Supporting Information

To be published in: New Journal of Chemistry
Manuscript ID: NJ-ART-01-2015-000120

Physicochemical properties of the ternary complexes of Pt(II) with uracil and small peptide moieties: an experimental and computational study

Shilpi Mandal[a], Gunajyoti Das*[b] and Hassan Askari[a]

[a]*Centre of Advanced Study and Department of Chemistry, North-Eastern Hill University, Shillong-793022, Meghalaya, India.*
[b]*Department of Chemistry, Central Institute of Technology, Kokrajhar-783370, BTAD, Assam, India.*
*E-mail: guna_das@yahoo.co.in

Contents:

Table S1. ZPVE corrected values (scaled with 0.97) of total electronic energies[a] (E_c) and Gibbs free energies (G_c) of the systems studied in gas and aqueous phase at B3PW91 level.

Table S2. NPA charges on some chemically meaningful atoms of the ligands and the metal complexes calculated at B3PW91 level in aqueous phase.

Table S3 Experimental and calculated IR spectral data (frequencies are in cm^{-1}) of the Pt(II) complexes (theoretical gas phase values are in parentheses)

Table S4. Calculated bond lengths (in angstrom), bond angles and dihedral angles (in degrees) of the ligands and the metal complexes calculated at B3PW91 level in vacuum and aqueous environment.

Table S5. DNA binding-affinities of the three ternary complexes of Pt(II)

Fig. S1 Experimental UV-vis spectrum of CT-DNA in aqueous phase

Fig. S2 TG/DTA curves of the metal complexes prepared in solid state

Fig. S3 Mass spectrum of the metal complexes prepared by solid state technique

Fig. S4 The potential energy surfaces corresponding to the three dihedrals α_1, α_2 and α_3 of zwitterion *l*-alanyl-*l*-glutamine at B3PW91/6-31++G(d,p) level in the aqueous phase

Fig. S5 B3PW91/6-31++G(d,p) level optimized structures of the seven possible conformers of zwitterion *l*-alanyl-*l*-glutamine corresponding to the three dihedrals α_1, α_2 and α_3 in aqueous phase (energy in Hartree)

Fig. S6 Experimental FT-IR spectra of the ligands and their ternary complexes with Pt(II)

Fig. S7 Experimental UV-vis spectra of the synthesized complexes in deionized water

Fig. S8 Theoretical UV-vis spectra of the complexes in gas and aqueous phases

► Cartesian coordinates of the optimized structures of the ligands their metal complexes in gas and aqueous phases using the B3PW91 level of theory

Table S1. ZPVE corrected values (scaled with 0.97) of total electronic energies[a] (E_c) and Gibbs free energies (G_c) of the systems studied in gas and aqueous phase at B3PW91 level.

Systems	Phases	E_c	G_c	E_c[b]	G_c[b]
Ura	Aqueous	-414.619174	-414.562066	-414.781257	-414.724633
	Gas	-414.601344	-414.544340	-414.763147	-414.706643
GV	Aqueous	-609.991018	-609.809153	-610.223776	-610.042676
	Gas	-609.972580	-609.791439	-610.205853	-610.025700
AG	Aqueous	-778.627827	-778.422084	-778.926281	-778.720530
	Gas	-778.598825	-778.394370	-778.897785	-778.694373
GL	Aqueous	-649.025580	-649.060411	-649.515052	-649.307296
	Gas	-649.248983	-649.041982	-649.496594	-649.290600
Pt(Ura)(GV)	Aqueous	-1142.644650	-1142.405060	-1142.989276	-1142.751281
	Gas	-1142.595199	-1142.356582	-1142.938910	-1142.702006
Pt(Ura)(GV)[c]	Aqueous	-1142.598921	-1142.363241	------	------
Pt(Ura)(AG)	Aqueous	-1311.277350	-1311.013695	-1311.687335	-1311.426340
	Gas	-1311.222364	-1310.959816	-1311.631179	-1311.370387
Pt(Ura)(GL)	Aqueous	-1181.676176	-1181.653861	-1182.278333	-1182.014216
	Gas	-1181.869852	-1181.604912	-1182.227688	-1181.964280

[a]energies in Hartrees; [b]at B3LYP level; [c]triplet.

Table S2. NPA charges on some chemically meaningful atoms of the ligands and the metal complexes calculated at B3PW91 level in aqueous phase.

