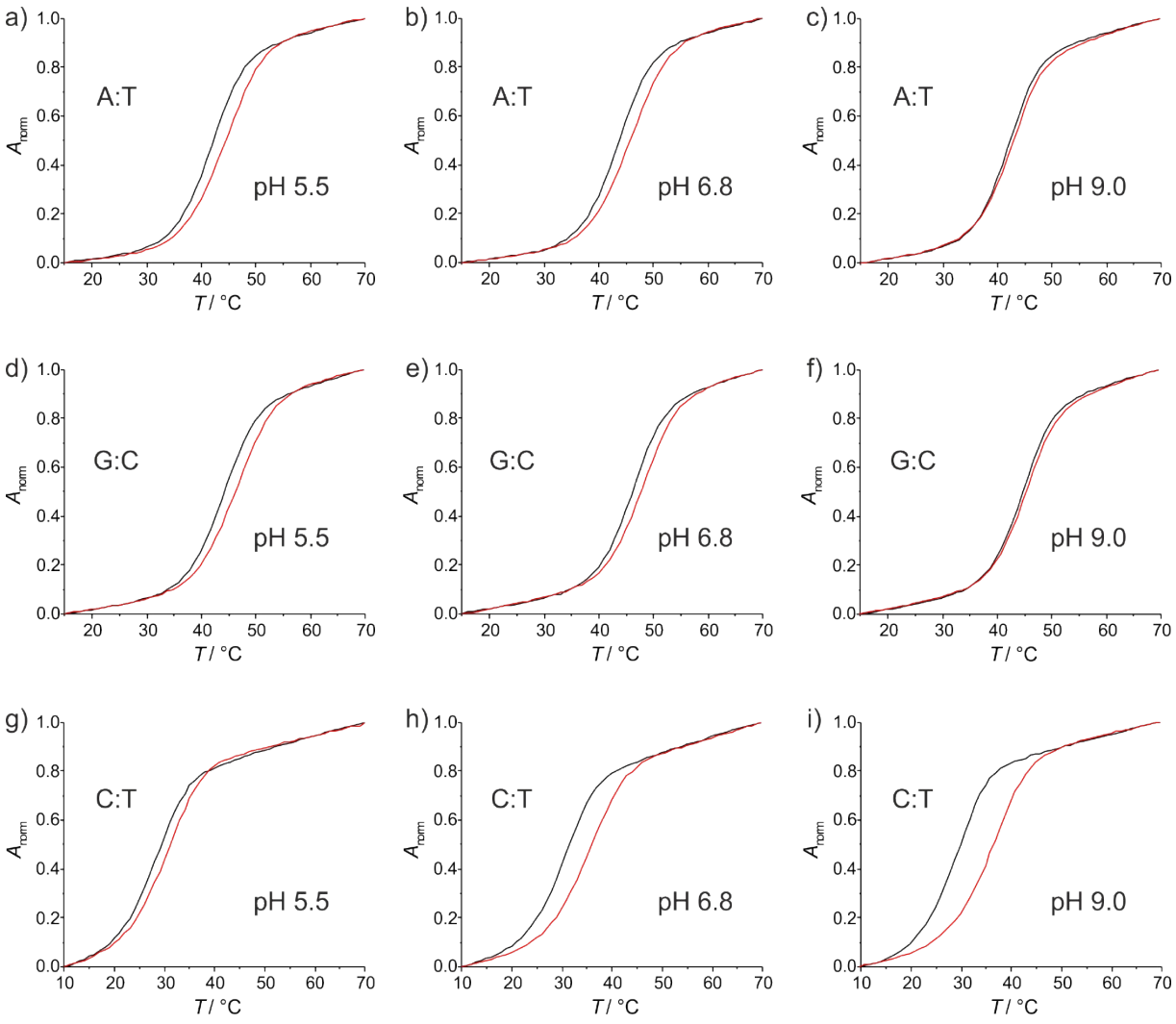


Figure S4. Melting curves of oligonucleotide duplexes identical to the one shown in Chart 2, but comprising a central **A**:**T** (a – c), **G**:**C** (d – f) or **C**:**T** (g – i) instead of the **P**:**X** base pair in the absence or presence of one equivalent of $AgNO_3$ (— 0 equiv., — 1 equiv.). a), d) and g) were recorded at pH 5.5, b), e) and h) were recorded at pH 6.8, c), f) and i) were recorded at pH 9.0. The **C**:**T** mispair is well-known to bind one Ag^+ to form a **C**–Ag^+–$\mathbf{T}_{-H}$ base pair.[1]

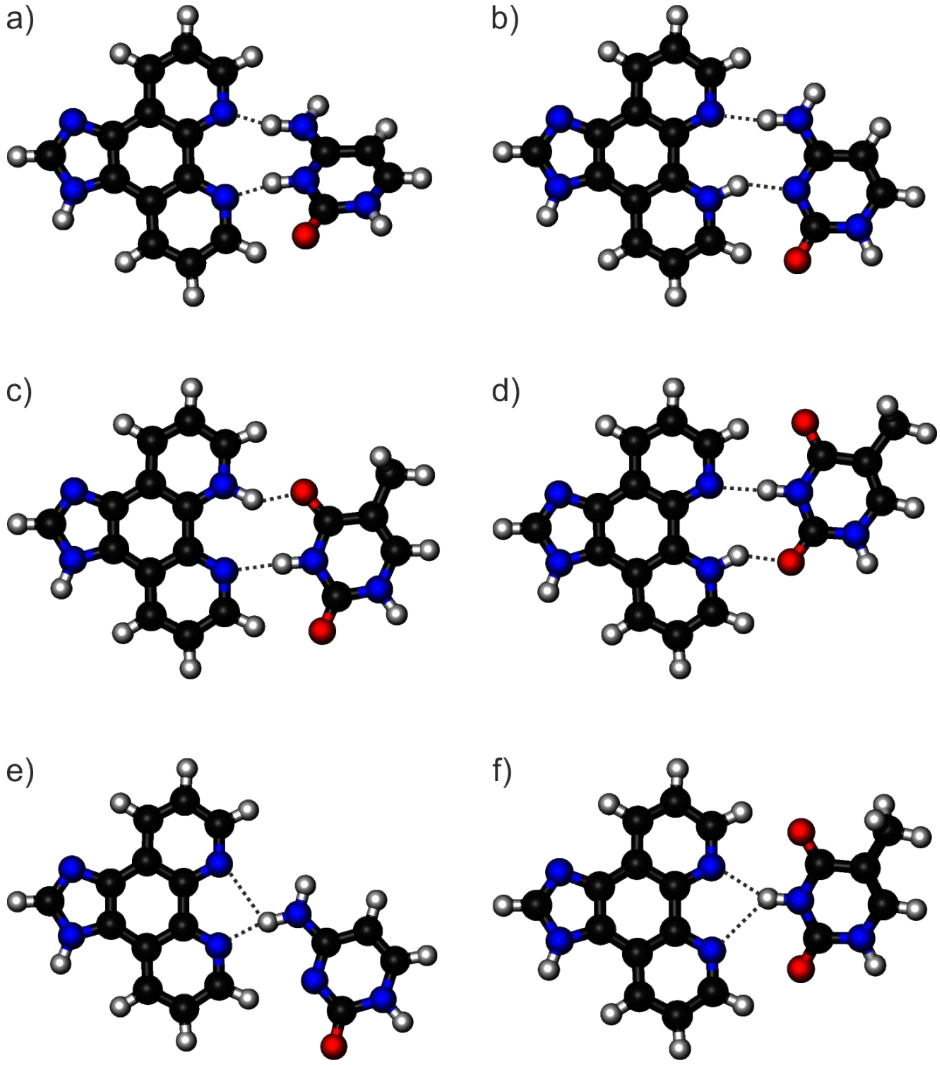


Figure S5. Geometry-optimized structures of possible hydrogen-bonded base pairs. a) **P**:**C**(H)$^+$; b) **P**(H(N1))$^+$:**C**; c) **P**(H(N10))$^+$:**T**; d) **P**(H(N1))$^+$:**T**; e) **P**:**C**; f) **P**:**T**. The close structural resemblance of the base pairs comprising two hydrogen bonds (top and middle rows) is clearly visible. All base pairs were calculated without symmetry constraints in the gas phase.

Table S1. Normalized proton-binding energies of **P** and **C** (E / kcal mol^{-1}).[a]

	Protonation site	Gas phase	COSMO
P(H(N1))$^+$	N1	–82.0	–37.0
P(H(N10))$^+$	N10	–84.1	–37.1
P(H(im))$^+$	$N_{imidazole}$	–65.0	–31.6
P(H(im)H(N1))$^{2+}$	$N_{imidazole}$	+9.0	–26.8
P(H(im)H(N10))$^{2+}$	$N_{imidazole}$	+11.1	–26.6
C(H)$^+$	N3	–67.3	–31.9

[a] Proton-binding energies were calculated according to: ligand + H_3O^+ ⇌ protonated ligand + H_2O

Table S2. Melting temperatures (T_m / °C) of the oligonucleotide duplexes comprising a central **A**:**T**, **G**:**C** or **C**:**T** base pair (rather than a **P**:**X** base pair) and change in T_m (ΔT_m / °C) upon the addition of one equivalent of $AgNO_3$.

pH	**A**:**T**			**G**:**C**			**C**:**T**		
	0 equiv.	1 equiv.	ΔT_m	0 equiv.	1 equiv.	ΔT_m	0 equiv.	1 equiv.	ΔT_m
5.5	42	45	+3	44	47	+3	29	31	+2
6.8	44	46	+2	46	48	+2	31	36	+5
9.0	42	43	+1	45	46	+1	30	35	+5

Table S3. Base pairing energies ΔE_{BP} of hydrogen-bond mediated base pairs (kcal mol^{-1}).[a]

Entry	Base pair	Conditions	Gas phase	In water
1	**P**(H(Im))$^+$:**C**(H)$^+$	Strongly acidic	+28.1[b]	–9.4
2	**P**(H(N1))$^+$:**C**	Acidic / neutral	–27.3	–10.0
3	**P**:**C**(H)$^+$	Acidic / neutral	–27.6	–12.0
4	**P**:**C**	Neutral / alkaline	–15.6	–7.4
5	**P**(H(Im)H(N1))$^{2+}$:**T**	Strongly acidic	–32.0	–9.2
6	**P**(H(Im)H(N10))$^{2+}$:**T**	Strongly acidic	–33.7	–9.5
7	**P**(H(N1))$^+$:**T**	Acidic	–21.3	–9.7
8	**P**(H(N10))$^+$:**T**	Acidic	–24.2	–9.8
9	**P**:**T**	Neutral	–12.2	–4.9

[a] All base pairs were optimized without symmetry constraints. The reactions given below have been used to compute the base pairing energies. To determine the protonation state of protonated starting materials, compounds with the more negative proton-binding energies were considered to be protonated first (i.e. order of protonation: **P**(N10), **C**, **P**(Im), **T**).

entry 1 **P**(H(N10))$^+$ + **C**(H)$^+$ → **P**(H(Im))$^+$:**C**(H)$^+$
entry 2 **P**(H(N10))$^+$ + **C** → **P**(H(N1))$^+$:**C**
entry 3 **P**(H(N10))$^+$ + **C** → **P**:**C**(H)$^+$
entry 4 **P** + **C** → **P**:**C**
entry 5 **P**(H(Im)H(N10))$^{2+}$ + **T** → **P**(H(Im)H(N1))$^{2+}$:**T**
entry 6 **P**(H(Im)H(N10))$^{2+}$ + **T** → **P**(H(Im)H(N10))$^{2+}$:**T**
entry 7 **P**(H(N10))$^+$ + **T** → **P**(H(N1))$^+$:**T**
entry 8 **P**(H(N10))$^+$ + **T** → **P**(H(N10))$^+$:**T**
entry 9 **P** + **T** → **P**

[b] Positive value because it refers to the interaction between two positively charged molecules.

Equations used to fit the pD-dependent chemical shift values.

The following equations were applied to fit the pD-dependent chemical shift values. Equation (3) was derived in analogy to equations (1) and (2), taken from the literature.[2]

(1)
$$\delta_{obsd} = \frac{\delta_A + \delta_{HA} \cdot 10^{\left(pK_{HA} - pH\right)}}{1 + 10^{\left(pK_{HA} - pH\right)}}$$

(2)
$$\delta_{obsd} = \frac{\delta_A + \delta_{HA} \cdot 10^{\left(pK_{HA} - pH\right)} + \delta_{H_2A} \cdot 10^{\left(pK_{H_2A} + pK_{HA} - 2pH\right)}}{1 + 10^{\left(pK_{HA} - pH\right)} + 10^{\left(pK_{H_2A} + pK_{HA} - 2pH\right)}}$$

(3)
$$\delta_{obsd} = \frac{\delta_A + \delta_{HA} \cdot 10^{\left(pK_{HA} - pH\right)} + \delta_{H_2A} \cdot 10^{\left(pK_{H_2A} + pK_{HA} - 2pH\right)} + \delta_{H_3A} \cdot 10^{\left(pK_{H_3A} + pK_{H_2A} + pK_{HA} - 3pH\right)}}{1 + 10^{\left(pK_{HA} - pH\right)} + 10^{\left(pK_{H_2A} + pK_{HA} - 2pH\right)} + 10^{\left(pK_{H_3A} + pK_{H_2A} + pK_{HA} - 3pH\right)}}$$

The following abbreviations have been used:

δ_{obsd} experimental chemical shift

pH experimental pD value

δ_A chemical shift of fully deprotonated compound A

δ_{HA} chemical shift of singly protonated compound HA

δ_{H_2A} chemical shift of doubly protonated compound H_2A

δ_{H_3A} chemical shift of triply protonated compound H_3A

pK_{HA} pK_a value of HA

pK_{H_2A} pK_a value of H_2A

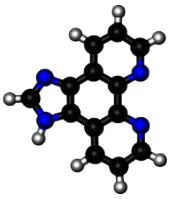
pK_{H_3A} pK_a value of H_3A

Full computational details.

All calculations were performed with the Amsterdam Density Functional (ADF) program.[3] The numerical integration was carried out using the procedure developed by te Velde *et al*..[4] The molecular orbitals were expanded in a large uncontracted set of Slater type orbitals (STOs): TZ2P. The TZ2P basis set has the triple-ξ quality for all atoms and has been enhanced with two sets of polarization functions, that is, 2p and 3d on H; 3d and 4f on carbon, nitrogen and oxygen; 5d and 4f on silver.[5] Core shells of the atoms were treated by the frozen-core approximation. An auxiliary set of s, p, d, f and g STOs were used to fit the molecular density and to represent the Coulomb and exchange potentials accurately in each self-consistent field (SCF) cycle. Equilibrium structures were obtained by optimizations using analytical gradient techniques.[6] Geometries and energies were calculated at the BLYP level of generalized gradient approximation (GGA). BLYP described the exchange by Slater's Xα potential,[7] with nonlocal corrections due to Becke[8] added self-consistently, and the gradient-corrected functional of Lee, Yang and Parr[9] is used for the correlation. Dispersion corrections are applied using the DFT-D method, developed by Grimme.[10] In this approach, the density functional is augmented with an empirical term correcting for long-range dispersion effects, described by a sum of damped interatomic potentials of the form $C_6/(R^6+c)$ added to the usual DFT energy. Scalar relativistic effects were accounted for using the zeroth-order regular approximation (ZORA).[11] Solvation in water is simulated using the conductor-like screening model (COSMO).[12]

Cartesian coordinates and energies of geometry-optimized structures

P, *E* = -3920.25 kcal mol^{-1}



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N	-2.780188	1.123265	0.000004
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H	-1.179249	3.369528	0.000022
H	3.139664	3.199302	-0.000007
H	1.049801	4.570784	0.000026
H	-1.092938	-3.480878	-0.000002
H	1.144796	-4.613754	0.000014
H	3.206307	-3.197184	0.000021
H	-4.601455	-0.000442	-0.000003
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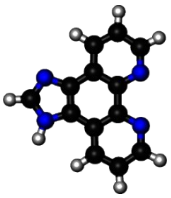
P (COSMO), *E* = -3936.50 kcal mol^{-1}



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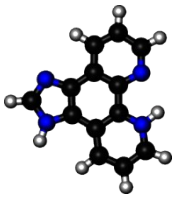
N	2.184944	1.379386	-0.003579
C	2.172250	2.715580	-0.001487
C	0.993644	3.490605	0.002808
C	-1.469641	0.665905	0.000809
C	-1.432963	-0.727581	-0.000366
C	-0.224331	-1.485507	0.000116
C	1.010602	-0.754194	-0.001414
C	-0.177657	-2.896774	0.003363
C	1.054303	-3.529137	0.002806
C	2.219079	-2.733546	-0.000205
N	2.209726	-1.396990	-0.001687
N	-2.785057	1.117893	-0.000076
C	-3.519205	0.010629	-0.002199
N	-2.755187	-1.126733	-0.002188
H	-1.166102	3.384592	0.006675
H	3.143661	3.207806	-0.003775
H	1.055082	4.575282	0.005134
H	-1.101434	-3.469847	0.007424
H	1.133818	-4.612402	0.005426
H	3.198336	-3.209827	-0.001305
H	-4.599437	-0.031591	-0.004821
H	-3.106069	-2.077277	-0.006174

P(H(N1))$^{+}$, *E* = -3880.18 kcal mol^{-1}



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C	2.037699	-3.253870	0.000002
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N	2.000320	-0.799592	0.000030
C	3.331036	-0.813118	0.000032
C	4.094961	-2.007639	0.000004
C	1.237580	-4.445620	-0.000006
C	-0.166272	-4.380025	0.000025
C	-0.889639	-3.153705	0.000038
C	-0.079911	-1.972991	0.000006
C	-2.293042	-2.990609	0.000065
C	-2.864690	-1.719585	0.000017
C	-2.039098	-0.594218	-0.000077
N	-0.702445	-0.759848	-0.000057
N	1.667107	-5.753136	-0.000042
C	0.560907	-6.474007	-0.000034
N	-0.580994	-5.699647	0.000016
H	3.993587	-4.174168	-0.000037
H	3.828342	0.154454	0.000056
H	5.179838	-1.947308	-0.000001
H	-2.938503	-3.865549	0.000114
H	-3.941417	-1.587774	0.000042
H	-2.406312	0.425496	-0.000156
H	0.511368	-7.555334	-0.000066
H	-1.532445	-6.047869	0.000028
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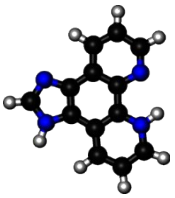
P(H(N1))$^{+}$ (COSMO), *E* = -3935.55 kcal mol^{-1}



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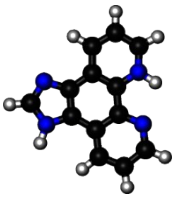
C	2.040712	-3.248077	0.001033
C	1.366420	-1.989891	-0.001806
N	2.018710	-0.797409	-0.002559
C	3.351831	-0.818738	-0.000402
C	4.109223	-2.012838	0.003027
C	1.242990	-4.439984	0.001192
C	-0.154260	-4.367823	0.002015
C	-0.877084	-3.141415	0.002589
C	-0.081206	-1.961793	-0.001210
C	-2.282213	-3.010599	0.005307
C	-2.869931	-1.751294	0.003040
C	-2.056153	-0.616656	-0.002215
N	-0.721311	-0.759068	-0.004071
N	1.655722	-5.762142	-0.002445
C	0.528632	-6.466727	-0.004290
N	-0.587008	-5.674335	-0.001402
H	3.996881	-4.171497	0.006859
H	3.855241	0.145897	-0.000427
H	5.194251	-1.960500	0.006133
H	-2.902832	-3.901992	0.009699
H	-3.947128	-1.630596	0.004159
H	-2.433650	0.397224	-0.006228
H	0.457511	-7.545652	-0.007844
H	-1.547470	-5.998931	-0.001130
H	-0.118482	0.067290	-0.007260

P(H(N10))$^+$, *E* = -3882.27 kcal mol^{-1}



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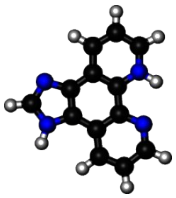
N	-0.641794	0.822383	-0.000025
C	-1.988768	0.808838	-0.000031
C	-2.689144	2.017224	0.000008
C	0.246921	4.386841	0.000027
C	1.646360	4.279917	0.000028
C	2.347617	3.034007	0.000036
C	1.547617	1.848627	0.000012
C	3.751602	2.859336	0.000035
C	4.270321	1.575163	0.000001
C	3.388654	0.467075	-0.000030
N	2.063890	0.594799	-0.000021
N	-0.154769	5.705556	-0.000019
C	0.968425	6.395425	-0.000067
N	2.090561	5.585772	-0.000007
H	-2.499498	4.175601	0.000062
H	-2.465593	-0.164636	-0.000067
H	-3.774063	1.999835	0.000007
H	4.413934	3.721893	0.000055
H	5.343552	1.407091	-0.000006
H	3.782371	-0.546994	-0.000066
H	1.048057	7.474763	-0.000163
H	3.052635	5.904236	-0.000021
H	-0.095617	-0.046603	-0.000053