Ura		GV		AG	GL		Pt(Ura)(GV)	Pt(Ura)(AG)	Pt(Ura)(GL)
Atoms	Charges	Atoms	Charges	Charges	Charges	Atoms	Charges	Charges	Charges
N_{15}	-0.621	N_6	-0.821	-0.819	-0.821	Pt	0.843	0.854	0.840
N_{10}	-0.664	O_7	-0.815	-0.793	-0.811	N_6	-0.852	-0.853	-0.854
O_{11}	-0.662	O_8	-0.747	-0.767	-0.752	N_{10}	-0.653	-0.651	-0.654
O_{16}	-0.674	C_1	0.803	0.811	0.800	O_7	-0.786	-0.779	-0.792
C_{16}	0.813	C_2	-0.177	-0.179	-0.181	O_{11}	-0.671	-0.669	-0.670
C_{12}	0.643	N_3	-0.642	-0.652	-0.646	O_8	-0.672	-0.689	-0.670
C_{13}	-0.407	$H(N_3H)$	0.446	0.443	0.444	C_1	0.824	0.833	0.819
$H(C_{13}H)$	0.282	C_4	0.658	0.671	0.660	C_2	-0.167	-0.171	-0.169
		$O (C_4O)$	-0.655	-0.645	-0.653	N_3	-0.658	-0.663	-0.660
		C_5	-0.343	-0.155	-0.345	$H(N_3H)$	0.463	0.457	0.465
						$H(N_3H)$	0.463	0.457	0.465
						C_4	0.679	0.689	0.679
						$O (C_4O)$	-0.668	-0.662	-0.667
						C_5	-0.350	-0.164	-0.350

Atomic charges in a. u.

Table S3 Experimental and calculated IR spectral data (frequencies are in cm^{-1}) of the Pt(II) complexes (theoretical gas phase values are in parentheses)

Systems			v(N$_3$-H)	v$_{as}$(N-H)	v$_s$(N-H)	v(C$_4$=O)	v$_{as}$(COO$^-$)	v$_s$(COO$^-$)	v(C$_5$-N$_6$)	v(C$_4$-N$_3$)	v(M-O)	v(M-N)	Δδ
GV	Expt.	A	3428	3251	3071	1689	1625	1406	1132	1228	------	------	219
	Theori.	I	3477 (3482)	3401 (3405)	3332 (3321)	1713 (1753)	1645 (1765)	1344 (1326)	1035 (1068)	1258 (1248)	------	-------	301 (439)
		II	3455 (3462)	3379 (3382)	3315 (3307)	1691 (1732)	1630 (1748)	1358 (1329)	1050 (1078)	1231 (1227)	------	-------	272 (419)
Pt(Ura)(GV)	Expt.	A	3431	3252	3131	1695	1645	1400	1127	1234	527w	480w	245
		B	3436	3259	3116	1717	1649	1400	1124	1236	545s	477w	249
	Theori.	I	3476 (3464)	3422 (3465)	3354 (3376)	1713 (1728)	1683 (1748)	1312 (1318)	1056 (1044)	1206 (1190)	544 (558)	460 (481)	371 (430)
		II	3455 (3442)	3391 (3436)	3328 (3353)	1691 (1745)	1657 (1726)	1320 (1303)	1041 (1029)	1201 (1182)	535 (552)	452 (442)	337 (423)
AG	Expt.	A	3430	3230	3110	1687	1603	1454	1130	1230	------	-------	149
	Theori	I	3468 (3480)	3394 (3392)	3323 (3310)	1712 (1751)	1642 (1746)	1361 (1327)	1045 (1089)	1281 (1213)	------	-------	281 (419)
		II	3450 (3463)	3374 (3370)	3308 (3295)	1677 (1729)	1605 (1729)	1372 (1356)	1088 (1130)	1209 (1210)	------	-------	233 (373)
Pt(Ura)(AG)	Expt.	A	3435	3232	3176	1717	1667	1419	1124	1237	546s	477w	248
		B	3429	3237	3116	1718	1664	1419	1123	1237	546s	475w	245
	Theori.	I	3480 (3461)	3406 (3454)	3338 3369)	1711 (1722)	1666 (1729)	1316 (1306)	1121 (1031)	1218 (1242)	540 (541)	475 (470)	350 (423)
		II	3459 (3439)	3379 (3425)	3368 (3388)	1690 (1740)	1642 (1705)	1323 (1308)	1027 (1092)	1246 (1215)	533 (537)	471 (476)	319 (397)
GL	Expt.	A	3443	3236	3067	1691	1626	1440	1102	1229	-----	------	186
	Theori.	I	3463 (3476)	3383 (3405)	3333 (3322)	1716 (1756)	1642 (1761)	1322 (1361)	1016 (1021)	1249 (1249)	------	------	320 (400)
		II	3446 (3456)	3375 (3383)	3319 (3308)	1694 (1734)	1629 (1742)	1362 (1363)	1036 (1075)	1259 (1239)	------	------	267 (379)
Pt(Ura)(GL)	Expt.	A	3449	3250	3120	1717	1650	1419	1097	1237	545s	475w	231
		B	3434	3242	3121	1717	1645	1418	1093	1236	545s	473w	227
	Theori.	I	3475 (3460)	3422 (3464)	3354 (3381)	1713 (1728)	1683 (1748)	1329 (1333)	1067 (1061)	1197 (1221)	551 (552)	453 (447)	354 (415)
		II	3453 (3438)	3388 (3436)	3326 (3353)	1691 (1745)	1656 (1726)	1333 (1363)	1021 (1013)	1224 (1217)	546 (547)	446 (439)	323 (363)

			v(N$_{15}$-H)	v(N$_{10}$-H)	v(C$_{12}$=O)	v(C$_{16}$=O)	v(N$_{15}$-H)*	v(N$_{10}$-H)*	v(C$_{12}$=O)*	v(C$_{16}$=O)*
Ura	Expt.	A	3447	3413	1735	1765	3381-3395	------	1602-1636	1725-1740
		B					3382-3385	------	1602-1670	1728-1739
	Theori.	I	3480 (3506)	3458 (3466)	1658 (1694)	1708 (1725)	3471-3475 (3488-3490)	------	1716-1717 (1629-1630)	1703-1705 (1755-1756)
		II	3459 (3483)	3437 (3444)	1681 (1753)	1732 (1747)	3450-3455 (3466-3467)	------	1677-1678 (1731-1733)	1719-1726 (1746-1751)

A=Solid state; B= Solution phase products; I= at B3PW91; II= B3LYP; w=weak; s=strong. For theoretical data, the frequencies below 1,800 cm^{-1} are scaled with 0.977 and for those above 1,800 cm^{-1} a correction factor 0.955 is used

Table S4. Calculated bond lengths (in angstrom), bond angles and dihedral angles (in degrees) of the ligands and the metal complexes calculated at B3PW91 level in vacuum and aqueous environment.