P(H(N10))$^+$ (COSMO), *E* = -3935.68 kcal mol^{-1}



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C	0.097576	1.958202	0.001146
N	-0.655598	0.821733	-0.000663
C	-1.997608	0.810441	-0.002591
C	-2.696582	2.019382	-0.001749
C	0.242338	4.381919	0.000304
C	1.636937	4.271286	-0.002499
C	2.335906	3.027418	-0.003162
C	1.541244	1.841011	0.001067
C	3.740150	2.876463	-0.006425
C	4.275938	1.599803	-0.001646
C	3.406185	0.485246	0.004981
N	2.076804	0.593008	0.005085
N	-0.142187	5.712611	0.003257
C	1.000131	6.389378	0.002976
N	2.097642	5.568087	-0.000801
H	-2.508456	4.167939	-0.000746
H	-2.472188	-0.161823	-0.006956
H	-3.780538	2.004069	-0.003937
H	4.383031	3.752714	-0.012506
H	5.350694	1.443135	-0.002013
H	3.814050	-0.523487	0.010529
H	1.096800	7.466216	0.006177
H	3.065306	5.870582	0.000447
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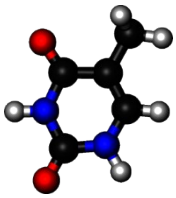
T, *E* = -2157.12 kcal mol^{-1}



N	-2.556120	-0.384314	-0.007471
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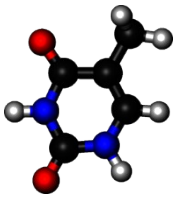
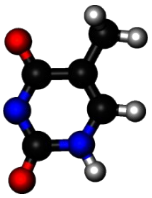
N	-4.667674	-1.344634	-0.039560
C	-5.245871	-0.085154	-0.035643
C	-4.513626	1.056918	-0.017939
C	-3.045894	0.949699	-0.002268
O	-2.263413	1.896323	0.014225
O	-2.790783	-2.689459	-0.029113
C	-5.121410	2.435824	-0.013500
H	-1.544129	-0.490778	0.003218
H	-5.241154	-2.179660	-0.052944
H	-6.332104	-0.076523	-0.047865
H	-4.797514	2.994147	0.874813
H	-6.216715	2.380830	-0.025007
H	-4.779753	3.007740	-0.886404

T (COSMO), *E* = -2170.86 kcal mol^{-1}



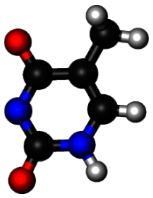
N	-2.560980	-0.382247	-0.006074
C	-3.300404	-1.554604	-0.025675
N	-4.665330	-1.341079	-0.039434
C	-5.241714	-0.088484	-0.035257
C	-4.505340	1.056062	-0.016913
C	-3.052552	0.937538	-0.002185
O	-2.252470	1.890879	0.013467
O	-2.786597	-2.682297	-0.029924
C	-5.126456	2.429768	-0.014119
H	-1.548945	-0.493952	0.004148
H	-5.253853	-2.167569	-0.054330
H	-6.325678	-0.082622	-0.049396
H	-4.817729	2.992958	0.876974
H	-6.219493	2.356151	-0.027380
H	-4.797202	3.005448	-0.889763

T_{-H}, *E* = -2093.67 kcal mol^{-1}



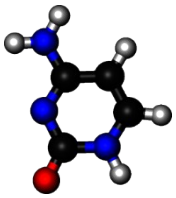
N	-2.477333	-0.387800	-0.006766
C	-3.242639	-1.502531	-0.024548
N	-4.679102	-1.328172	-0.039641
C	-5.274771	-0.087196	-0.036024
C	-4.515192	1.035981	-0.018098
C	-3.024858	0.878062	-0.002645
O	-2.313674	1.915896	0.013783
O	-2.841206	-2.689031	-0.029525
C	-5.107053	2.422525	-0.013304
H	-5.225586	-2.180543	-0.052596
H	-6.365745	-0.068000	-0.048205
H	-4.775379	2.984468	0.873083
H	-6.208738	2.384642	-0.025556
H	-4.756372	2.998724	-0.883081

T_{-1} (COSMO), *E* = -2163.79 kcal mol^{-1}



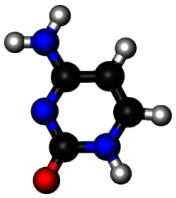
N	-2.495600	-0.387156	-0.006366
C	-3.277777	-1.496823	-0.024921
N	-4.671315	-1.329889	-0.039060
C	-5.263828	-0.088835	-0.035695
C	-4.509031	1.043081	-0.017954
C	-3.045948	0.878343	-0.002634
O	-2.283208	1.896807	0.013870
O	-2.818364	-2.677184	-0.029900
C	-5.120495	2.423235	-0.013935
H	-5.243887	-2.167489	-0.052608
H	-6.349141	-0.081069	-0.048162
H	-4.808542	2.988473	0.875896
H	-6.216127	2.362218	-0.026791
H	-4.788647	3.002234	-0.887548

C, *E* = -1894.56 kcal mol^{-1}



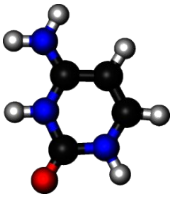
N	0.004808	-0.261151	0.002130
C	-0.014578	2.421139	-0.023002
N	-1.191266	1.811715	0.034079
C	-1.261595	0.435989	0.042279
C	1.207105	0.371869	-0.051436
C	1.255125	1.735257	-0.069063
N	-0.023297	3.790587	-0.064117
H	2.093555	-0.254679	-0.079548
H	2.198081	2.269354	-0.120123
O	-2.288457	-0.232036	0.085384
H	0.829366	4.309688	0.091356
H	-0.909741	4.254401	0.097530
H	-0.056794	-1.274110	0.015373

C (COSMO), *E* = -1913.95 kcal mol^{-1}



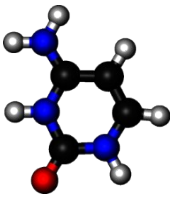
N	-0.004937	-0.259497	0.001414
C	-0.009144	2.433351	-0.025259
N	-1.196553	1.797864	0.027012
C	-1.231944	0.432527	0.041397
C	1.201026	0.376604	-0.052132
C	1.248965	1.738337	-0.067631
N	-0.020473	3.783709	-0.037690
H	2.079597	-0.256616	-0.081005
H	2.189527	2.275625	-0.110025
O	-2.295634	-0.229938	0.087987
H	0.842685	4.309205	-0.078925
H	-0.900307	4.285103	-0.010144
H	-0.045554	-1.274175	0.012898

C(H)$^+$, *E* = -1839.80 kcal mol^{-1}



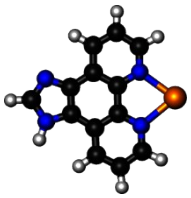
N	-0.016198	-0.277103	-0.001332
C	0.017682	2.483868	0.002221
N	-1.150656	1.779937	0.041157
C	-1.270832	0.359859	0.043592
C	1.173563	0.383484	-0.041353
C	1.236659	1.751259	-0.041206
N	-0.020981	3.819517	0.006067
H	2.064035	-0.236589	-0.073084
H	2.187966	2.269181	-0.073451
O	-2.332333	-0.208064	0.080025
H	0.840970	4.352852	-0.022922
H	-0.891991	4.339411	0.036696
H	-2.050558	2.259004	0.073857
H	-0.050255	-1.294928	-0.001834

C(H)$^+$ (COSMO), *E* = -1907.85 kcal mol^{-1}



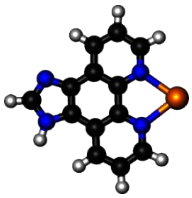
N	-0.025843	-0.267075	-0.000567
C	0.019980	2.480080	0.002631
N	-1.149389	1.771085	0.042083
C	-1.252814	0.377755	0.043187
C	1.173470	0.386190	-0.041764
C	1.240323	1.748305	-0.040974
N	-0.029513	3.805182	0.006133
H	2.051400	-0.246045	-0.075638
H	2.185906	2.273354	-0.074312
O	-2.333501	-0.205342	0.079359
H	0.829966	4.340586	-0.026001
H	-0.909660	4.308554	0.032748
H	-2.036260	2.269774	0.073258
H	-0.052126	-1.282688	-0.002559

P-Ag^{+}, *E* = -3829.43 kcal mol^{-1}



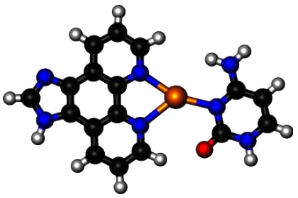
C	-0.000075	2.900087	0.348765
C	-0.000049	1.488350	0.346156
C	-0.000062	0.798724	-0.904953
N	-0.000061	1.501238	-2.076451
C	-0.000092	2.839004	-2.052849
C	-0.000111	3.579564	-0.856682
C	0.000010	0.714259	1.549381
C	0.000019	-0.681617	1.500650
C	-0.000041	-1.422559	0.283878
C	-0.000068	-0.670125	-0.938908
C	-0.000057	-2.833541	0.204008
C	-0.000107	-3.452777	-1.033650
C	-0.000115	-2.652249	-2.189318
N	-0.000085	-1.315513	-2.139916
N	0.000073	1.167593	2.853005
C	0.000135	0.071844	3.587000
N	0.000101	-1.080794	2.824430
Ag	0.000068	0.147155	-3.921480
H	0.000139	-2.028925	3.180791
H	-0.000070	3.417087	1.304359
H	-0.000099	3.342136	-3.015270
H	-0.000138	4.664797	-0.897011
H	-0.000032	-3.427786	1.114861
H	-0.000122	-4.534523	-1.126480
H	-0.000129	-3.104605	-3.176592
H	0.000208	0.035161	4.668750

P-Ag^{+} (COSMO), *E* = -3889.14 kcal mol^{-1}



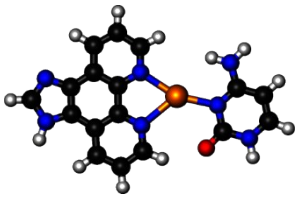
C	0.006062	2.910214	0.359498
C	0.004735	1.498775	0.370300
C	0.004058	0.805506	-0.881217
N	0.003451	1.493777	-2.056877
C	0.004058	2.830338	-2.042796
C	0.005661	3.581145	-0.852040
C	0.000496	0.721277	1.574213
C	-0.001749	-0.672556	1.518296
C	0.002977	-1.414221	0.300999
C	0.004571	-0.663399	-0.917113
C	0.006127	-2.824568	0.229586
C	0.008332	-3.439849	-1.011052
C	0.007378	-2.635597	-2.166386
N	0.005720	-1.299471	-2.120747
N	-0.004176	1.155012	2.893540
C	-0.009982	0.037265	3.612133
N	-0.009282	-1.089367	2.832839
Ag	-0.004345	0.142696	-3.961948
H	-0.013661	-2.045626	3.168347
H	0.007141	3.445212	1.304693
H	0.002374	3.323548	-3.010244
H	0.005999	4.665871	-0.898366
H	0.007906	-3.410917	1.144476
H	0.010515	-4.521197	-1.105888
H	0.007644	-3.085384	-3.154781
H	-0.016112	-0.019811	4.691587

P–Ag^{+}–C, *E* = -5771.01 kcal mol^{-1}



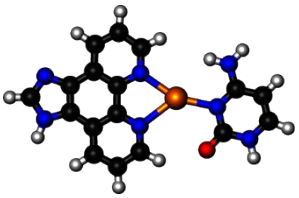
C	-2.883167	2.731750	0.000166
C	-2.789192	1.324637	0.000053
C	-1.495475	0.719327	0.000202
N	-0.364081	1.485220	0.000349
C	-0.481797	2.819910	0.000447
C	-1.720531	3.484399	0.000392
C	-3.934814	0.465287	-0.000206
C	-3.787525	-0.923845	-0.000204
C	-2.520374	-1.578913	0.000038
C	-1.361192	-0.738885	0.000191
C	-2.322952	-2.978569	0.000151
C	-1.034655	-3.487203	0.000395
C	0.053562	-2.591173	0.000426
N	-0.112865	-1.267656	0.000352
N	-5.269718	0.824361	-0.000493
C	-5.923546	-0.320432	-0.000618
N	-5.079686	-1.415679	-0.000478
Ag	1.609750	0.381297	0.000081
N	3.769124	0.055149	-0.000166
C	4.132807	-1.292446	-0.000107
N	5.523013	-1.556010	-0.000164
C	6.475304	-0.582211	-0.000274
C	6.110253	0.730842	-0.000339
C	4.705986	1.024703	-0.000278
N	4.289884	2.308916	-0.000313
O	3.328470	-2.216779	-0.000024
H	-3.868631	3.189184	0.000060
H	0.444917	3.385930	0.000528
H	-1.748030	4.570188	0.000485
H	-3.179831	-3.648925	0.000062
H	-0.853171	-4.558116	0.000535
H	1.082362	-2.940125	0.000478
H	-6.999745	-0.434624	-0.000822
H	-5.364036	-2.387477	-0.000564
H	5.778074	-2.539361	-0.000097
H	7.509166	-0.911590	-0.000301
H	6.849542	1.523338	-0.000427
H	4.951639	3.073005	-0.000367
H	3.294286	2.507342	-0.000298

P–Ag^{+}–C (planar), *E* = -5771.00 kcal mol^{-1}



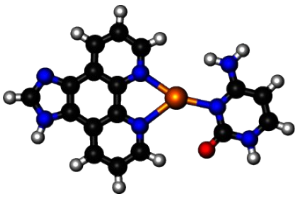
C	-2.881023	2.732238	0.000000
C	-2.788523	1.324992	0.000000
C	-1.495413	0.718316	0.000000
N	-0.363328	1.483058	0.000000
C	-0.479584	2.817879	0.000000
C	-1.717599	3.483715	0.000000
C	-3.935049	0.466851	0.000000
C	-3.789137	-0.922442	0.000000
C	-2.522715	-1.578847	0.000000
C	-1.362553	-0.740104	0.000000
C	-2.327010	-2.978774	0.000000
C	-1.039334	-3.488923	0.000000
C	0.049939	-2.594124	0.000000
N	-0.114744	-1.270319	0.000000
N	-5.269630	0.827275	0.000000
C	-5.924588	-0.316924	0.000000
N	-5.081809	-1.413014	0.000000
Ag	1.609838	0.377571	0.000000
N	3.770265	0.056674	0.000000
C	4.136761	-1.290158	0.000000
N	5.527645	-1.550662	0.000000
C	6.477761	-0.574689	0.000000
C	6.109839	0.737600	0.000000
C	4.704914	1.028332	0.000000
N	4.285980	2.311692	0.000000
O	3.334247	-2.216114	0.000000
H	-3.865980	3.190714	0.000000
H	0.447745	3.382876	0.000000
H	-1.743953	4.569516	0.000000
H	-3.184699	-3.648088	0.000000
H	-0.859085	-4.560050	0.000000
H	1.078062	-2.944800	0.000000
H	-7.000867	-0.430063	0.000000
H	-5.367086	-2.384545	0.000000
H	5.784973	-2.533424	0.000000
H	7.512364	-0.901699	0.000000
H	6.847445	1.531645	0.000000
H	4.946082	3.077229	0.000000
H	3.289986	2.508072	0.000000

P-Ag^{+}-C (COSMO), *E* = -5826.23 kcal mol^{-1}



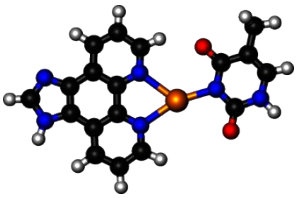
C	-2.840433	2.754232	0.007989
C	-2.782366	1.344335	0.003957
C	-1.499744	0.713972	0.002139
N	-0.353560	1.454156	0.003905
C	-0.436237	2.790820	0.009311
C	-1.661417	3.481666	0.010952
C	-3.943217	0.502417	0.001624
C	-3.815427	-0.887989	0.000203
C	-2.560630	-1.565303	-0.000110
C	-1.389244	-0.746763	-0.000389
C	-2.399165	-2.968986	-0.000135
C	-1.120302	-3.503581	-0.001399
C	-0.016199	-2.627416	-0.002592
N	-0.150124	-1.299470	-0.001969
N	-5.283304	0.866870	-0.001032
C	-5.943425	-0.286271	-0.004259
N	-5.106707	-1.371110	-0.003304
Ag	1.617328	0.319151	-0.002688
N	3.783753	0.048879	-0.005961
C	4.219659	-1.263683	0.003407
N	5.603717	-1.469216	0.015545
C	6.513172	-0.452188	0.013195
C	6.089060	0.841503	-0.001305
C	4.674963	1.072889	-0.009144
N	4.202579	2.329034	-0.019358
O	3.443276	-2.236242	0.002797
H	-3.809434	3.244716	0.009445
H	0.503782	3.333208	0.010829
H	-1.665904	4.567159	0.014603
H	-3.274189	-3.613691	0.001676
H	-0.959284	-4.577348	-0.001095
H	1.004256	-3.001802	-0.004005
H	-7.018455	-0.399176	-0.007630
H	-5.391456	-2.343586	-0.006546
H	5.918704	-2.434388	0.023838
H	7.556821	-0.741674	0.023016
H	6.784614	1.671645	-0.004612
H	4.834855	3.119003	-0.020214
H	3.201792	2.497976	-0.027619

P-Ag^{+}-C (planar, COSMO), *E* = -5826.25 kcal mol^{-1}



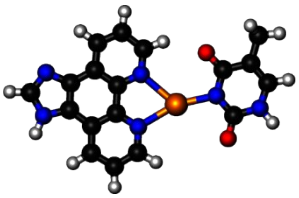
C	-2.843963	2.751990	0.000000
C	-2.783254	1.342199	0.000000
C	-1.499471	0.714273	0.000000
N	-0.354726	1.456791	0.000000
C	-0.439820	2.793398	0.000000
C	-1.666363	3.481710	0.000000
C	-3.942491	0.497992	0.000000
C	-3.812049	-0.892170	0.000000
C	-2.556001	-1.567048	0.000000
C	-1.386224	-0.746306	0.000000
C	-2.391759	-2.970426	0.000000
C	-1.111865	-3.502533	0.000000
C	-0.009433	-2.624187	0.000000
N	-0.146135	-1.296618	0.000000
N	-5.283310	0.859741	0.000000
C	-5.941196	-0.294663	0.000000
N	-5.102347	-1.377837	0.000000
Ag	1.617360	0.329939	0.000000
N	3.781368	0.046842	0.000000
C	4.210132	-1.268074	0.000000
N	5.593112	-1.480929	0.000000
C	6.507808	-0.468667	0.000000
C	6.090606	0.827357	0.000000
C	4.677894	1.066252	0.000000
N	4.211575	2.324648	0.000000
O	3.428555	-2.236525	0.000000
H	-3.813811	3.240748	0.000000
H	0.499357	3.337134	0.000000
H	-1.672992	4.567198	0.000000
H	-3.265494	-3.616896	0.000000
H	-0.948924	-4.576015	0.000000
H	1.012009	-2.995949	0.000000
H	-7.015981	-0.409658	0.000000
H	-5.385101	-2.350905	0.000000
H	5.903294	-2.447741	0.000000
H	7.549831	-0.763715	0.000000
H	6.790497	1.653878	0.000000
H	4.847326	3.111923	0.000000
H	3.211328	2.497676	0.000000