Bond Distance	GV	Pt(Ura)(GV)	MD^A	AG	Pt(Ura)(AG)	MD^B	GL	Pt(Ura)(GL)	MD^C
C_1–C_2	1.568 (1.551)	1.557 (1.559)	0.011 (0.008)	1.562 (1.547)	1.555 (1.557)	0.007 (0.010)	1.561 (1.546)	1.555 (1.556)	0.006 (0.010)
C_2–N_3	1.463 (1.459)	1.473 (1.481)	0.010 (0.022)	1.462 (1.456)	1.469 (1.479)	0.007 (0.023)	1.463 (1.459)	1.472 (1.481)	0.009 (0.008)
N_3-H	1.011 (1.010)	1.010 (1.010)	0.001 (0.000)	1.011 (1.010)	1.011 (1.011)	0.000 (0.001)	1.011 (1.010)	1.011 (1.011)	0.000 (0.001)
C_4–N_3	1.354 (1.368)	1.362 (1.374)	0.008 (0.006)	1.356 (1.370)	1.364 (1.378)	0.008 (0.008)	1.356 (1.370)	1.364 (1.375)	0.008 (0.005)
C_4=O	1.229 (1.222)	1.229 (1.219)	0.000 (0.003)	1.228 (1.221)	1.229 (1.219)	0.001 (0.002)	1.229 (1.221)	1.229 (1.218)	0.000 (0.003)
C_4–C_5	1.527 (1.527)	1.524 (1.532)	0.003 (0.005)	1.536 (1.534)	1.531 (1.538)	0.005 (0.004)	1.527 (1.527)	1.523 (1.532)	0.004 (0.005)
C_5-N_6	1.502 (1.472)	1.494 (1.494)	0.008 (0.022)	1.518 (1.479)	1.501 (1.501)	0.017 (0.022)	1.503 (1.472)	1.493 (1.493)	0.010 (0.021)
C_1-O_7	1.282 (1.345)	1.315 (1.329)	0.033 (0.016)	1.273 (1.337)	1.307 (1.318)	0.034 (0.019)	1.281 (1.343)	1.316 (1.330)	0.035 (0.013)
C_1-O_8	1.242 (1.207)	1.224 (1.212)	0.018 (0.005)	1.250 (1.212)	1.229 (1.218)	0.021 (0.006)	1.244 (1.208)	1.224 (1.212)	0.020 (0.004)
Pt–O_7	--------	2.051 (2.022); *0.390 (0.434)	--------	--------	2.052 (2.024); *0.375 (0.418)	--------	--------	2.053 (2.021); *0.385 (0.432)	--------
Pt–O_{11}	--------	2.092 (2.106); *0.371 (0.351)	--------	--------	2.082 (2.099); *0.382 (0.361)	--------	--------	2.091 (2.105); *0.375 (0.352)	--------
Pt–N_6	--------	2.091 (2.099); *0.414 (0.368)	--------	--------	2.091 (2.099); *0.410 (0.369)	--------	--------	2.090 (2.100); *0.416 (0.368)	--------
Pt–N_{10}	--------	2.053 (2.028); *0.413 (0.446)	--------	--------	2.053 (2.029); *0.415 (0.447)	--------	--------	2.057 (2.028); *0.411 (0.447)	--------
Bond Angle									
N_3–C_2–C_1	109.1 (110.7)	105.7 (105.7)	3.4 (5.0)	109.9 (111.4)	106.6 (106.4)	3.3 (5.0)	110.3 (112.1)	106.6 (106.4)	3.7 (5.7)
C_4-C_5-N_6	104.3 (105.6)	109.1 (110.7)	4.8 (5.1)	104.1 (103.8)	107.1 (108.8)	3.0 (5.0)	104.4 (105.1)	108.9 (110.6)	4.5 (5.5)
C_2-C_1-O_7	117.3 (117.1)	110.8 (109.8)	6.5 (7.3)	117.8 (117.6)	111.5 (110.2)	6.3 (7.4)	118.3 (117.9)	111.4 (110.1)	6.9 (7.8)
C_2-N_3-C_4	121.5 (123.1)	119.8 (118.8)	1.7 (4.3)	120.7 (122.0)	119.0 (118.1)	1.7 (3.9)	121.6 (123.2)	119.4 (118.6)	2.2 (4.6)
N_3–C_4–C_5	113.7 (113.4)	115.7 (115.8)	2.0 (2.4)	115.2 (114.5)	116.7 (116.8)	1.5 (2.3)	113.6 (113.2)	115.8 (115.8)	2.2 (2.6)
Dihedrals									
C_2-N_3-C_4-C_5	140.6 (151.8)	138.2 (135.8)	2.4 (16)	141.1 (149.7)	139.6 (136.9)	1.5 (12.8)	139.8 (150.8)	138.4 (135.6)	1.4 (15.2)
H-N_3-C_4-O	-179.0 (-177.7)	180.0 (-177.1)	1.0 (0.6)	-178.8 (-175.0)	-178.3 (-175.4)	0.5 (0.4)	-178.4 (-176.1)	-179.2 (-176.3)	0.8 (0.2)
C_1-C_2-N_3-C_4	-56.5 (-61.6)	-44.1 (-47.1)	12.4 (14.5)	-55.5 (-57.8)	-43.8 (-45.8)	11.7 (12)	-61.0 (-64.7)	-44.6 (-47.9)	16.4 (16.8)
N_3-C_4-C_5-N_6	-79.2 (-71.6)	-66.9 (-64.8)	12.3 (6.8)	-69.5 (-71.0)	-68.7 (-66.5)	0.8 (4.5)	-78.9 (-73.3)	-68.3 (-65.2)	10.6 (8.1)
N_3-C_2-C_1-O_7	-18.7 (-22.6)	-49.2 (-47.2)	30.5 (24.6)	-19.2 (-25.7)	-47.2 (-46.4)	28.0 (20.7)	-9.9 (-17.3)	-47.0 (-45.9)	37.1 (28.6)
N_3-C_2-C_1-O_8	164.4 (161.7)	129.6 (129.6)	34.8 (32.1)	163.7 (158.6)	132.7 (131.1)	31.0 (27.5)	172.8 (166.9)	133.0 (131.8)	39.8 (35.1)
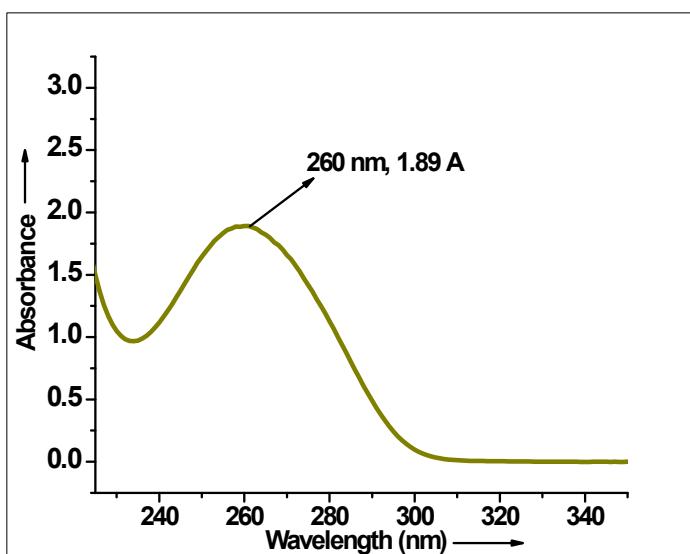
MD^A; MD^B and MD^C are the largest variations of Pt(Ura)(GV), Pt(Ura)(AG) and Pt(Ura)(GL) from their constituent dipeptide molecules; *Wiberg bond indices. Values in parentheses are from gas phase calculations.