P-Ag^{+}-T_{-H}, *E* = -6048.89 kcal mol^{-1}



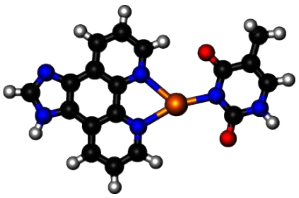
C	-2.626963	2.794583	-0.001706
C	-2.795293	1.393049	-0.000856
C	-1.624864	0.578471	-0.000814
N	-0.386016	1.119788	-0.001524
C	-0.237147	2.443231	-0.002199
C	-1.343891	3.321061	-0.002457
C	-4.069754	0.734005	0.000007
C	-4.147172	-0.660642	0.000862
C	-3.008220	-1.521720	0.000911
C	-1.725920	-0.883986	0.000052
C	-3.052265	-2.932684	0.001748
C	-1.866185	-3.650912	0.001733
C	-0.646013	-2.949397	0.000851
N	-0.577829	-1.613746	0.000040
N	-5.334818	1.299332	0.000184
C	-6.162441	0.272629	0.001235
N	-5.504195	-0.942041	0.001611
Ag	1.425997	-0.485060	-0.000978
N	3.515392	-0.062944	-0.001088
C	4.407422	-1.111273	-0.000661
N	5.773389	-0.752545	-0.000543
C	6.212268	0.555386	-0.000811
C	5.337711	1.591736	-0.001183
C	3.894365	1.280789	-0.001419
O	3.034536	2.188236	-0.001871
O	4.090725	-2.309734	-0.000365
C	5.765696	3.036952	-0.001278
H	-3.510037	3.427803	-0.001721
H	0.793994	2.794078	-0.002484
H	-1.179311	4.395594	-0.003213
H	-4.010396	-3.449240	0.002408
H	-1.863879	-4.737225	0.002383
H	0.305279	-3.474911	0.000796
H	-7.243189	0.330890	0.001755
H	-5.935278	-1.857248	0.002326
H	6.427505	-1.525441	-0.000333
H	7.290710	0.694105	-0.000675
H	6.860432	3.123788	-0.000905
H	5.362844	3.557930	0.878393
H	5.363470	3.557659	-0.881393

P-Ag^{+}-T$_{-H}$ (planar), *E* = -6048.90 kcal mol^{-1}



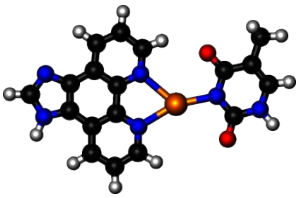
C	-2.618724	-2.743260	0.000000
C	-2.883603	-1.356715	0.000000
C	-1.772391	-0.463053	0.000000
N	-0.499013	-0.917286	0.000000
C	-0.258871	-2.227270	0.000000
C	-1.302233	-3.179641	0.000000
C	-4.200612	-0.787482	0.000000
C	-4.374420	0.598471	0.000000
C	-3.297845	1.536372	0.000000
C	-1.974475	0.988903	0.000000
C	-3.439535	2.940926	0.000000
C	-2.305998	3.739566	0.000000
C	-1.040146	3.124171	0.000000
N	-0.879638	1.796388	0.000000
N	-5.423482	-1.439137	0.000000
C	-6.320261	-0.472169	0.000000
N	-5.747716	0.785215	0.000000
Ag	1.197570	0.809068	0.000000
N	3.311252	0.532719	0.000000
C	4.128380	1.640463	0.000000
N	5.515998	1.377331	0.000000
C	6.044591	0.102924	0.000000
C	5.244015	-0.991628	0.000000
C	3.782548	-0.781481	0.000000
O	2.987742	-1.746491	0.000000
O	3.729277	2.814164	0.000000
C	5.771034	-2.403759	0.000000
H	-3.455948	-3.435959	0.000000
H	0.794096	-2.505838	0.000000
H	-1.063604	-4.240207	0.000000
H	-4.431155	3.389843	0.000000
H	-2.378918	4.823449	0.000000
H	-0.127550	3.714294	0.000000
H	-7.394331	-0.605094	0.000000
H	-6.241151	1.668380	0.000000
H	6.114915	2.193758	0.000000
H	7.130073	0.039397	0.000000
H	6.869157	-2.414598	0.000000
H	5.405496	-2.951222	-0.879907
H	5.405496	-2.951222	0.879907

P-Ag^{+}-T_{-H} (COSMO), *E* = -6078.77 kcal mol^{-1}



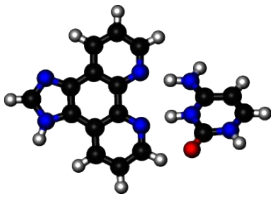
C	-2.677678	2.798418	-0.004070
C	-2.824610	1.393866	-0.002326
C	-1.641136	0.592506	0.005203
N	-0.408498	1.157945	0.011000
C	-0.290209	2.486503	0.009918
C	-1.405415	3.349184	0.002152
C	-4.090106	0.720388	-0.007434
C	-4.149899	-0.674526	-0.003733
C	-3.000028	-1.518987	0.003733
C	-1.725960	-0.870310	0.006678
C	-3.043316	-2.930045	0.006896
C	-1.854376	-3.641369	0.009535
C	-0.638270	-2.933875	0.010576
N	-0.571723	-1.595831	0.009776
N	-5.369237	1.261181	-0.017225
C	-6.178222	0.206841	-0.019633
N	-5.495001	-0.980248	-0.011613
Ag	1.410348	-0.460805	0.007569
N	3.542271	-0.065097	-0.001857
C	4.427545	-1.112761	-0.009896
N	5.785815	-0.792575	-0.018320
C	6.251419	0.501890	-0.019587
C	5.393302	1.556267	-0.012273
C	3.956129	1.266209	-0.002241
O	3.096737	2.189570	0.006032
O	4.076454	-2.318359	-0.010246
C	5.860974	2.990685	-0.013574
H	-3.565790	3.423810	-0.009562
H	0.727296	2.869384	0.014688
H	-1.257889	4.425281	0.001422
H	-4.001865	-3.442246	0.006759
H	-1.844873	-4.726748	0.011026
H	0.309881	-3.462475	0.011838
H	-7.258535	0.239883	-0.027897
H	-5.908085	-1.905543	-0.014434
H	6.440264	-1.567599	-0.023728
H	7.330494	0.613986	-0.026106
H	6.956389	3.040773	-0.020462
H	5.485951	3.523626	0.871424
H	5.474882	3.525847	-0.892501

P-Ag^{+}-T$_{-H}$ (planar, COSMO), *E* = -6078.71 kcal mol^{-1}



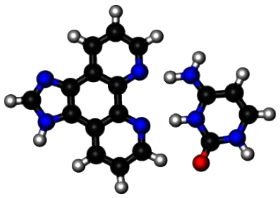
C	-2.675155	-2.749241	0.000000
C	-2.916952	-1.357786	0.000000
C	-1.789995	-0.478683	0.000000
N	-0.521889	-0.959398	0.000000
C	-0.313896	-2.276858	0.000000
C	-1.368426	-3.212741	0.000000
C	-4.225056	-0.770666	0.000000
C	-4.378454	0.617067	0.000000
C	-3.287582	1.536411	0.000000
C	-1.972997	0.974928	0.000000
C	-3.425262	2.941136	0.000000
C	-2.287056	3.731062	0.000000
C	-1.026183	3.106782	0.000000
N	-0.870156	1.776262	0.000000
N	-5.465296	-1.395884	0.000000
C	-6.343143	-0.398128	0.000000
N	-5.741143	0.832186	0.000000
Ag	1.183641	0.774606	0.000000
N	3.338298	0.537064	0.000000
C	4.144696	1.646473	0.000000
N	5.522718	1.426247	0.000000
C	6.081283	0.169045	0.000000
C	5.302463	-0.945169	0.000000
C	3.847688	-0.761052	0.000000
O	3.057678	-1.743976	0.000000
O	3.706443	2.823369	0.000000
C	5.874071	-2.341383	0.000000
H	-3.518542	-3.433734	0.000000
H	0.727371	-2.589902	0.000000
H	-1.148777	-4.276462	0.000000
H	-4.416180	3.386595	0.000000
H	-2.350746	4.814613	0.000000
H	-0.115507	3.697650	0.000000
H	-7.418886	-0.503621	0.000000
H	-6.215754	1.727809	0.000000
H	6.119247	2.246739	0.000000
H	7.165638	0.135840	0.000000
H	6.970268	-2.310920	0.000000
H	5.533697	-2.901868	-0.882000
H	5.533697	-2.901868	0.882000

P-C(H)$^+$, *E* = -5804.41 kcal mol^{-1}



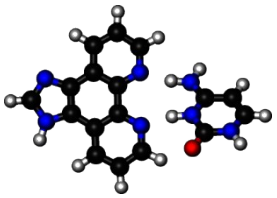
C	-2.459813	2.890831	0.476069
C	-2.351438	1.501988	0.252417
C	-1.060621	0.936531	-0.002685
N	0.038491	1.736946	-0.085273
C	-0.094603	3.049290	0.132190
C	-1.319182	3.673204	0.431478
C	-3.488405	0.633444	0.258160
C	-3.337304	-0.732193	0.019067
C	-2.074021	-1.354924	-0.199343
C	-0.911806	-0.509840	-0.180640
C	-1.899384	-2.740838	-0.407591
C	-0.623888	-3.252886	-0.561310
C	0.465207	-2.367166	-0.482766
N	0.333019	-1.048814	-0.302259
N	-4.815841	0.959969	0.464825
C	-5.461292	-0.184230	0.353167
N	-4.619609	-1.247079	0.082499
N	2.972734	-0.324355	0.031981
C	3.758254	-1.334159	0.600148
N	5.144468	-1.078326	0.518692
C	5.681195	-0.002256	-0.128422
C	4.884055	0.936683	-0.714247
C	3.465284	0.772806	-0.614388
N	2.583498	1.629516	-1.115238
O	3.306414	-2.342109	1.107247
H	1.907888	-0.495254	-0.002695
H	-3.442429	3.309614	0.675186
H	0.817614	3.640251	0.055166
H	-1.356777	4.744981	0.603990
H	-2.765490	-3.398466	-0.436143
H	-0.451707	-4.313892	-0.715245
H	1.483798	-2.743382	-0.531799
H	-6.530201	-0.320225	0.454340
H	-4.898811	-2.212989	-0.036459
H	5.738752	-1.787724	0.939021
H	6.764550	0.057299	-0.142076
H	5.303633	1.796318	-1.223182
H	2.924609	2.447606	-1.605340
H	1.558822	1.558296	-0.819852

P-C(H)$^+$ (planar), *E* = -5803.44 kcal mol^{-1}



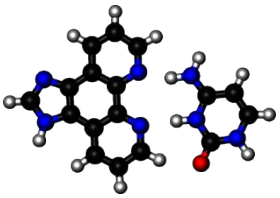
C	-2.608845	2.933775	0.000000
C	-2.454249	1.531724	0.000000
C	-1.134913	0.966385	0.000000
N	-0.048793	1.787606	0.000000
C	-0.226807	3.112521	0.000000
C	-1.484102	3.738587	0.000000
C	-3.580270	0.651816	0.000000
C	-3.393832	-0.727797	0.000000
C	-2.110543	-1.346306	0.000000
C	-0.952366	-0.490727	0.000000
C	-1.929508	-2.746342	0.000000
C	-0.649530	-3.262422	0.000000
C	0.432849	-2.364688	0.000000
N	0.303217	-1.030740	0.000000
N	-4.925109	0.975628	0.000000
C	-5.545726	-0.187452	0.000000
N	-4.671369	-1.258789	0.000000
N	3.111961	-0.431181	0.000000
C	3.956645	-1.552499	0.000000
N	5.326111	-1.226751	0.000000
C	5.809281	0.050645	0.000000
C	4.962319	1.116995	0.000000
C	3.551927	0.865918	0.000000
N	2.645622	1.828403	0.000000
O	3.570184	-2.705853	0.000000
H	2.060424	-0.591729	0.000000
H	-3.615323	3.343031	0.000000
H	0.680131	3.716809	0.000000
H	-1.555901	4.822359	0.000000
H	-2.795194	-3.405327	0.000000
H	-0.464134	-4.332475	0.000000
H	1.449387	-2.745826	0.000000
H	-6.618264	-0.332382	0.000000
H	-4.928480	-2.238021	0.000000
H	5.954415	-2.025727	0.000000
H	6.889200	0.155711	0.000000
H	5.333732	2.134879	0.000000
H	2.976915	2.785320	0.000000
H	1.580402	1.634605	0.000000

P-C(H)$^+$ (COSMO), *E* = -5861.59 kcal mol^{-1}



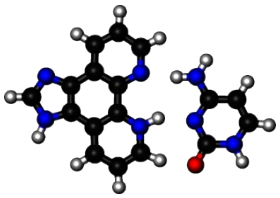
C	-2.463317	2.895692	0.505096
C	-2.367862	1.506876	0.275739
C	-1.074654	0.939183	0.036073
N	0.033363	1.726004	-0.018655
C	-0.088277	3.038440	0.199072
C	-1.315284	3.669137	0.479490
C	-3.505060	0.635770	0.256422
C	-3.346366	-0.726090	0.005430
C	-2.081681	-1.347438	-0.206478
C	-0.924751	-0.504156	-0.164458
C	-1.910368	-2.729552	-0.434859
C	-0.632068	-3.234478	-0.598362
C	0.455791	-2.346692	-0.506152
N	0.321790	-1.033596	-0.295195
N	-4.846615	0.942542	0.443915
C	-5.477123	-0.218698	0.306064
N	-4.619523	-1.253966	0.041665
N	2.999816	-0.314207	0.052209
C	3.787175	-1.286077	0.652105
N	5.154594	-1.081082	0.506378
C	5.693398	-0.045737	-0.205132
C	4.898328	0.881987	-0.808558
C	3.486886	0.745872	-0.664128
N	2.604175	1.587448	-1.184155
O	3.316010	-2.251016	1.258221
H	1.949604	-0.473501	0.043991
H	-3.439484	3.333828	0.693959
H	0.829285	3.621419	0.136690
H	-1.348829	4.740781	0.653666
H	-2.779589	-3.381311	-0.474557
H	-0.457592	-4.291521	-0.775900
H	1.476479	-2.714959	-0.582577
H	-6.544595	-0.372864	0.385722
H	-4.880954	-2.222983	-0.100221
H	5.761441	-1.768637	0.943455
H	6.775179	-0.015058	-0.245757
H	5.310459	1.712788	-1.367239
H	2.940982	2.390632	-1.702365
H	1.604821	1.539193	-0.874824

P-C(H)$^+$ (planar, COSMO), *E* = -5860.09 kcal mol^{-1}



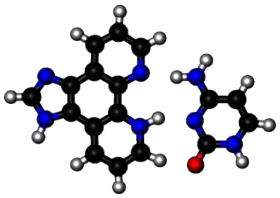
C	-2.624585	2.946177	0.000000
C	-2.487860	1.541507	0.000000
C	-1.169820	0.972365	0.000000
N	-0.074665	1.779018	0.000000
C	-0.235837	3.105758	0.000000
C	-1.491064	3.740280	0.000000
C	-3.613972	0.657334	0.000000
C	-3.423172	-0.721832	0.000000
C	-2.139870	-1.341673	0.000000
C	-0.987004	-0.485403	0.000000
C	-1.959617	-2.741584	0.000000
C	-0.675442	-3.251871	0.000000
C	0.404675	-2.349442	0.000000
N	0.271876	-1.016207	0.000000
N	-4.970023	0.962777	0.000000
C	-5.576880	-0.218954	0.000000
N	-4.691893	-1.265205	0.000000
N	3.174851	-0.439473	0.000000
C	4.020457	-1.546580	0.000000
N	5.372758	-1.229467	0.000000
C	5.856547	0.048872	0.000000
C	5.011292	1.115978	0.000000
C	3.607468	0.862774	0.000000
N	2.698952	1.822424	0.000000
O	3.615446	-2.710183	0.000000
H	2.142673	-0.604538	0.000000
H	-3.621108	3.378312	0.000000
H	0.676156	3.700196	0.000000
H	-1.554639	4.824177	0.000000
H	-2.825407	-3.398592	0.000000
H	-0.487769	-4.321254	0.000000
H	1.423835	-2.724970	0.000000
H	-6.645720	-0.380786	0.000000
H	-4.935483	-2.248730	0.000000
H	6.015196	-2.016218	0.000000
H	6.934625	0.145606	0.000000
H	5.374749	2.135563	0.000000
H	3.019736	2.783255	0.000000
H	1.665680	1.620234	0.000000

P(H(N1))$^{+}$-C, *E* = -5804.12 kcal mol^{-1}



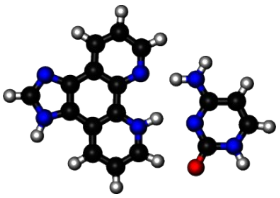
C	-2.995992	-2.577979	0.000000
C	-2.714825	-1.194353	0.000000
C	-1.346414	-0.772279	0.000000
N	-0.324823	-1.670671	0.000000
C	-0.626465	-2.969323	0.000000
C	-1.943618	-3.474446	0.000000
C	-3.741273	-0.198284	0.000000
C	-3.414816	1.159876	0.000000
C	-2.074785	1.640013	0.000000
C	-1.039315	0.648327	0.000000
C	-1.717840	3.007448	0.000000
C	-0.386098	3.385948	0.000000
C	0.600484	2.395338	0.000000
N	0.257371	1.095094	0.000000
N	-5.109497	-0.379664	0.000000
C	-5.608389	0.841195	0.000000
N	-4.630848	1.818003	0.000000
N	2.993637	0.140853	0.000000
C	3.876615	1.198733	0.000000
N	5.260242	0.887111	0.000000
C	5.739378	-0.388307	0.000000
C	4.868650	-1.435287	0.000000
C	3.465242	-1.120680	0.000000
N	2.556366	-2.116327	0.000000
O	3.548205	2.391884	0.000000
H	1.089243	0.447099	0.000000
H	-4.033796	-2.899255	0.000000
H	0.216303	-3.659552	0.000000
H	-2.112521	-4.547560	0.000000
H	-2.499253	3.763945	0.000000
H	-0.090046	4.429918	0.000000
H	1.678239	2.583860	0.000000
H	-6.660700	1.094536	0.000000
H	-4.790507	2.818185	0.000000
H	5.888035	1.685519	-0.000001
H	6.817977	-0.506135	0.000000
H	5.216271	-2.462432	0.000000
H	2.860628	-3.079151	0.000000
H	1.556706	-1.877440	0.000000

P(H(N1))$^{+}$-C (planar), *E* = -5804.12 kcal mol^{-1}



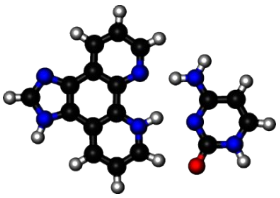
C	-2.995877	-2.577927	0.000000
C	-2.714737	-1.194324	0.000000
C	-1.346347	-0.772232	0.000000
N	-0.324745	-1.670588	0.000000
C	-0.626352	-2.969252	0.000000
C	-1.943494	-3.474384	0.000000
C	-3.741202	-0.198285	0.000000
C	-3.414784	1.159875	0.000000
C	-2.074761	1.640052	0.000000
C	-1.039286	0.648365	0.000000
C	-1.717793	3.007464	0.000000
C	-0.386032	3.385943	0.000000
C	0.600543	2.395340	0.000000
N	0.257393	1.095117	0.000000
N	-5.109404	-0.379719	0.000000
C	-5.608344	0.841120	0.000000
N	-4.630839	1.817955	0.000000
N	2.993509	0.140829	0.000000
C	3.876481	1.198706	0.000000
N	5.260094	0.887066	0.000000
C	5.739240	-0.388364	0.000000
C	4.868510	-1.435332	0.000000
C	3.465121	-1.120674	0.000000
N	2.556281	-2.116330	0.000000
O	3.548088	2.391837	0.000000
H	1.089191	0.447094	0.000000
H	-4.033671	-2.899185	0.000000
H	0.216428	-3.659453	0.000000
H	-2.112396	-4.547496	0.000000
H	-2.499173	3.763990	0.000000
H	-0.089989	4.429911	0.000000
H	1.678251	2.583863	0.000000
H	-6.660648	1.094415	0.000000
H	-4.790530	2.818132	0.000000
H	5.887876	1.685477	0.000000
H	6.817841	-0.506206	0.000000
H	5.216094	-2.462480	0.000000
H	2.860566	-3.079151	0.000000
H	1.556663	-1.877454	0.000000

P(H(N1))$^{+}$-C (COSMO), *E* = -5859.65 kcal mol^{-1}



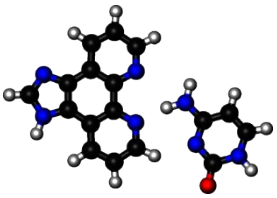
C	-2.995698	-2.594785	-0.001315
C	-2.735111	-1.206817	-0.000682
C	-1.369567	-0.774959	0.005358
N	-0.339105	-1.662264	0.011380
C	-0.621123	-2.966486	0.011463
C	-1.933833	-3.481617	0.004827
C	-3.764529	-0.211230	-0.005170
C	-3.437844	1.146160	-0.003582
C	-2.100102	1.631807	0.000823
C	-1.068982	0.645197	0.004468
C	-1.751627	2.999901	0.000652
C	-0.418953	3.379256	0.004785
C	0.566377	2.388930	0.009560
N	0.224145	1.090672	0.008876
N	-5.141397	-0.377279	-0.009755
C	-5.626647	0.860084	-0.010150
N	-4.643087	1.812688	-0.005694
N	3.042521	0.185315	0.003384
C	3.958682	1.201668	0.000652
N	5.322977	0.859201	-0.006525
C	5.766095	-0.431049	-0.013979
C	4.866224	-1.452736	-0.012581
C	3.473930	-1.098484	-0.002545
N	2.538588	-2.062794	0.001078
O	3.653404	2.417752	0.004592
H	1.033463	0.436837	0.010215
H	-4.025279	-2.939693	-0.006468
H	0.229816	-3.644613	0.016843
H	-2.093217	-4.555437	0.004427
H	-2.537801	3.748800	-0.001497
H	-0.126071	4.422986	0.005479
H	1.637283	2.579596	0.013275
H	-6.673708	1.128083	-0.014284
H	-4.785964	2.816228	-0.006368
H	5.987518	1.626951	-0.008005
H	6.840128	-0.572046	-0.020875
H	5.177818	-2.490980	-0.018670
H	2.817171	-3.034914	-0.002513
H	1.541903	-1.806402	0.005694

P(H(N1))$^{+}$-C (planar, COSMO), *E* = -5859.63 kcal mol^{-1}



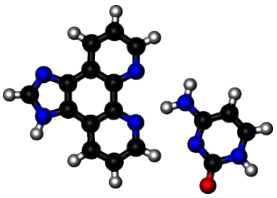
C	-2.996020	-2.594811	0.000000
C	-2.735665	-1.206780	0.000000
C	-1.370118	-0.774863	0.000000
N	-0.339532	-1.661997	0.000000
C	-0.621364	-2.966214	0.000000
C	-1.934020	-3.481504	0.000000
C	-3.765084	-0.211141	0.000000
C	-3.438359	1.146255	0.000000
C	-2.100596	1.631899	0.000000
C	-1.069562	0.645276	0.000000
C	-1.752031	2.999943	0.000000
C	-0.419282	3.379171	0.000000
C	0.566013	2.388789	0.000000
N	0.223603	1.090591	0.000000
N	-5.141980	-0.377163	0.000000
C	-5.627213	0.860187	0.000000
N	-4.643604	1.812793	0.000000
N	3.043399	0.185033	0.000000
C	3.959388	1.201531	0.000000
N	5.323778	0.859268	0.000000
C	5.767106	-0.430910	0.000000
C	4.867381	-1.452750	0.000000
C	3.475017	-1.098684	0.000000
N	2.539804	-2.063178	0.000000
O	3.653822	2.417556	0.000000
H	1.032482	0.436393	0.000000
H	-4.025557	-2.939939	0.000000
H	0.229624	-3.644254	0.000000
H	-2.093238	-4.555360	0.000000
H	-2.538139	3.748911	0.000000
H	-0.126346	4.422893	0.000000
H	1.636923	2.579233	0.000000
H	-6.674308	1.128202	0.000000
H	-4.786493	2.816333	0.000000
H	5.988154	1.627149	0.000000
H	6.841161	-0.571871	0.000000
H	5.179132	-2.490968	0.000000
H	2.818540	-3.035254	0.000000
H	1.543236	-1.806902	0.000000

P-C, *E* = -5830.41 kcal mol^{-1}



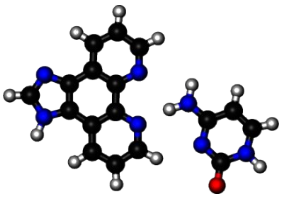
C	0.008493	-2.199588	-3.696345
C	0.003606	-0.903954	-3.140166
C	-0.012949	-0.769579	-1.713031
N	-0.024342	-1.854538	-0.894194
C	-0.019628	-3.063890	-1.453487
C	-0.003282	-3.292987	-2.846021
C	0.014329	0.288195	-3.938405
C	0.008238	1.544170	-3.334072
C	-0.007988	1.743277	-1.921074
C	-0.018066	0.567678	-1.099900
C	-0.014226	3.004462	-1.285229
C	-0.028894	3.067701	0.098142
C	-0.036478	1.863049	0.832915
N	-0.031686	0.662233	0.251121
N	0.030958	0.403737	-5.321837
C	0.034872	1.702352	-5.549718
N	0.021617	2.447172	-4.384876
N	-0.008155	0.348358	3.685267
C	0.010159	0.885659	4.943532
N	0.031778	-0.051130	6.040008
C	0.035138	-1.403106	5.860860
C	0.017169	-1.922018	4.601702
C	-0.004530	-0.977732	3.502092
N	-0.022760	-1.435576	2.232755
O	0.009651	2.089207	5.209164
H	-0.029230	-0.778645	1.430253
H	0.021259	-2.304985	-4.777919
H	-0.029596	-3.912705	-0.768523
H	-0.000214	-4.309794	-3.231596
H	-0.007081	3.914971	-1.882887
H	-0.033878	4.020419	0.621199
H	-0.044311	1.851425	1.922541
H	0.047008	2.174854	-6.523281
H	0.022024	3.456420	-4.316335
H	0.045785	0.359062	6.967499
H	0.052325	-2.016851	6.756634
H	0.018945	-2.993815	4.430900
H	-0.013352	-2.427257	2.046944

P-C (planar), *E* = -5830.40 kcal mol^{-1}



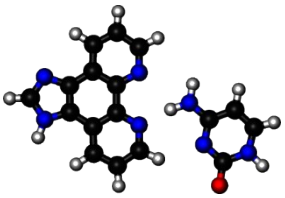
C	-3.697324	-2.199321	0.000000
C	-3.140611	-0.903898	0.000000
C	-1.713330	-0.770062	0.000000
N	-0.894895	-1.855348	0.000000
C	-1.454646	-3.064493	0.000000
C	-2.847324	-3.293053	0.000000
C	-3.938488	0.288539	0.000000
C	-3.333687	1.544307	0.000000
C	-1.920501	1.742870	0.000000
C	-1.099669	0.567000	0.000000
C	-1.284270	3.003883	0.000000
C	0.099203	3.066692	0.000000
C	0.833618	1.861834	0.000000
N	0.251458	0.661149	0.000000
N	-5.321987	0.404593	0.000000
C	-5.549427	1.703290	0.000000
N	-4.384240	2.447701	0.000000
N	3.684679	0.348189	0.000000
C	4.942683	0.886424	0.000000
N	6.039987	-0.049634	0.000000
C	5.861849	-1.401781	0.000000
C	4.602934	-1.921576	0.000000
C	3.502518	-0.978015	0.000000
N	2.233326	-1.436592	0.000000
O	5.207445	2.090149	0.000000
H	1.430692	-0.779819	0.000000
H	-4.779024	-2.304216	0.000000
H	-0.769923	-3.913542	0.000000
H	-3.233229	-4.309753	0.000000
H	-1.881832	3.914445	0.000000
H	0.622689	4.019182	0.000000
H	1.923283	1.849800	0.000000
H	-6.522912	2.176150	0.000000
H	-4.315315	3.456916	0.000000
H	6.967363	0.361059	0.000000
H	6.758296	-2.014768	0.000000
H	4.432799	-2.993477	0.000000
H	2.048105	-2.428423	0.000000

P-C (COSMO), *E* = -5857.87 kcal mol^{-1}



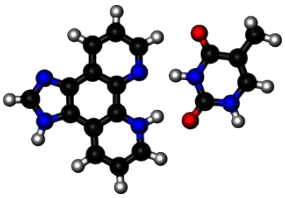
C	0.017703	-2.227272	-3.636742
C	0.008856	-0.911599	-3.124695
C	0.024283	-0.734740	-1.701946
N	0.044641	-1.796266	-0.849469
C	0.051714	-3.026556	-1.368796
C	0.039645	-3.295024	-2.754179
C	-0.014008	0.258555	-3.955092
C	-0.021130	1.532383	-3.386223
C	-0.006140	1.769096	-1.979616
C	0.017857	0.617508	-1.127457
C	-0.013701	3.050643	-1.385549
C	0.003329	3.156361	-0.004109
C	0.026510	1.974049	0.763509
N	0.033477	0.752021	0.224365
N	-0.030282	0.346800	-5.342873
C	-0.046216	1.651086	-5.595644
N	-0.041364	2.407962	-4.453591
N	0.030149	0.362364	3.758907
C	0.040906	0.798990	5.048171
N	-0.015499	-0.165072	6.077645
C	-0.083290	-1.506530	5.827589
C	-0.095601	-1.955853	4.542061
C	-0.034048	-0.963707	3.498181
N	-0.037879	-1.347332	2.209201
O	0.099155	2.012055	5.370302
H	-0.000171	-0.655113	1.435946
H	0.007404	-2.378570	-4.712601
H	0.068327	-3.851774	-0.657973
H	0.047400	-4.321639	-3.109796
H	-0.033333	3.937948	-2.013160
H	-0.002396	4.125160	0.487015
H	0.038094	2.003131	1.851896
H	-0.063312	2.105101	-6.576545
H	-0.049102	3.420379	-4.411910
H	-0.005657	0.175734	7.034055
H	-0.123037	-2.156925	6.693165
H	-0.147936	-3.013581	4.308278
H	-0.084900	-2.330433	1.977352

P-C (planar, COSMO), *E* = -5857.88 kcal mol^{-1}



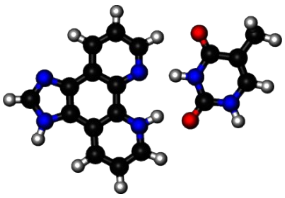
C	-3.640546	-2.225990	0.000000
C	-3.126270	-0.911161	0.000000
C	-1.703079	-0.736729	0.000000
N	-0.852378	-1.799917	0.000000
C	-1.373820	-3.029339	0.000000
C	-2.759760	-3.295389	0.000000
C	-3.954958	0.260404	0.000000
C	-3.384084	1.533305	0.000000
C	-1.976931	1.767757	0.000000
C	-1.126296	0.614637	0.000000
C	-1.381030	3.048549	0.000000
C	0.000650	3.151889	0.000000
C	0.766649	1.968309	0.000000
N	0.225875	0.746918	0.000000
N	-5.342644	0.351008	0.000000
C	-5.593466	1.655777	0.000000
N	-4.450091	2.410663	0.000000
N	3.755746	0.362068	0.000000
C	5.043302	0.803717	0.000000
N	6.076387	-0.158114	0.000000
C	5.831374	-1.502165	0.000000
C	4.547505	-1.956532	0.000000
C	3.499932	-0.966397	0.000000
N	2.212039	-1.354197	0.000000
O	5.360695	2.019392	0.000000
H	1.437026	-0.663019	0.000000
H	-4.716717	-2.375276	0.000000
H	-0.664330	-3.855898	0.000000
H	-3.117154	-4.321385	0.000000
H	-2.007153	3.937262	0.000000
H	0.493355	4.119869	0.000000
H	1.855077	1.995739	0.000000
H	-6.573848	2.111039	0.000000
H	-4.406669	3.422950	0.000000
H	7.031562	0.186207	0.000000
H	6.699867	-2.150037	0.000000
H	4.317850	-3.016463	0.000000
H	1.983301	-2.339169	0.000000

P(H(N1))$^{+}$-T, *E* = -6060.68 kcal mol^{-1}



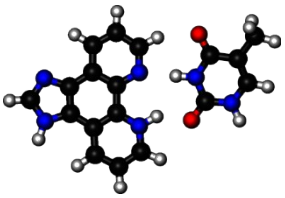
C	-0.002833	4.666223	2.128006
C	-0.002055	3.309024	2.518974
C	-0.000250	2.306947	1.499937
N	0.001070	2.626591	0.175262
C	0.000466	3.918817	-0.163842
C	-0.001489	4.970708	0.780224
C	-0.001894	2.894809	3.890161
C	0.000306	1.538158	4.231402
C	0.001524	0.494804	3.264907
C	0.000803	0.907957	1.888468
C	0.003264	-0.886163	3.560682
C	0.003994	-1.831703	2.543151
C	0.002798	-1.390838	1.219139
N	0.001356	-0.075327	0.940906
N	-0.003523	3.687774	5.018179
C	-0.001887	2.837153	6.026990
N	0.000453	1.519251	5.614860
N	0.002187	1.578976	-2.584778
C	-0.002499	0.213370	-2.691221
N	-0.005985	-0.262625	-3.983394
C	-0.004882	0.571261	-5.098772
C	-0.000160	1.923891	-4.994775
C	0.003564	2.521305	-3.652079
O	0.007545	3.725384	-3.407133
O	-0.003593	-0.543250	-1.697277
C	0.001226	2.850983	-6.181939
H	-0.004185	5.431939	2.898628
H	0.002048	4.132450	-1.232555
H	-0.001672	5.999996	0.432741
H	0.004110	-1.211017	4.598443
H	0.005393	-2.895358	2.756573
H	0.002904	-2.043440	0.354001
H	-0.002552	3.101414	7.076656
H	0.002048	0.708143	6.221449
H	0.003699	1.931882	-1.613148
H	-0.009684	-1.270783	-4.092297
H	-0.008058	0.057530	-6.054879
H	-0.002370	2.286856	-7.121308
H	0.884772	3.502103	-6.153795
H	-0.877477	3.508482	-6.150847
H	0.000038	0.137041	-0.087356

P(H(N1))$^{+}$-T (planar), *E* = -6060.69 kcal mol^{-1}



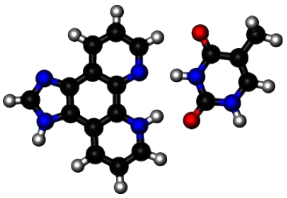
C	2.126960	4.666144	0.000000
C	2.518133	3.309016	0.000000
C	1.499330	2.306706	0.000000
N	0.174651	2.626172	0.000000
C	-0.164755	3.918325	0.000000
C	0.779113	4.970384	0.000000
C	3.889346	2.895073	0.000000
C	4.230889	1.538500	0.000000
C	3.264621	0.494931	0.000000
C	1.888107	0.907779	0.000000
C	3.560688	-0.885990	0.000000
C	2.543342	-1.831727	0.000000
C	1.219232	-1.391154	0.000000
N	0.940728	-0.075716	0.000000
N	5.017143	3.688339	0.000000
C	6.026102	2.837978	0.000000
N	5.614367	1.519954	0.000000
N	-2.583789	1.578225	0.000000
C	-2.690978	0.212702	0.000000
N	-3.983411	-0.262624	0.000000
C	-5.098276	0.571914	0.000000
C	-4.993494	1.924500	0.000000
C	-3.650518	2.521150	0.000000
O	-3.404820	3.725107	0.000000
O	-1.697373	-0.544398	0.000000
C	-6.180030	2.852304	0.000000
H	2.897451	5.431976	0.000000
H	-1.233571	4.131648	0.000000
H	0.431416	5.999602	0.000000
H	4.598528	-1.210586	0.000000
H	2.756908	-2.895343	0.000000
H	0.354235	-2.043941	0.000000
H	7.075674	3.102650	0.000000
H	6.221133	0.708964	0.000000
H	-1.611906	1.930638	0.000000
H	-4.092880	-1.270725	0.000000
H	-6.054711	0.058790	0.000000
H	-7.119806	2.288886	0.000000
H	-6.149985	3.506607	-0.881105
H	-6.149985	3.506607	0.881105
H	-0.087596	0.136356	0.000000

P(H(N1))$^{+}$-T (COSMO), *E* = -6116.26 kcal mol^{-1}



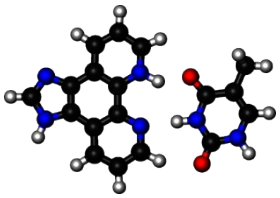
C	-0.189159	4.664985	2.128649
C	-0.093969	3.313662	2.527189
C	-0.097476	2.305999	1.510662
N	-0.170500	2.619517	0.186089
C	-0.258003	3.908510	-0.154395
C	-0.276287	4.963874	0.781620
C	0.008958	2.903377	3.896096
C	0.101441	1.550477	4.230057
C	0.087387	0.504721	3.265472
C	-0.019151	0.909645	1.900373
C	0.164151	-0.870811	3.573202
C	0.128603	-1.818262	2.560255
C	0.014717	-1.385282	1.238178
N	-0.052405	-0.074492	0.956321
N	0.039439	3.686525	5.039692
C	0.148851	2.815823	6.038058
N	0.189611	1.518056	5.604305
N	-0.006231	1.578331	-2.599963
C	-0.192056	0.220938	-2.724838
N	-0.192644	-0.243424	-4.018880
C	-0.018744	0.577883	-5.114166
C	0.164357	1.920352	-4.992494
C	0.172103	2.496849	-3.652440
O	0.320749	3.706680	-3.401400
O	-0.347007	-0.529391	-1.739117
C	0.354058	2.832655	-6.177644
H	-0.190033	5.441945	2.887169
H	-0.296188	4.118265	-1.220596
H	-0.350259	5.989722	0.433782
H	0.248410	-1.180159	4.610653
H	0.183307	-2.879498	2.772867
H	-0.030073	-2.050215	0.385580
H	0.203790	3.064289	7.088449
H	0.272025	0.696462	6.192182
H	-0.016397	1.924361	-1.624466
H	-0.325530	-1.241098	-4.149159
H	-0.040125	0.074760	-6.073930
H	0.321781	2.261051	-7.111661
H	1.317632	3.356205	-6.111996
H	-0.429455	3.602299	-6.201985
H	-0.153065	0.154214	-0.051430

P(H(N1))$^{+}$-T (planar, COSMO), *E* = -6116.20 kcal mol^{-1}



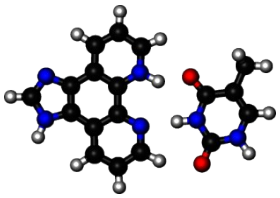
C	2.135315	4.668055	0.000000
C	2.535049	3.313798	0.000000
C	1.517726	2.306639	0.000000
N	0.191329	2.622479	0.000000
C	-0.149899	3.914577	0.000000
C	0.786342	4.970008	0.000000
C	3.906878	2.900548	0.000000
C	4.243340	1.545275	0.000000
C	3.277825	0.500415	0.000000
C	1.909379	0.908432	0.000000
C	3.587660	-0.876846	0.000000
C	2.572930	-1.823071	0.000000
C	1.247047	-1.386707	0.000000
N	0.963637	-0.074520	0.000000
N	5.051565	3.682658	0.000000
C	6.053232	2.808801	0.000000
N	5.620273	1.510097	0.000000
N	-2.616332	1.583402	0.000000
C	-2.732056	0.212266	0.000000
N	-4.024578	-0.256612	0.000000
C	-5.127327	0.572840	0.000000
C	-5.014905	1.928497	0.000000
C	-3.677137	2.510117	0.000000
O	-3.435647	3.731061	0.000000
O	-1.740650	-0.546012	0.000000
C	-6.208324	2.849797	0.000000
H	2.894711	5.444160	0.000000
H	-1.216819	4.125273	0.000000
H	0.437118	5.998047	0.000000
H	4.627966	-1.188486	0.000000
H	2.786482	-2.885473	0.000000
H	0.392052	-2.049834	0.000000
H	7.105588	3.055110	0.000000
H	6.210107	0.685914	0.000000
H	-1.641835	1.930276	0.000000
H	-4.147613	-1.264017	0.000000
H	-6.084820	0.064853	0.000000
H	-7.139279	2.272331	0.000000
H	-6.192360	3.502770	-0.883326
H	-6.192360	3.502770	0.883326
H	-0.048455	0.156295	0.000000

P(H(N10))$^{+}$-T, *E* = -6063.62 kcal mol^{-1}



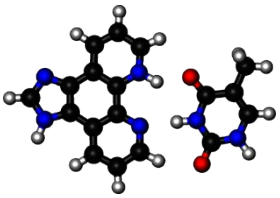
C	0.001050	-2.625021	-2.996311
C	0.000570	-1.218876	-2.876838
C	-0.001015	-0.623793	-1.578276
N	-0.001998	-1.466637	-0.502053
C	-0.001557	-2.806655	-0.606983
C	0.000035	-3.423239	-1.860326
C	0.001438	-0.342386	-4.004646
C	0.000155	1.043681	-3.825248
C	-0.001276	1.671902	-2.544508
C	-0.001674	0.818352	-1.390755
C	-0.002008	3.070284	-2.334509
C	-0.002820	3.560626	-1.042589
C	-0.002922	2.648971	0.035365
N	-0.002463	1.322707	-0.127040
N	0.003467	-0.675464	-5.344125
C	0.003027	0.482984	-5.973139
N	0.001350	1.560719	-5.105665
N	-0.000171	0.634657	2.755911
C	0.001978	1.708693	3.645007
N	0.003612	1.300322	4.979227
C	0.002791	-0.020861	5.378987
C	0.000354	-1.055178	4.492482
C	-0.001150	-0.721582	3.076204
O	-0.003249	-1.564550	2.151037
O	0.002721	2.883797	3.298645
C	-0.000674	-2.506011	4.903404
H	0.002375	-3.053853	-3.994743
H	-0.002348	-3.338088	0.337724
H	0.000465	-4.506418	-1.925477
H	-0.001700	3.748678	-3.184836
H	-0.003153	4.628330	-0.843416
H	-0.002970	3.007473	1.064014
H	0.003356	0.619616	-7.046643
H	0.000695	2.538288	-5.371260
H	-0.001024	0.852484	1.745582
H	0.005418	2.049137	5.664396
H	0.004260	-0.180372	6.453051
H	0.000897	-2.601471	5.994960
H	0.881468	-3.020544	4.499979
H	-0.885230	-3.018513	4.502705
H	-0.002865	-1.125292	0.494698

P(H(N10))$^{+}$-T (planar), *E* = -6063.62 kcal mol^{-1}



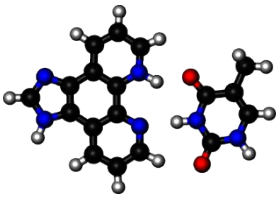
C	-2.996372	-2.625009	0.000000
C	-2.876795	-1.218867	0.000000
C	-1.578184	-0.623835	0.000000
N	-0.502007	-1.466738	0.000000
C	-0.607091	-2.806765	0.000000
C	-1.860440	-3.423291	0.000000
C	-4.004596	-0.342383	0.000000
C	-3.825198	1.043679	0.000000
C	-2.544454	1.671882	0.000000
C	-1.390678	0.818344	0.000000
C	-2.334507	3.070272	0.000000
C	-1.042609	3.560683	0.000000
C	0.035373	2.649069	0.000000
N	-0.127003	1.322792	0.000000
N	-5.344076	-0.675500	0.000000
C	-5.973108	0.482936	0.000000
N	-5.105640	1.560704	0.000000
N	2.755854	0.634578	0.000000
C	3.644840	1.708699	0.000000
N	4.979097	1.300441	0.000000
C	5.378956	-0.020706	0.000000
C	4.492535	-1.055110	0.000000
C	3.076241	-0.721634	0.000000
O	2.151098	-1.564669	0.000000
O	3.298370	2.883790	0.000000
C	4.903704	-2.505893	0.000000
H	-3.994858	-3.053758	0.000000
H	0.337538	-3.338305	0.000000
H	-1.925644	-4.506489	0.000000
H	-3.184883	3.748599	0.000000
H	-0.843487	4.628411	0.000000
H	1.064021	3.007593	0.000000
H	-7.046655	0.619603	0.000000
H	-5.371249	2.538271	0.000000
H	1.745457	0.852234	0.000000
H	5.664219	2.049310	0.000000
H	6.453037	-0.180136	0.000000
H	5.995280	-2.601132	0.000000
H	4.501740	-3.019501	-0.883345
H	4.501740	-3.019501	0.883345
H	0.494800	-1.125475	0.000000

P(H(N10))$^{+}$-T (COSMO), *E* = -6116.30 kcal mol^{-1}



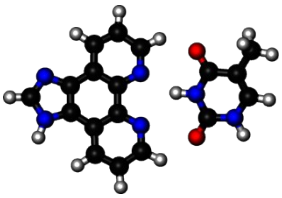
C	-0.073515	-2.632582	-3.007038
C	-0.039110	-1.226328	-2.895726
C	0.003761	-0.631969	-1.599059
N	0.015183	-1.470872	-0.523150
C	-0.016192	-2.809032	-0.619375
C	-0.063247	-3.427413	-1.869943
C	-0.039817	-0.345042	-4.021701
C	0.001028	1.037961	-3.834304
C	0.040261	1.662092	-2.553402
C	0.039099	0.807198	-1.404378
C	0.082404	3.059609	-2.351397
C	0.120142	3.548963	-1.058991
C	0.110826	2.636253	0.016617
N	0.070387	1.309114	-0.138191
N	-0.068689	-0.655929	-5.372548
C	-0.044900	0.522693	-5.983927
N	-0.003096	1.572647	-5.103627
N	-0.022057	0.638434	2.776025
C	-0.110949	1.694897	3.667806
N	-0.121590	1.300665	4.993561
C	-0.051858	-0.012157	5.402049
C	0.037580	-1.044294	4.517829
C	0.057590	-0.717111	3.103608
O	0.139252	-1.563802	2.183660
O	-0.174059	2.882429	3.318712
C	0.116382	-2.489401	4.940710
H	-0.107219	-3.075604	-3.997377
H	-0.000458	-3.343541	0.321456
H	-0.089040	-4.509275	-1.931150
H	0.083625	3.730845	-3.205788
H	0.153712	4.615629	-0.860260
H	0.127954	2.996896	1.042260
H	-0.056420	0.679706	-7.053125
H	0.021357	2.554834	-5.352451
H	-0.004939	0.854543	1.764118
H	-0.187921	2.041137	5.684550
H	-0.072656	-0.163325	6.475200
H	0.084286	-2.571310	6.032712
H	1.044431	-2.949467	4.574884
H	-0.717660	-3.062909	4.514058
H	0.059694	-1.107480	0.452270

P(H(N10))$^{+}$-T (planar, COSMO), *E* = -6116.28 kcal mol^{-1}



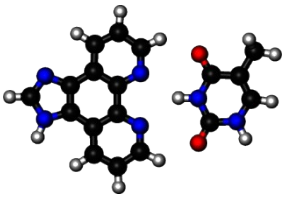
C	-3.008811	-2.634879	0.000000
C	-2.898284	-1.228090	0.000000
C	-1.601428	-0.632402	0.000000
N	-0.524758	-1.470388	0.000000
C	-0.620301	-2.808881	0.000000
C	-1.871028	-3.428789	0.000000
C	-4.024671	-0.347194	0.000000
C	-3.837111	1.036463	0.000000
C	-2.556094	1.661719	0.000000
C	-1.406737	0.807235	0.000000
C	-2.354251	3.059894	0.000000
C	-1.061678	3.550245	0.000000
C	0.014174	2.637665	0.000000
N	-0.140371	1.309854	0.000000
N	-5.375744	-0.658529	0.000000
C	-5.987073	0.520391	0.000000
N	-5.106458	1.570942	0.000000
N	2.781298	0.641867	0.000000
C	3.676020	1.699587	0.000000
N	5.001257	1.303226	0.000000
C	5.406561	-0.012529	0.000000
C	4.519307	-1.045923	0.000000
C	3.105282	-0.716916	0.000000
O	2.182904	-1.564632	0.000000
O	3.330057	2.889720	0.000000
C	4.938361	-2.494192	0.000000
H	-3.999145	-3.079169	0.000000
H	0.321319	-3.342151	0.000000
H	-1.931853	-4.510953	0.000000
H	-3.208908	3.730714	0.000000
H	-0.863018	4.617453	0.000000
H	1.039706	2.999116	0.000000
H	-7.056407	0.677207	0.000000
H	-5.354723	2.553550	0.000000
H	1.769726	0.858418	0.000000
H	5.694336	2.044722	0.000000
H	6.479893	-0.164631	0.000000
H	6.030710	-2.576983	0.000000
H	4.540374	-3.011817	-0.883340
H	4.540374	-3.011817	0.883340
H	0.451208	-1.105799	0.000000

P-T, *E* = -6089.57 kcal mol^{-1}



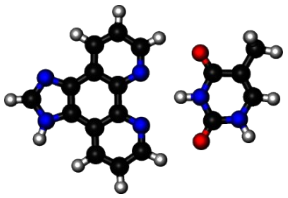
C	-2.394685	2.664538	-0.362227
C	-2.427249	1.267836	-0.173864
C	-1.191127	0.546807	-0.198013
N	-0.001701	1.173432	-0.387366
C	0.000421	2.495569	-0.557407
C	-1.171104	3.283083	-0.558586
C	-3.640496	0.530335	0.038151
C	-3.608369	-0.853399	0.205476
C	-2.408486	-1.626162	0.182621
C	-1.179773	-0.910815	-0.015571
C	-2.343908	-3.027766	0.336977
C	-1.109396	-3.656060	0.287862
C	0.045275	-2.867635	0.089548
N	0.015121	-1.543823	-0.050190
N	-4.942766	1.007138	0.105146
C	-5.683204	-0.064734	0.309194
N	-4.933371	-1.223874	0.378816
N	2.879862	0.086860	-0.205693
C	3.481277	-1.134571	-0.487980
N	4.867832	-1.138578	-0.260053
C	5.587163	-0.047952	0.189299
C	4.992325	1.141424	0.446865
C	3.540787	1.263066	0.229716
O	2.920772	2.313239	0.407442
O	2.910234	-2.138816	-0.899943
C	5.735496	2.356806	0.937693
H	-3.329990	3.217876	-0.346066
H	0.979718	2.951651	-0.672319
H	-1.099419	4.358271	-0.704698
H	-3.255735	-3.603796	0.489468
H	-1.022358	-4.734487	0.396994
H	1.030709	-3.324445	0.029892
H	-6.760221	-0.079811	0.415176
H	-5.285554	-2.159483	0.532212
H	1.848402	0.150002	-0.311152
H	5.327518	-2.015816	-0.471540
H	6.653827	-0.210709	0.318056
H	6.804829	2.141158	1.054851
H	5.327131	2.692709	1.900398
H	5.609755	3.192584	0.236391

P-T (planar), *E* = -6089.44 kcal mol^{-1}



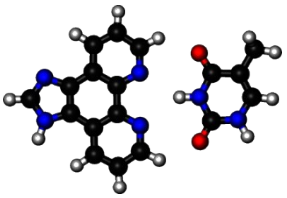
C	-2.531677	-2.860737	0.000000
C	-2.683751	-1.459255	0.000000
C	-1.506601	-0.643161	0.000000
N	-0.261285	-1.183478	0.000000
C	-0.147714	-2.512291	0.000000
C	-1.252953	-3.391408	0.000000
C	-3.963892	-0.810867	0.000000
C	-4.051543	0.579779	0.000000
C	-2.916516	1.444823	0.000000
C	-1.621837	0.822488	0.000000
C	-2.980680	2.854561	0.000000
C	-1.802131	3.582233	0.000000
C	-0.574415	2.885120	0.000000
N	-0.481707	1.555052	0.000000
N	-5.227395	-1.387230	0.000000
C	-6.062076	-0.366399	0.000000
N	-5.411324	0.853248	0.000000
N	2.652503	0.333041	0.000000
C	3.163029	1.627048	0.000000
N	4.564954	1.676220	0.000000
C	5.384196	0.563675	0.000000
C	4.878483	-0.692496	0.000000
C	3.415654	-0.864555	0.000000
O	2.873251	-1.969185	0.000000
O	2.499802	2.659051	0.000000
C	5.731237	-1.934804	0.000000
H	-3.421545	-3.484805	0.000000
H	0.869919	-2.890860	0.000000
H	-1.088522	-4.466572	0.000000
H	-3.946865	3.357611	0.000000
H	-1.810926	4.669589	0.000000
H	0.371315	3.419423	0.000000
H	-7.142507	-0.431577	0.000000
H	-5.846054	1.766398	0.000000
H	1.622475	0.236434	0.000000
H	4.953856	2.611349	0.000000
H	6.451467	0.767486	0.000000
H	6.797681	-1.677583	0.000000
H	5.508185	-2.552561	-0.880263
H	5.508185	-2.552561	0.880263

P-T (COSMO), *E* = -6112.21 kcal mol^{-1}



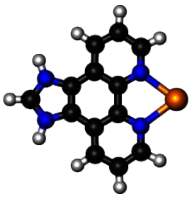
C	-2.504415	2.706660	0.019235
C	-2.529058	1.295569	0.009683
C	-1.280507	0.589659	0.024614
N	-0.088913	1.247422	0.043686
C	-0.102292	2.583452	0.051691
C	-1.282216	3.357103	0.041026
C	-3.743016	0.531691	-0.015725
C	-3.702216	-0.861979	-0.023904
C	-2.491220	-1.616342	-0.004623
C	-1.260414	-0.879506	0.018694
C	-2.435422	-3.027186	-0.004965
C	-1.198021	-3.648579	0.014668
C	-0.037195	-2.846199	0.034374
N	-0.055570	-1.510032	0.036826
N	-5.059567	0.979945	-0.037889
C	-5.790536	-0.129298	-0.059140
N	-5.023278	-1.264557	-0.051190
N	3.047110	-0.018016	0.025550
C	3.677347	-1.256075	0.014308
N	5.060100	-1.184439	-0.029758
C	5.769683	-0.004974	-0.059886
C	5.152210	1.205339	-0.044551
C	3.693745	1.238437	0.003436
O	3.026635	2.286953	0.025712
O	3.077969	-2.338860	0.042706
C	5.904143	2.512027	-0.074273
H	-3.442535	3.254601	0.009306
H	0.871543	3.062518	0.066106
H	-1.219613	4.441957	0.049588
H	-3.354829	-3.607240	-0.019823
H	-1.110954	-4.731544	0.015502
H	0.947351	-3.304058	0.048676
H	-6.870312	-0.174335	-0.082118
H	-5.371136	-2.216040	-0.068747
H	2.016017	-0.023140	0.048683
H	5.552629	-2.071384	-0.039821
H	6.847980	-0.113855	-0.093752
H	6.984415	2.332250	-0.108435
H	5.670004	3.114121	0.814292
H	5.613022	3.106948	-0.950796

P-T (planar, COSMO), *E* = -6112.24 kcal mol^{-1}



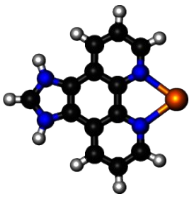
C	-2.562233	-2.868389	0.000000
C	-2.714628	-1.465362	0.000000
C	-1.535159	-0.649132	0.000000
N	-0.288723	-1.196368	0.000000
C	-0.181111	-2.528197	0.000000
C	-1.286033	-3.405525	0.000000
C	-3.992990	-0.814737	0.000000
C	-4.079078	0.576787	0.000000
C	-2.941489	1.438043	0.000000
C	-1.648606	0.815953	0.000000
C	-3.013946	2.848175	0.000000
C	-1.837881	3.579323	0.000000
C	-0.608936	2.885592	0.000000
N	-0.505820	1.553299	0.000000
N	-5.263645	-1.380832	0.000000
C	-6.092579	-0.342570	0.000000
N	-5.431675	0.857718	0.000000
N	2.717983	0.341073	0.000000
C	3.236006	1.630202	0.000000
N	4.620334	1.680800	0.000000
C	5.432027	0.568695	0.000000
C	4.923839	-0.691579	0.000000
C	3.473307	-0.853097	0.000000
O	2.899993	-1.956042	0.000000
O	2.542282	2.655412	0.000000
C	5.788805	-1.926647	0.000000
H	-3.446996	-3.498998	0.000000
H	0.832316	-2.916630	0.000000
H	-1.125417	-4.480256	0.000000
H	-3.982325	3.342547	0.000000
H	-1.849399	4.665703	0.000000
H	0.330144	3.431066	0.000000
H	-7.172232	-0.396116	0.000000
H	-5.864853	1.773658	0.000000
H	1.690296	0.253296	0.000000
H	5.032644	2.607797	0.000000
H	6.496942	0.772878	0.000000
H	6.849547	-1.652331	0.000000
H	5.579907	-2.546161	-0.882907
H	5.579907	-2.546161	0.882907

P(H(Im))$^{+}$-Ag^{+}, *E* = -3705.41 kcal mol^{-1}



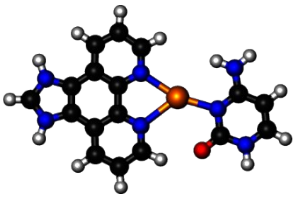
C	0.00000463	2.87839947	0.19468388
C	0.00000473	1.46709525	0.23260850
C	0.00001506	0.73683586	-0.99625895
N	0.00002465	1.40062278	-2.18393075
C	0.00002441	2.73859065	-2.20180618
C	0.00001454	3.52015552	-1.03107922
C	-0.00000496	0.69313361	1.43526118
C	-0.00000456	-0.69313269	1.43525540
C	0.00000558	-1.46710607	0.23260541
C	0.00001549	-0.73684959	-0.99626259
C	0.00000630	-2.87841332	0.19467532
C	0.00001658	-3.52016982	-1.03109039
C	0.00002600	-2.73860211	-2.20181883
N	0.00002547	-1.40063384	-2.18393801
N	-0.00001609	1.08671990	2.77267936
C	-0.00002227	0.00001790	3.56123100
N	-0.00001546	-1.08669397	2.77267818
Ag	0.00004042	0.00000307	-4.04857086
H	-0.00001808	-2.04046116	3.12472466
H	-0.00000312	3.45796927	1.11526187
H	0.00003232	3.21371205	-3.17869739
H	0.00001483	4.60349745	-1.10403611
H	-0.00000112	-3.45798771	1.11525179
H	0.00001750	-4.60351388	-1.10404630
H	0.00003419	-3.21372003	-3.17871234
H	-0.00003118	0.00002105	4.64285853
H	-0.00001927	2.04049050	3.12471813

P(H(Im))$^{+}$-Ag^{+} (COSMO), *E* = -3879.96 kcal mol^{-1}



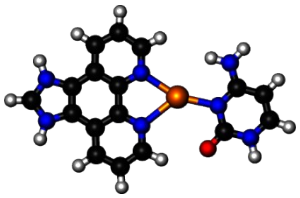
C	0.01423540	2.87063308	0.20748537
C	0.01079302	1.46128018	0.23885133
C	0.01034431	0.73551483	-0.99085639
N	0.00906678	1.39663364	-2.17881340
C	0.01031327	2.73334642	-2.19126761
C	0.01382678	3.51250297	-1.01910160
C	0.00454318	0.69176333	1.43931558
C	0.00555658	-0.69176048	1.43932993
C	0.01191263	-1.46129654	0.23886959
C	0.01041187	-0.73555332	-0.99084575
C	0.01444472	-2.87065296	0.20737383
C	0.01360344	-3.51251872	-1.01920700
C	0.00956315	-2.73334914	-2.19134361
N	0.00826779	-1.39663741	-2.17879918
N	-0.01637440	1.08623760	2.76775916
C	-0.02694064	0.00006174	3.55154956
N	-0.01524596	-1.08615504	2.76780456
Ag	-0.00958197	-0.00000701	-4.05945021
H	-0.01946259	-2.04007230	3.11218118
H	0.01800769	3.43373509	1.13653643
H	0.00796485	3.20611445	-3.16856472
H	0.01575508	4.59529032	-1.09002765
H	0.01798136	-3.43400804	1.13625028
H	0.01506414	-4.59530777	-1.09010777
H	0.00640773	-3.20606263	-3.16865622
H	-0.04486184	0.00002085	4.62836544
H	-0.02368938	2.04027987	3.11175029

P(H(Im))$^{+}$-Ag^{+}-C, *E* = -5660.52 kcal mol^{-1}



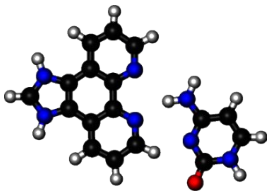
C	-0.00000571	2.75013285	2.95040331
C	0.00000110	1.34357205	2.84478782
C	0.00001449	0.74129666	1.54881106
N	0.00002066	1.51205104	0.42569905
C	0.00001399	2.84535374	0.55133575
C	0.00000080	3.50810517	1.79226854
C	-0.00000446	0.44577616	3.95860277
C	0.00000257	-0.93470974	3.81417360
C	0.00001596	-1.57908829	2.53916425
C	0.00002190	-0.71997315	1.39884487
C	0.00002356	-2.97650074	2.33508656
C	0.00003647	-3.46419426	1.03957201
C	0.00004163	-2.54920339	-0.03576227
N	0.00003453	-1.22715800	0.14690772
N	-0.00001701	0.69720906	5.33020460
C	-0.00001775	-0.46520230	6.00264165
N	-0.00000601	-1.46363755	5.10398323
Ag	0.00004221	0.44543025	-1.61069222
N	0.00006179	0.06222040	-3.75388575
C	0.00006993	-1.30430135	-4.03943636
N	0.00008282	-1.65169527	-5.40297582
C	0.00008743	-0.73654601	-6.41335832
C	0.00007944	0.59648372	-6.12879655
C	0.00006626	0.97823945	-4.74838907
N	0.00005794	2.28359349	-4.41159665
O	0.00006633	-2.17461340	-3.17188391
H	-0.00001591	3.23598996	3.92377683
H	0.00001932	3.41701144	-0.37156290
H	-0.00000405	4.59323524	1.82607316
H	0.00001936	-3.66155575	3.18043436
H	0.00004262	-4.53190088	0.84139108
H	0.00005169	-2.88064858	-1.07062669
H	-0.00002629	-0.57723453	7.07769798
H	-0.00000393	-2.44939765	5.35045483
H	0.00008868	-2.64886624	-5.60098791
H	0.00009756	-1.12888760	-7.42495846

P(H(Im))$^{+}$-Ag^{+}-C (COSMO), *E* = -5817.27 kcal mol^{-1}



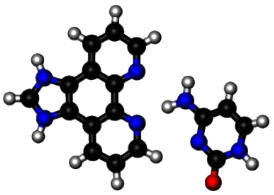
C	0.00676107	2.76865586	2.87662448
C	0.00201937	1.36116972	2.80403395
C	0.00422858	0.72897200	1.52547726
N	0.00359393	1.47191519	0.38391371
C	0.00412583	2.80843436	0.47335149
C	0.00757394	3.49769337	1.69914726
C	-0.00420958	0.49890540	3.94070020
C	0.00480220	-0.88191461	3.83510015
C	0.01452600	-1.55653043	2.57890977
C	0.00972185	-0.73315164	1.41441641
C	0.02516602	-2.95810141	2.42245488
C	0.02554498	-3.48911874	1.14257229
C	0.01632572	-2.60981794	0.04128336
N	0.01023432	-1.28200841	0.17573458
N	-0.02219754	0.79041621	5.29548087
C	-0.02674761	-0.35262650	5.99405398
N	-0.00983739	-1.37601955	5.12967976
Ag	-0.00288598	0.34412750	-1.59010394
N	-0.00556656	0.03804896	-3.74846155
C	-0.01688005	-1.28238608	-4.15983118
N	-0.01434224	-1.51326623	-5.53946638
C	-0.00266660	-0.51306824	-6.46719707
C	0.00875190	0.78847362	-6.06709488
C	0.00673793	1.04601965	-4.65777415
N	0.01660163	2.31007321	-4.20728397
O	-0.02869125	-2.24030809	-3.36541397
H	0.01135130	3.26301797	3.84385793
H	0.00288052	3.35383969	-0.46451878
H	0.01131575	4.58262369	1.70622250
H	0.03411734	-3.60154583	3.29762261
H	0.03247010	-4.56208500	0.97934079
H	0.01437522	-2.98174022	-0.97974474
H	-0.04346704	-0.43465320	7.06773538
H	-0.01397406	-2.35386995	5.39909699
H	-0.02422658	-2.48411925	-5.83666871
H	-0.00233914	-0.82183528	-7.50506308
H	0.01995439	1.60548403	-6.77810667
H	0.02231785	3.08901429	-4.85304218
H	0.01382802	2.49683935	-3.20964652
H	-0.03958716	1.71548910	5.71117583

P(H(Im))$^{+}$-C, *E* = -5772.78 kcal mol^{-1}



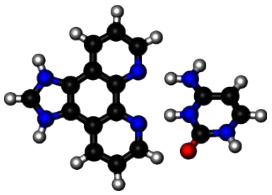
C	-0.00000339	2.18539083	3.59861659
C	0.00000023	0.90677262	3.00240150
C	0.00000746	0.80456629	1.57190551
N	0.00001084	1.91057671	0.79079132
C	0.00000730	3.10503148	1.38018490
C	0.00000018	3.30030077	2.77936793
C	-0.00000281	-0.32313300	3.72705689
C	0.00000094	-1.56402851	3.10196390
C	0.00000812	-1.71989081	1.68552565
C	0.00001141	-0.51449732	0.91182559
C	0.00001209	-2.96304937	1.01587184
C	0.00001903	-2.96965089	-0.36639021
C	0.00002189	-1.73486058	-1.05651141
N	0.00001820	-0.55114885	-0.43698873
N	-0.00000957	-0.57611734	5.09902665
C	-0.00001003	-1.90263992	5.31902293
N	-0.00000372	-2.51535298	4.12174336
N	0.00003436	-0.22647517	-3.68915428
C	0.00004055	-0.95113681	-4.85238527
N	0.00004629	-0.19252140	-6.06948066
C	0.00004573	1.17053523	-6.09099662
C	0.00003953	1.87582193	-4.92283098
C	0.00003377	1.10598853	-3.70179356
N	0.00002743	1.73624926	-2.49891463
O	0.00004144	-2.18152158	-4.91011509
H	0.00002338	1.18305134	-1.63846052
H	-0.00000888	2.29427998	4.68196811
H	0.00001020	3.96969731	0.71770587
H	-0.00000238	4.30493808	3.19226032
H	0.00000972	-3.89631683	1.57746305
H	0.00002230	-3.89895948	-0.92899383
H	0.00002733	-1.67830070	-2.14637987
H	-0.00001463	-2.38826244	6.28290416
H	-0.00000259	-3.52195842	3.99421208
H	0.00005087	-0.73232101	-6.92916989
H	0.00005040	1.64330236	-7.06807465
H	0.00003897	2.96078667	-4.91861623
H	0.00002670	2.74395378	-2.45113365
H	-0.00001360	0.12258675	5.83439362

P(H(Im))$^{+}$-C (COSMO), *E* = -5849.70 kcal mol^{-1}



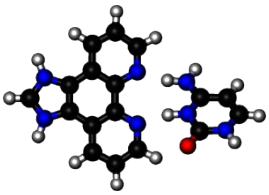
C	0.02386695	2.23435506	3.48368013
C	0.00087206	0.92913871	2.95060939
C	-0.18790906	0.75611248	1.54237693
N	-0.34474852	1.82254332	0.71522012
C	-0.31800989	3.04706519	1.24770903
C	-0.13706651	3.30678731	2.62275182
C	0.15478137	-0.25494912	3.73197048
C	0.12966907	-1.52389743	3.17911871
C	-0.05034768	-1.75055641	1.78257026
C	-0.21271902	-0.59334996	0.95792175
C	-0.06963971	-3.02791043	1.18529554
C	-0.24392035	-3.12195041	-0.18522445
C	-0.39450942	-1.93451578	-0.93007147
N	-0.38373680	-0.71644206	-0.38232542
N	0.34594898	-0.42408676	5.09610645
C	0.43449666	-1.73185382	5.37297243
N	0.30615951	-2.41504175	4.22776094
N	-0.20099137	-0.33275486	-3.86293973
C	-0.02184091	-0.82201608	-5.12072237
N	0.39260798	0.07537389	-6.12860545
C	0.60769923	1.40312962	-5.89044377
C	0.42867781	1.90392608	-4.63638461
C	0.02036105	0.97703659	-3.61214529
N	-0.16477933	1.40972964	-2.35007479
O	-0.20483407	-2.02511109	-5.43069247
H	-0.32021115	0.73543596	-1.57964655
H	0.16585851	2.38626104	4.55036039
H	-0.44750859	3.87729246	0.55532703
H	-0.12693333	4.32923417	2.98787033
H	0.05617616	-3.91716249	1.79708463
H	-0.25998378	-4.08519409	-0.68595646
H	-0.51317549	-1.95658794	-2.01164390
H	0.58196505	-2.16137794	6.34935005
H	0.32991524	-3.42670649	4.16152177
H	0.52809940	-0.30391380	-7.06062301
H	0.92137497	2.00036603	-6.73829850
H	0.59519483	2.95155520	-4.41133846
H	0.06086214	2.36693111	-2.11318409
H	0.40933452	0.31114484	5.79149840

P(H(Im))$^{+}$-C(H)$^{+}$, *E* = -5693.94 kcal mol^{-1}



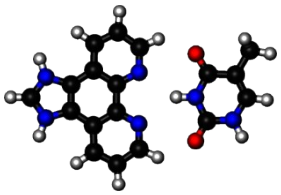
C	-2.48622669	2.92649562	0.44243540
C	-2.38211813	1.53444813	0.23756392
C	-1.09623794	0.95631076	-0.02158805
N	0.00445591	1.74557740	-0.11622463
C	-0.12241853	3.06023215	0.08589028
C	-1.34169608	3.70045189	0.38009507
C	-3.49507950	0.63896428	0.26198121
C	-3.36215440	-0.72414169	0.05094408
C	-2.09911119	-1.35172297	-0.17524241
C	-0.94833638	-0.49874487	-0.18473679
C	-1.93235213	-2.74065263	-0.36126418
C	-0.65599259	-3.24395086	-0.52829959
C	0.42859519	-2.34574852	-0.48399258
N	0.29535094	-1.02522840	-0.32271213
N	-4.85406716	0.87477479	0.46900576
C	-5.52980415	-0.28311499	0.38924714
N	-4.64572989	-1.26238603	0.13677360
N	3.03896047	-0.29824580	-0.00055347
C	3.78072045	-1.36127172	0.54552340
N	5.16904588	-1.13955486	0.51169681
C	5.74938624	-0.04689156	-0.06353446
C	4.99463475	0.94355153	-0.62826747
C	3.57614867	0.81282702	-0.58356420
N	2.72939418	1.71503646	-1.07923070
O	3.27115204	-2.37010751	0.98939651
H	1.99581661	-0.43592349	-0.03324098
H	-3.45049742	3.38718862	0.64688711
H	0.79060378	3.64863404	0.00669746
H	-1.37256513	4.77415688	0.53866723
H	-2.79226534	-3.40741740	-0.36497316
H	-0.47786325	-4.30563398	-0.66962421
H	1.44675629	-2.71986088	-0.54978717
H	-6.59724230	-0.40529504	0.50713821
H	-4.89804045	-2.24087425	0.03144522
H	5.73717682	-1.88163784	0.91526976
H	6.83404682	-0.01422062	-0.04233243
H	5.45573448	1.81286123	-1.08229917
H	3.09319043	2.53648478	-1.54682058
H	1.71253865	1.62325161	-0.88847047
H	-5.29029441	1.77382123	0.65194617

P(H(Im))$^{+}$-C(H)$^{+}$ (COSMO), *E* = -5852.87 kcal mol^{-1}



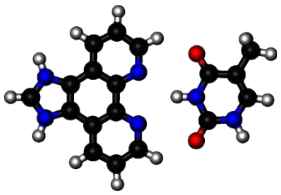
C	-2.44742164	2.90494272	0.52885370
C	-2.34980070	1.51963373	0.28791064
C	-1.06580319	0.94004219	0.04356196
N	0.04428866	1.72024539	-0.01022112
C	-0.07332167	3.03250937	0.21454827
C	-1.29440194	3.67048623	0.50509973
C	-3.47107112	0.64012787	0.25524632
C	-3.34722260	-0.71461122	0.00391891
C	-2.08541698	-1.34516472	-0.20532365
C	-0.92797063	-0.50666759	-0.15709082
C	-1.92870070	-2.72749818	-0.43340394
C	-0.65156228	-3.23909660	-0.58550122
C	0.44028587	-2.35665819	-0.48654665
N	0.31472286	-1.04167973	-0.28214793
N	-4.82445775	0.88881575	0.42446393
C	-5.50512977	-0.25582043	0.27947952
N	-4.63058343	-1.23874789	0.02652824
N	2.99628041	-0.29954773	0.04014804
C	3.77652825	-1.26987794	0.65410957
N	5.14547403	-1.07417026	0.50919810
C	5.69158120	-0.04843177	-0.21065799
C	4.90335598	0.87942306	-0.82408908
C	3.49085891	0.75203526	-0.68394964
N	2.61463380	1.59269238	-1.21790132
O	3.29696609	-2.22475416	1.26872506
H	1.94883074	-0.45656343	0.03652587
H	-3.41775203	3.35202458	0.72492710
H	0.84517388	3.61251968	0.15058773
H	-1.32045195	4.73998558	0.68729645
H	-2.80233875	-3.37167489	-0.48090186
H	-0.48215882	-4.29663073	-0.76024393
H	1.45864462	-2.73156267	-0.55436375
H	-6.57371109	-0.36776084	0.35280137
H	-4.88662276	-2.20864449	-0.12279698
H	5.74742076	-1.76066266	0.95422755
H	6.77319151	-0.02522520	-0.25011244
H	5.32170977	1.70163695	-1.39024271
H	2.95468147	2.39227423	-1.73878535
H	1.61810400	1.54644656	-0.91691989
H	-5.25152399	1.78957998	0.61330487

P(H(Im))$^{+}$-T, *E* = -6035.85 kcal mol^{-1}



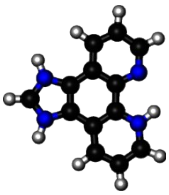
C	0.00102036	-2.82853381	-2.39069688
C	0.00053136	-1.42555856	-2.54467249
C	0.00146593	-0.60135057	-1.37329102
N	0.00257281	-1.13847659	-0.13469561
C	0.00295297	-2.46594728	-0.00940202
C	0.00227284	-3.35345569	-1.11093901
C	-0.00080236	-0.74353692	-3.79750014
C	-0.00096746	0.64279578	-3.90296838
C	-0.00002176	1.50616844	-2.76717474
C	0.00112865	0.86822313	-1.48459619
C	-0.00044557	2.91633751	-2.82613746
C	0.00023549	3.62798802	-1.63978298
C	0.00141322	2.91600899	-0.41726982
N	0.00186000	1.58518186	-0.34050460
N	-0.00221196	-1.23472506	-5.10288703
C	-0.00313775	-0.21250162	-5.97707127
N	-0.00243638	0.93038035	-5.26798851
N	0.00135590	0.39407831	2.78801681
C	0.00095605	1.68683578	3.30147858
N	-0.00130995	1.72728451	4.69617939
C	-0.00294950	0.60504869	5.50507574
C	-0.00233707	-0.65136228	4.99438041
C	0.00004498	-0.81240977	3.53518010
O	0.00098537	-1.90636700	2.96567027
O	0.00237634	2.71318183	2.62486716
C	-0.00401430	-1.89570753	5.84448263
H	0.00042506	-3.48398243	-3.26037937
H	0.00371691	-2.82927382	1.01513756
H	0.00269210	-4.42681625	-0.94337779
H	-0.00116143	3.43356437	-3.78459679
H	-0.00004225	4.71437314	-1.63621772
H	0.00200925	3.43306507	0.53881687
H	-0.00448107	-0.29461563	-7.05324243
H	-0.00298773	1.85720149	-5.68026406
H	0.00264786	0.30933453	1.76427329
H	-0.00164526	2.65748129	5.09871327
H	-0.00471061	0.80204729	6.57304198
H	-0.00578349	-1.64101664	6.91071529
H	0.87737013	-2.51198427	5.62278429
H	-0.88491121	-2.51157918	5.61976675
H	-0.00253478	-2.21348627	-5.36935671

P(H(Im))$^{+}$-T (COSMO), *E* = -6104.73 kcal mol^{-1}



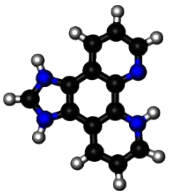
C	-0.03654799	-2.81769916	-2.43167790
C	-0.02080028	-1.41482483	-2.56851026
C	-0.04360933	-0.59791742	-1.39293657
N	-0.07310140	-1.14977785	-0.15223521
C	-0.08612846	-2.48223403	-0.05168225
C	-0.07159247	-3.35749729	-1.15793540
C	0.01999072	-0.73971047	-3.82407985
C	0.03414187	0.63988346	-3.92965137
C	0.00650402	1.49789937	-2.79047561
C	-0.03350268	0.86877845	-1.50473161
C	0.01569827	2.90542665	-2.86627315
C	-0.01468602	3.63180146	-1.68852406
C	-0.05475331	2.93355923	-0.46305797
N	-0.06461220	1.60126548	-0.36152955
N	0.05716104	-1.23505484	-5.11980033
C	0.09421673	-0.21264760	-5.98468212
N	0.08043607	0.93069498	-5.28612650
N	-0.02525557	0.38836107	2.83910188
C	-0.02030383	1.67625595	3.35996092
N	0.02996624	1.72416382	4.74300661
C	0.07199243	0.61044668	5.55126760
C	0.06411600	-0.64872784	5.04036218
C	0.00971982	-0.80759965	3.59089006
O	-0.00745982	-1.90938418	3.01582163
O	-0.05743776	2.70282835	2.66914149
C	0.10655510	-1.88604578	5.90086825
H	-0.02081024	-3.45331655	-3.31314879
H	-0.10626729	-2.87434013	0.95994744
H	-0.08513711	-4.43190311	-1.00115137
H	0.04628244	3.40027606	-3.83347781
H	-0.00900806	4.71772871	-1.69625721
H	-0.07953790	3.47640999	0.47667368
H	0.12815922	-0.29572659	-7.05787508
H	0.10292207	1.85414642	-5.70466762
H	-0.05591580	0.30393592	1.81237807
H	0.03402519	2.65028154	5.15732069
H	0.10881024	0.81271002	6.61580524
H	0.14092692	-1.61493511	6.96184708
H	0.98757103	-2.49602353	5.65878013
H	-0.77686952	-2.51350045	5.72004654
H	0.06268123	-2.21205351	-5.39099611

P(H(Im)H(N1))$^{2+}$, *E* = -3749.15 kcal mol^{-1}



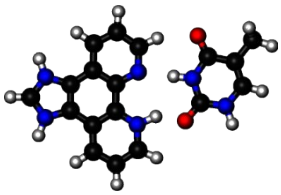
C	-2.92449815	0.16368291	0.00000041
C	-1.52749571	-0.04728783	0.00000038
C	-0.68494344	1.10355384	0.00000044
N	-1.15572841	2.36954024	0.00000053
C	-2.47709890	2.54422559	0.00000055
C	-3.39792925	1.46662734	0.00000050
C	-0.85864133	-1.31416796	0.00000030
C	0.52748162	-1.44759341	0.00000027
C	1.41090142	-0.31803491	0.00000033
C	0.75692794	0.94417900	0.00000042
C	2.82291976	-0.35234370	0.00000031
C	3.55326388	0.83305984	0.00000038
C	2.87555105	2.05592052	0.00000046
N	1.53020012	2.06950846	0.00000048
N	-1.37121618	-2.60951495	0.00000022
C	-0.36323508	-3.49678877	0.00000016
N	0.79288345	-2.81567794	0.00000019
H	-2.83433457	3.57167114	0.00000062
H	-4.46480362	1.67161262	0.00000052
H	3.35221877	-1.30255283	0.00000025
H	4.63866388	0.82628720	0.00000036
H	3.37538163	3.01938832	0.00000051
H	-0.46416927	-4.57414045	0.00000009
H	1.70733742	-3.26083843	0.00000015
H	1.00219527	2.95366564	0.00000054
H	-2.35490406	-2.86952372	0.00000022
H	-3.61982912	-0.67281480	0.00000037

P(H(Im)H(N1))$^{2+}$ (COSMO), *E* = -3924.35 kcal mol^{-1}



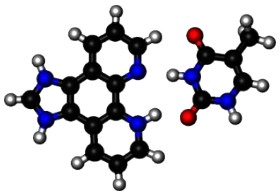
C	-2.91368314	0.14678905	0.00289360
C	-1.51575201	-0.03937713	0.00305799
C	-0.68178975	1.11700269	0.00228574
N	-1.17669960	2.37971700	-0.00235099
C	-2.50299597	2.52602589	-0.00541389
C	-3.40800738	1.44024723	-0.00206763
C	-0.85548476	-1.30522283	0.00337942
C	0.52538037	-1.43549726	0.00100401
C	1.40041316	-0.30962554	0.00088294
C	0.76005898	0.95673407	0.00233130
C	2.80832719	-0.37052403	-0.00299671
C	3.55295861	0.80224377	-0.00235836
C	2.89089323	2.03161421	0.00118462
N	1.54931768	2.06680562	0.00339691
N	-1.36735197	-2.59182214	0.00118946
C	-0.35692626	-3.47162764	-0.00212763
N	0.79671975	-2.79280373	-0.00201990
H	-2.87928037	3.54601590	-0.01157843
H	-4.47645983	1.63064385	-0.00441368
H	3.30431906	-1.33579496	-0.00673087
H	4.63601121	0.78281310	-0.00422197
H	3.39756627	2.98717697	0.00215575
H	-0.45493432	-4.54403139	-0.00792586
H	1.71437572	-3.22586680	-0.00699261
H	1.06090378	2.96527709	0.00653883
H	-2.34841661	-2.84994498	-0.00100465
H	-3.58074296	-0.71034111	0.00670624

P(H(Im)H(N1))$^{2+}$-T, *E* = -5938.28 kcal mol^{-1}



C	-0.00185810	-2.99396636	-1.91852992
C	-0.00128181	-1.63669060	-2.30890413
C	-0.00116408	-0.62872310	-1.29225609
N	-0.00112585	-0.95490819	0.02064173
C	-0.00141050	-2.24649075	0.37039362
C	-0.00191004	-3.30083126	-0.57012220
C	0.00012742	-1.18381026	-3.66362362
C	0.00078448	0.15915529	-4.01027858
C	-0.00088257	1.20529827	-3.03436639
C	-0.00115595	0.78340946	-1.66909345
C	-0.00264432	2.58255963	-3.34358711
C	-0.00449799	3.52336830	-2.32490993
C	-0.00346106	3.07217694	-1.00143117
N	-0.00180334	1.76007891	-0.71294560
N	0.00168056	-1.89630209	-4.86149822
C	0.00386113	-1.04007292	-5.89604700
N	0.00319176	0.20870073	-5.40358919
N	-0.00061587	0.09407699	2.77478688
C	0.00252951	1.45439520	2.86332909
N	0.00462665	1.94750018	4.13825007
C	0.00396915	1.12137251	5.26492084
C	0.00121747	-0.23471778	5.18061927
C	-0.00104827	-0.84591118	3.84700744
O	-0.00305099	-2.04734317	3.58872597
O	0.00355266	2.18954607	1.84074786
C	0.00073536	-1.14353083	6.38117682
H	-0.00215177	-3.78644730	-2.66405674
H	-0.00148735	-2.45104099	1.44438053
H	-0.00230364	-4.33079981	-0.22528684
H	-0.00304598	2.91147118	-4.38046466
H	-0.00690480	4.58849415	-2.53307064
H	-0.00437611	3.72941300	-0.13786477
H	0.00630224	-1.30851389	-6.94374688
H	0.00473440	1.04325506	-5.98388075
H	-0.00163140	-0.26587136	1.81492456
H	0.00715884	2.95713450	4.24318230
H	0.00593647	1.64803878	6.21364147
H	0.00276530	-0.56634677	7.31184387
H	0.88127478	-1.79889889	6.35968664
H	-0.88223775	-1.79568174	6.36148773
H	-0.00033729	1.58440837	0.35598330
H	0.00194488	-2.90818503	-4.96161864

P(H(Im)H(N1))$^{2+}$-T (COSMO), *E* = -6104.45 kcal mol^{-1}



C	0.27891357	-2.97266105	-1.93161450
C	0.14540281	-1.62190549	-2.31321569
C	0.14238665	-0.61496735	-1.29999583
N	0.23811463	-0.93365448	0.01729843
C	0.35960669	-2.22202818	0.35096104
C	0.39334893	-3.27388719	-0.58717199
C	0.00449444	-1.18517835	-3.66280097
C	-0.13365618	0.14779185	-4.00907909
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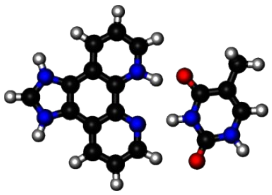
P(H(Im)H(N10))$^{2+}$-T, *E* = -5939.98 kcal mol^{-1}



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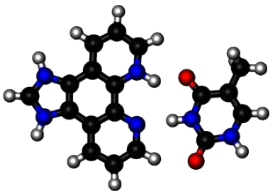
P(H(Im)H(N10))$^{2+}$-T (COSMO), *E* = -6104.69 kcal mol^{-1}



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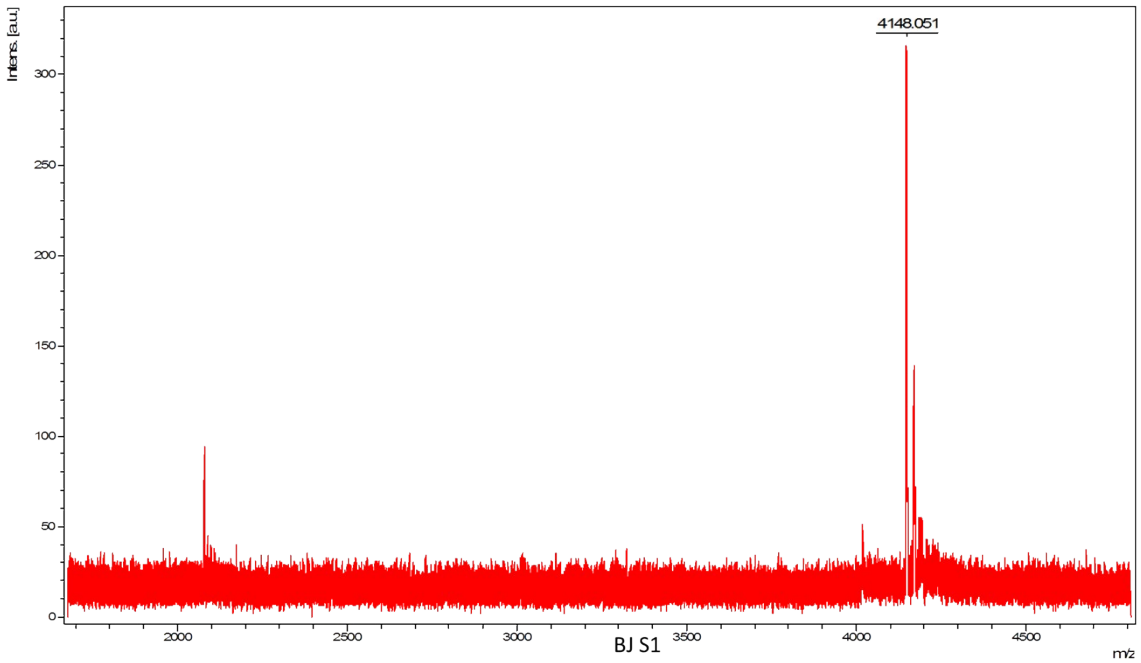
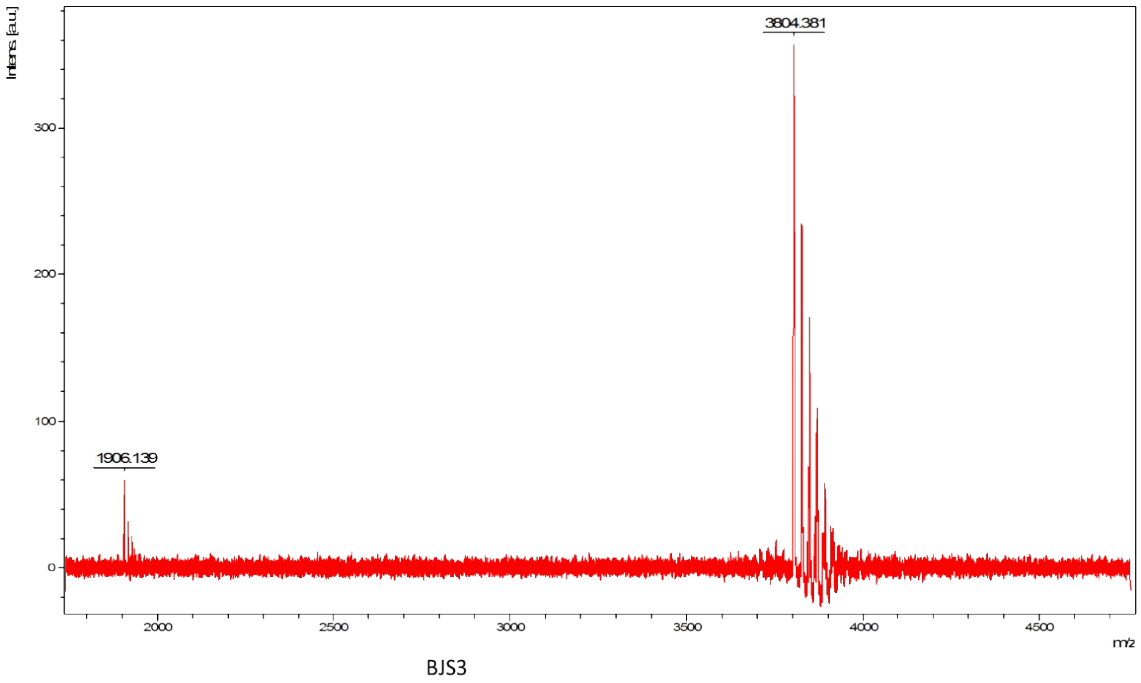
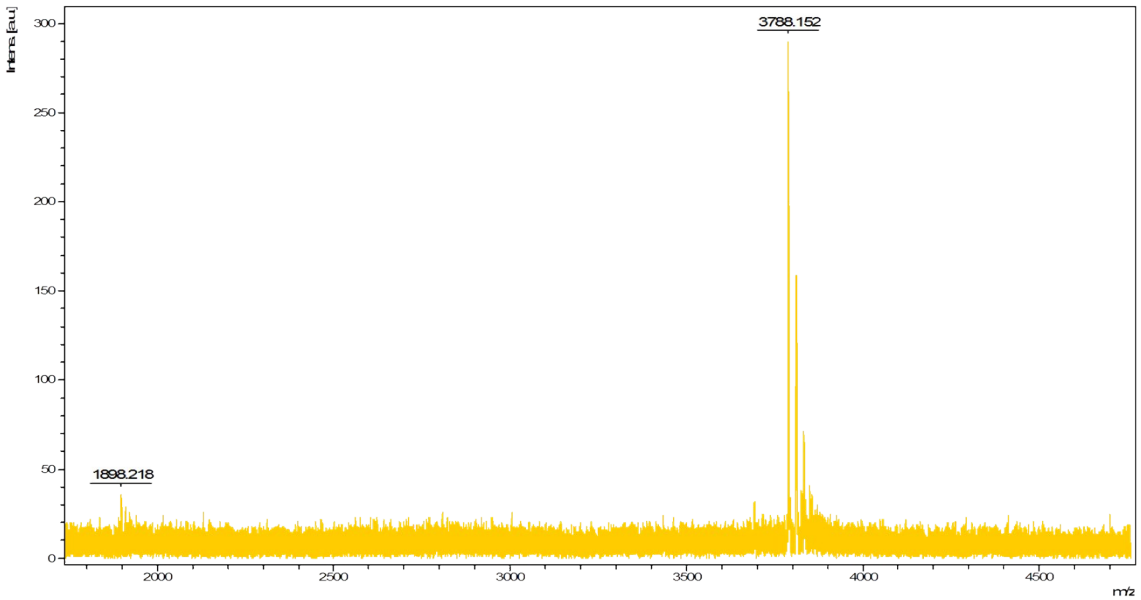


MALDI mass spectrum of 5'-d(GAGGGA**P**AGAAAG).



MALDI mass spectrum of 5'-d(CTTTCT**T**TCCCTC).



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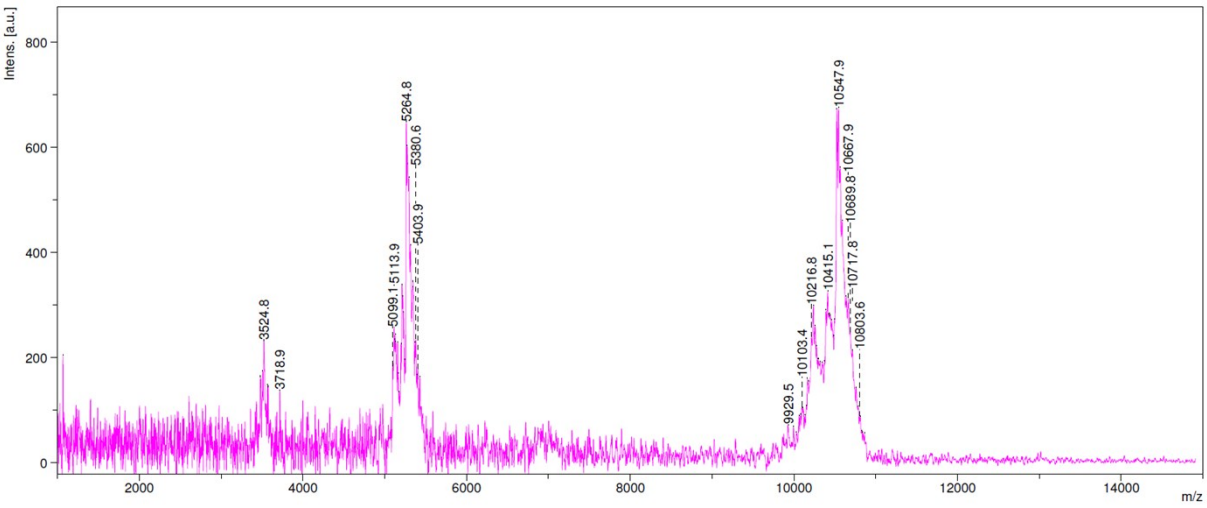
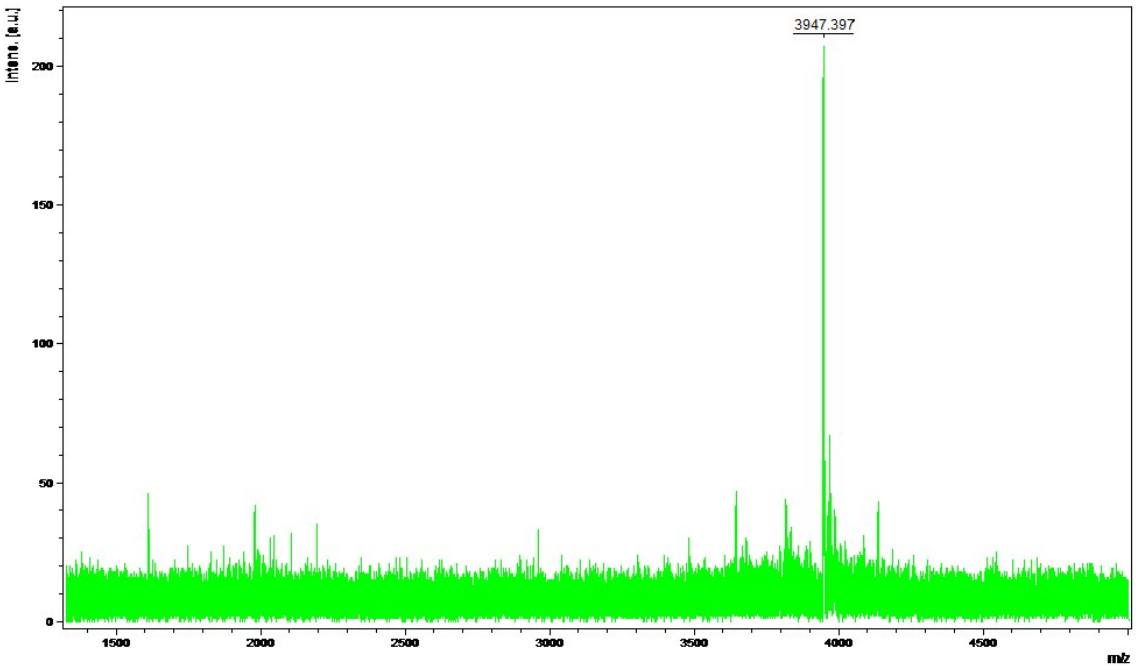
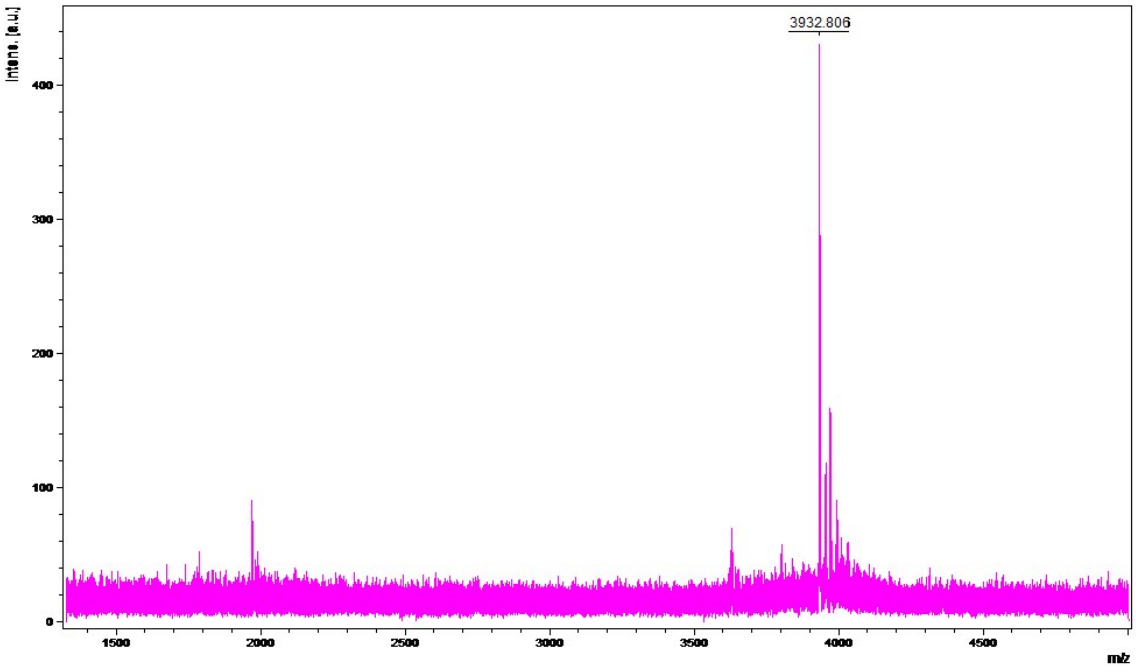
MALDI mass spectrum of 5’-d(CTTTCT**C**TCCCTC).



MALDI mass spectrum of 5’-d(dabcyl-CCTAGCACTAAATCT**P**CATGGTCGCGCTAGG-FAM).



MALDI mass spectrum of 5’-d(ACCATG**T**AGATTT).



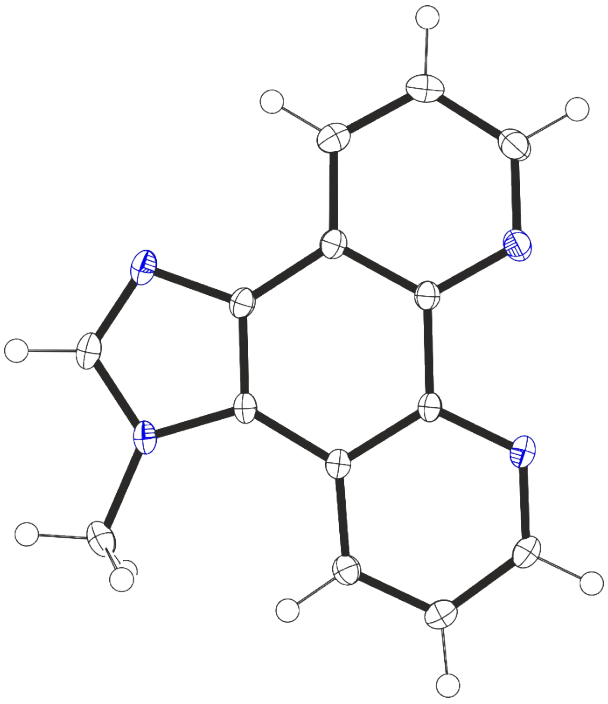
MALDI mass spectrum of 5’-d(ACCATG**C**AGATTT).

Synthesis and characterization of compound 1.

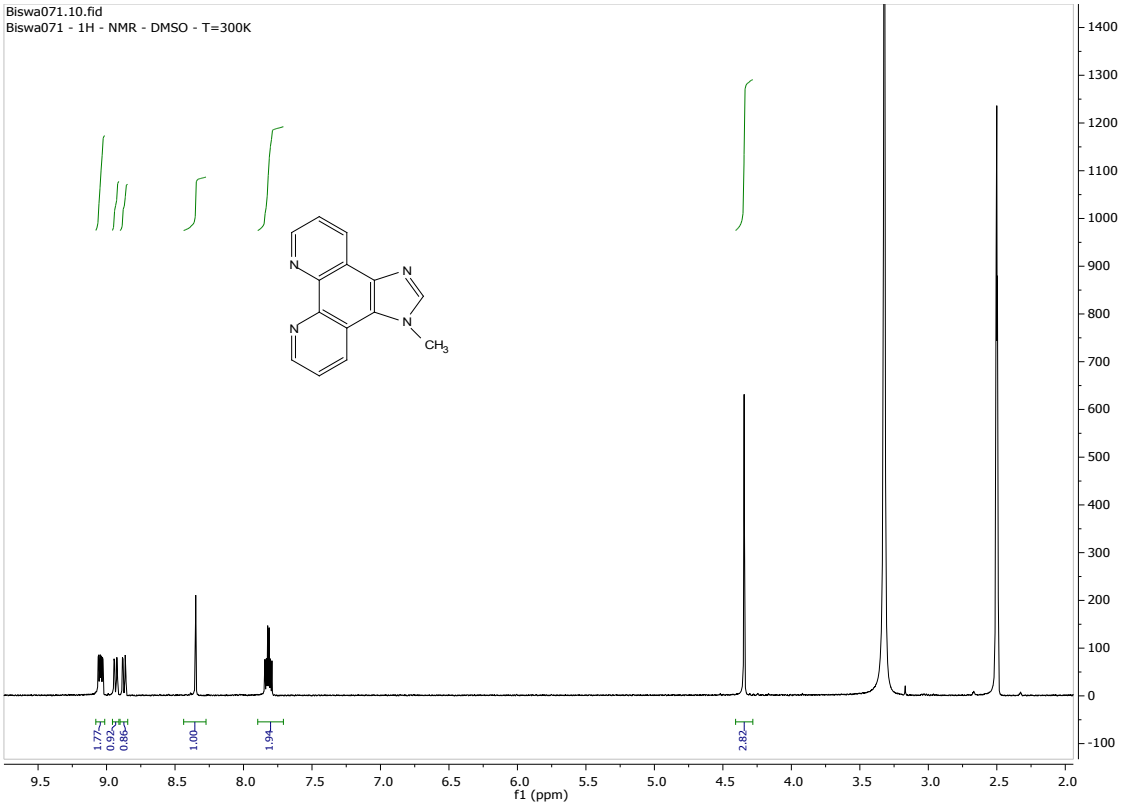
750 mg (3.4 mmol) of 1*H*-imidazo[4,5-*f*][1,10]phenanthroline[13] were suspended in dry acetonitrile and 272 mg (6.8 mmol) of NaH (60% in mineral oil) were added. The suspension was stirred at 0 °C for 30 min. After that, 316 µL (5.1 mmol) of methyl iodide were added and the resultant mixture was refluxed at 80 °C for 2 h. The solvent was evaporated to dryness and the product purified by flash column chromatography using 1% triethylamine in methanol as eluent. The product was obtained as a light brown solid with a yield of 621 mg (78%). The product was crystallized by the vapor diffusion method, dissolving the compound in methanol with *n*-hexane as antisolvent.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.07-9.02 (m, 2H, H2, H9), 8.93 (dd, J = 8.4, 1.7 Hz, 1H, H4), 8.87 (dd, J = 8.1, 1.8 Hz, 1H, H7), 8.35 (s, 1H, H_{im}), 7.85-7.78 (m, 2H, H3, H8), 4.34 (s, 3H, CH_3) ppm. ^{13}C NMR (101 MHz, DMSO-d_6): δ = 147.9, 147.3, 144.5, 129.4, 129.2, 123.5, 122.8, 34.8 ppm. HRMS: m/z $[M+H]^+$ calcd.: 235.0984, found: 235.0985.

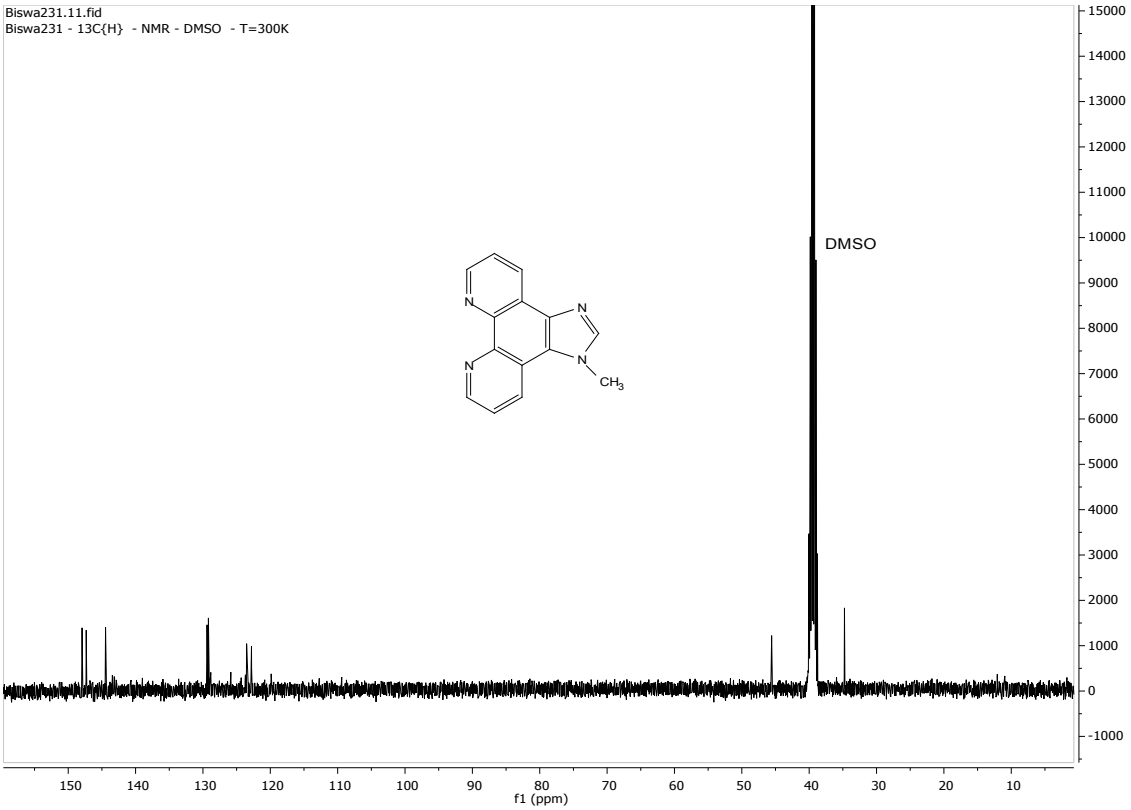
Crystallographic data and data collection and refinement details: empirical formula: $C_{14}H_{10}N_4$; formula weight: 234.26; crystal system: monoclinic; space group: $P2_1/n$; a: 9.3816(4) Å; b: 6.7781(3) Å; c: 16.9307(6) Å; β: 99.515(1)°; V: 1061.80(8) Å^3; Z: 4; ρ_{calcd}: 1.47 g cm^{-3}; μ(MoK_α): 0.09 mm^{-1}; crystal size: (0.18×0.10×0.09) mm^3; T: 100(2) K; θ range: 2.44–30.05°; hkl range: –13:13, –9:9, –23:23; Total/unique data/R_{int}: 16254/3118/0.031; observed data [$I > 2\sigma(I)$]: 2477; N_{ref}/N_{par}: 3118/164; R_1/wR_2 [$I > 2\sigma(I)$]: 0.0470/0.1287; R_1/wR_2 (all data): 0.0617/0.1397; S: 1.044; min./max. residual density: –0.31/0.48 e Å^{-3}; CCDC no.: 1489603.



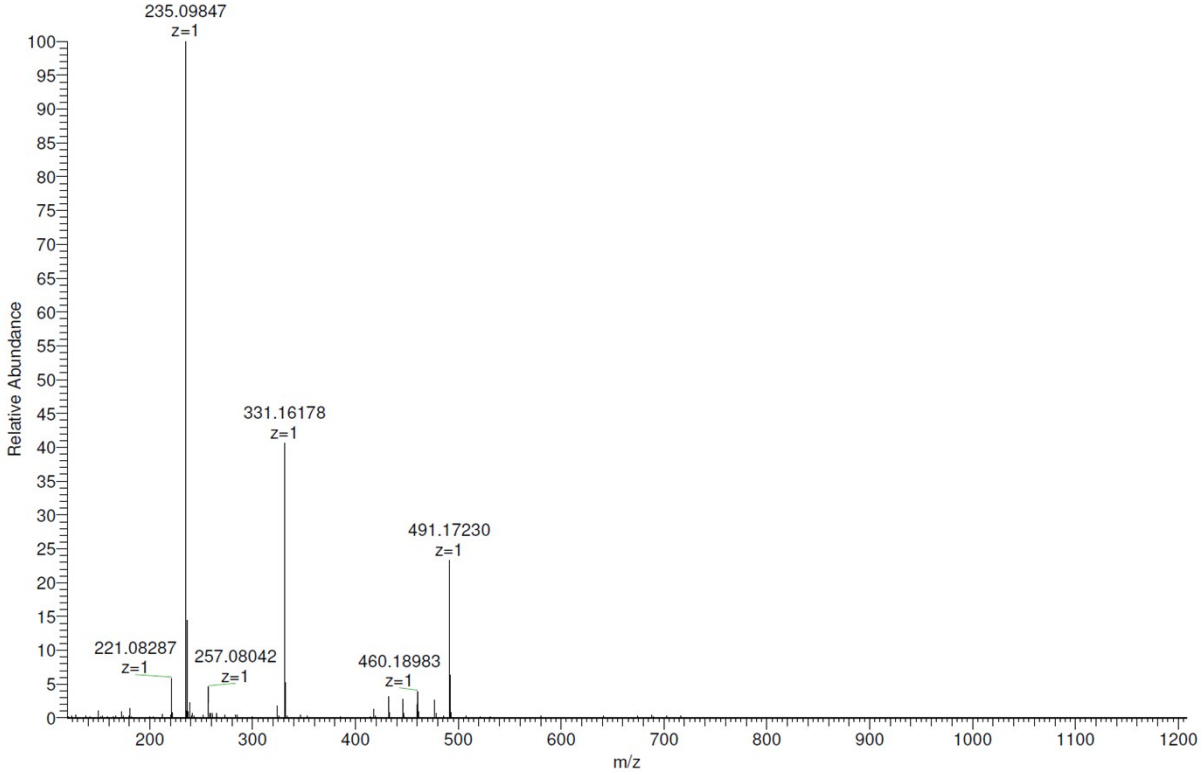
Molecular structure of compound **1**.



^{1}H NMR spectrum of compound **1** (400 MHz, DMSO-d_6).



^{13}C NMR spectrum of compound **1** (101 MHz, DMSO-d_6).

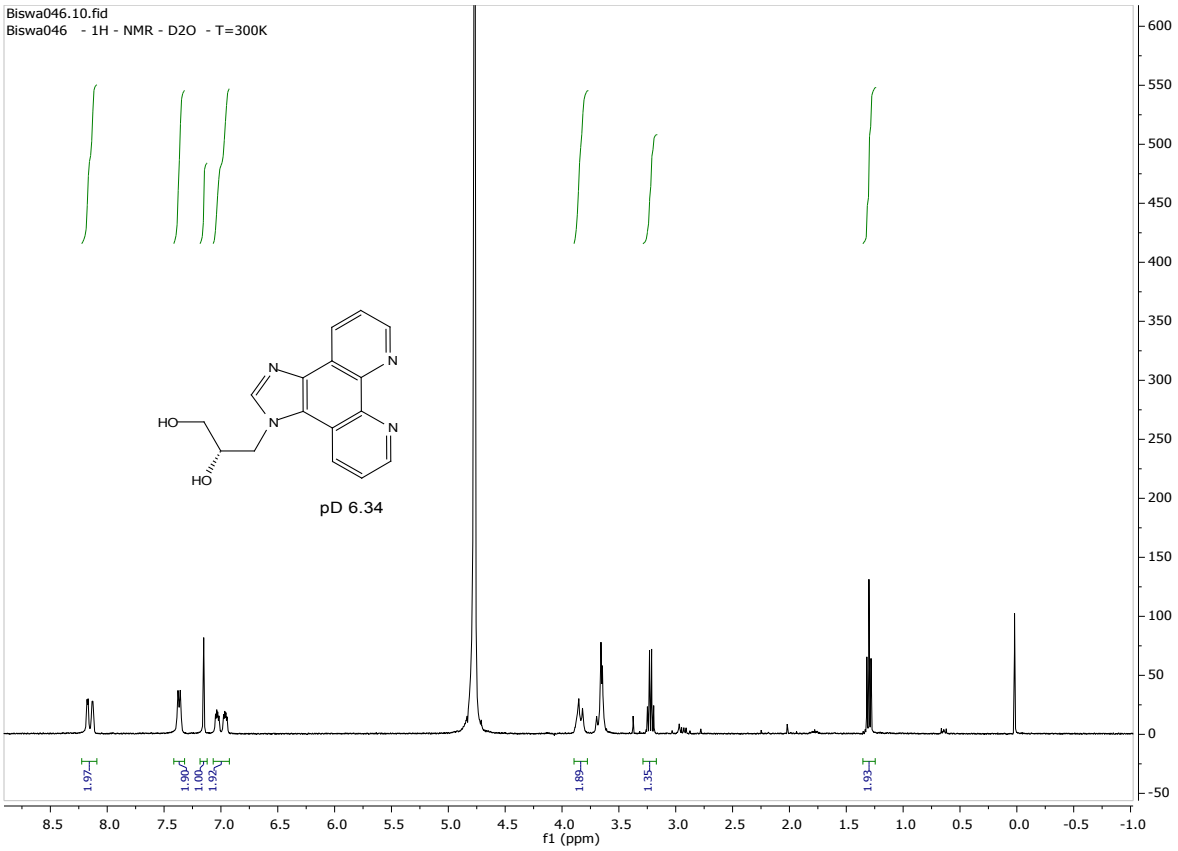


High-resolution mass spectrum of compound **1** (in CH_3OH).

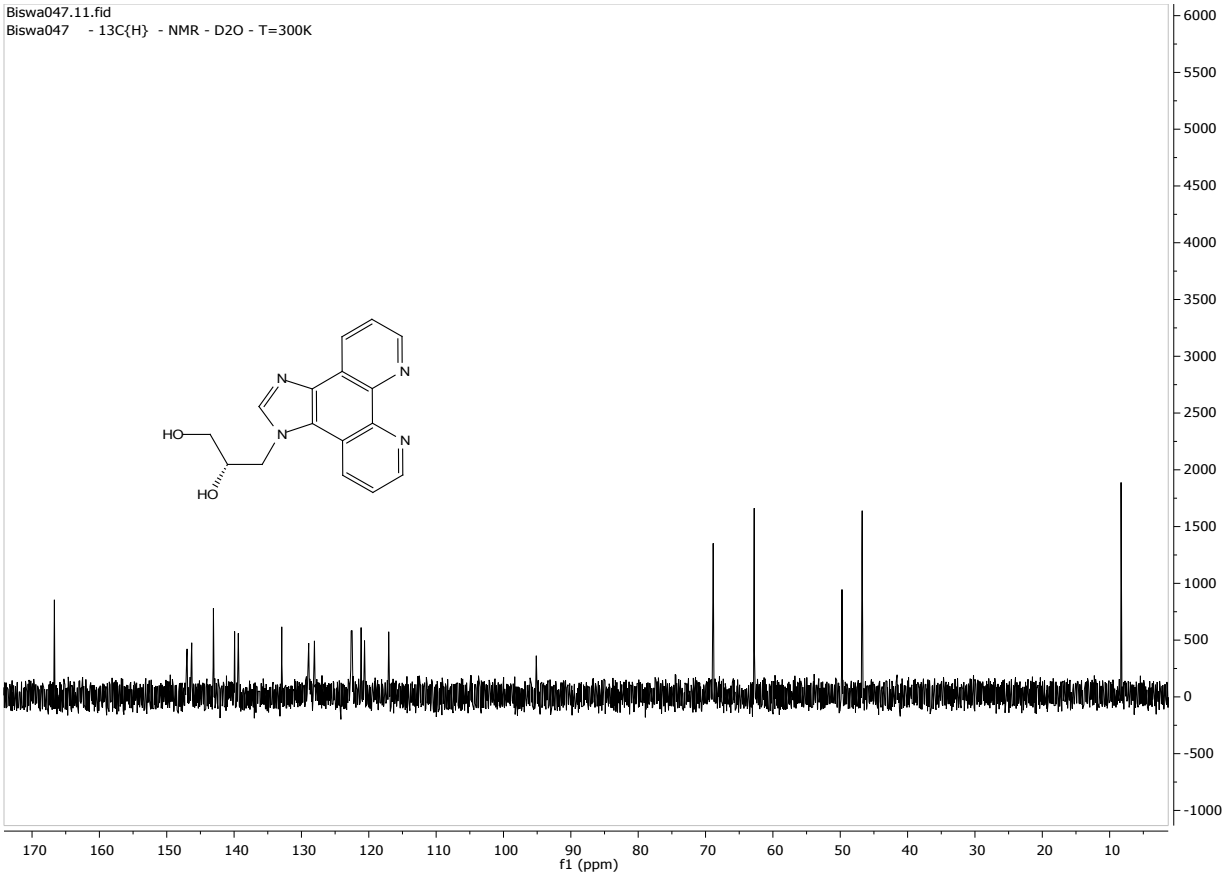
Characterization of compound P.

(*S*)-3-(1*H*-Imidazo[4,5-*f*][1,10]phenanthrolin-1-yl)propane-1,2-diol (compound **P**) was prepared as reported previously.[14]

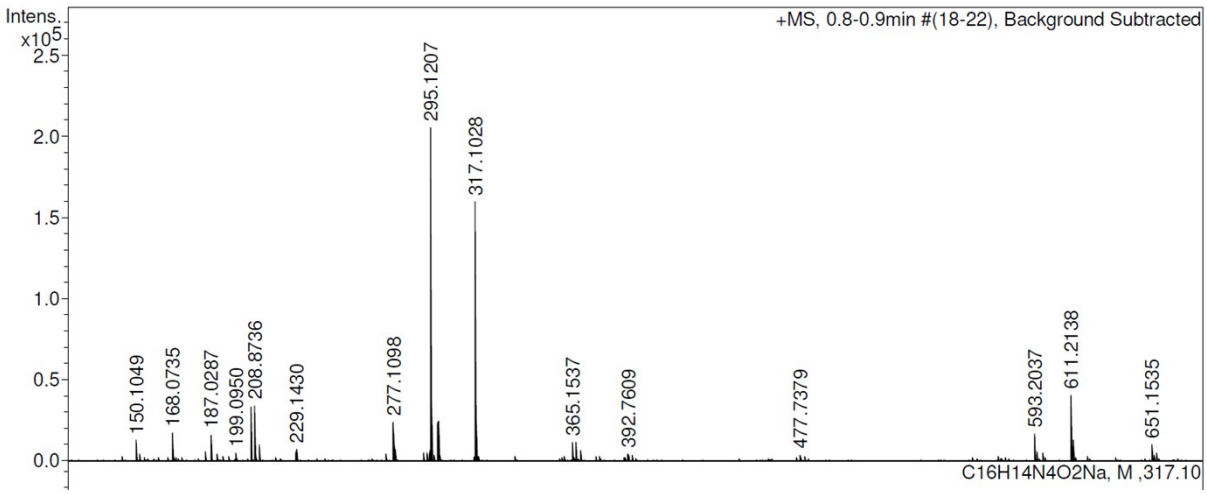
^{1}H NMR (400 MHz, D_2O, pD 6.3): δ = 8.15 (dd, *J* = 17.3, 4.1 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.15 (s, 1H), 7.00 (ddd, *J* = 28.5, 7.9, 4.1 Hz, 2H), 3.84 (d, J = 14.3 Hz, 2H), 3.22 (q, *J* = 7.3 Hz, 1H), 1.30 (t, *J* = 7.3 Hz, 2H) ppm. ^{13}C NMR (101 MHz, D_2O, pD 6.3): δ = 166.7, 147.0, 146.3, 143.1, 139.9, 139.4, 132.9, 128.9, 128.1, 122.5, 121.4, 120.6, 117.0, 68.9, 62.8, 49.7 ppm. HRMS: m/z $[M+H]^+$ calcd.: 295.1195, found: 295.1207.



^{1}H NMR spectrum of compound **P** (400 MHz, D_2O, pD 6.3).



^{13}C NMR spectrum of compound **P** (101 MHz, D_2O, pD 6.3).



High-resolution mass spectrum of compound **P** (in CH_3OH).

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