Table S5. DNA binding-affinities* of the three ternary complexes of Pt(II)

System	Single point energies at UFF level (kcal/mol)	$E_{\text{Binding-affinity}}$ (kcal/mol)
DNA	-9082.96611048	
Pt(Ura)(GV)	-147.64418800	
Pt(Ura)(AG)	-170.18546617	
Pt(Ura)(GL)	-148.18122431	
DNA-Pt(Ura)(GV)	-9256.86445240	-26.25415392
DNA-Pt(Ura)(AG)	-9290.18251919	-37.03094254
DNA-Pt(Ura)(GL)	-9259.47825098	-28.33091619
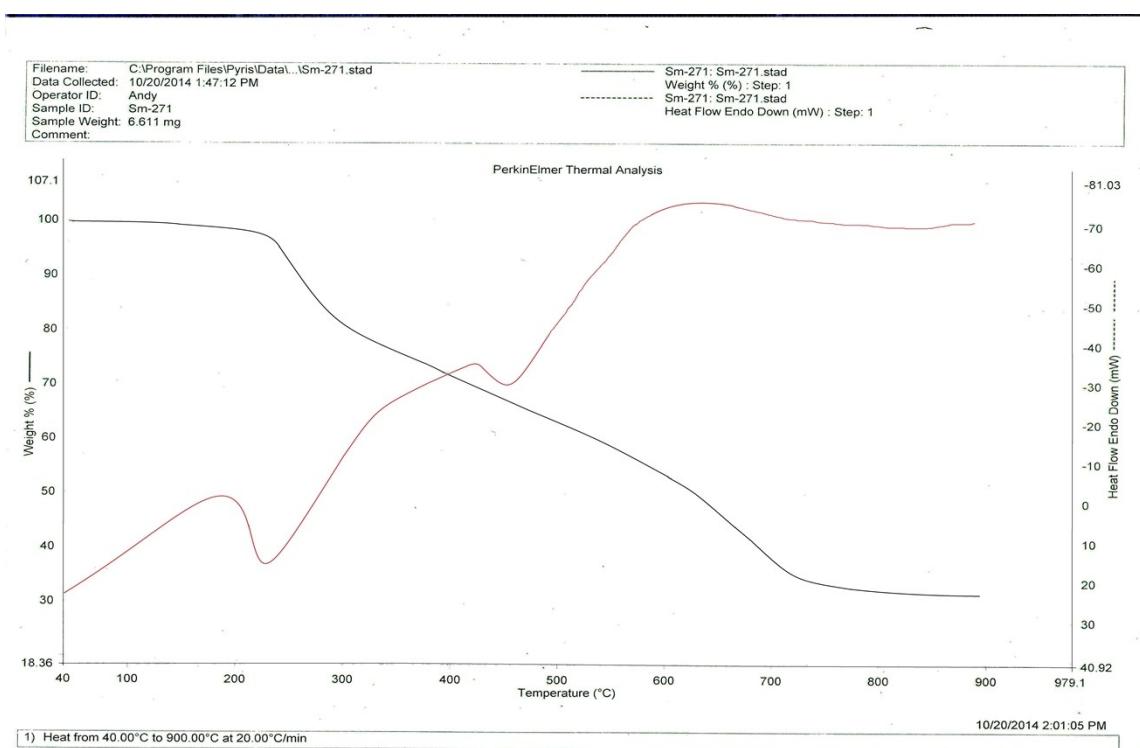
*The theoretical DNA binding-affinity order of the three ternary complexes were determined by performing single point energy calculations at UFF level[1] inbuilt in ARGUSLAB 4.0.1 program[2] on the molecular geometries of the highest ranking docked poses of the Pt(Ura)GV, Pt(Ura)AG and Pt(Ura)GL with the classical d(CGCGAATTCGCG)₂ B-DNA sequence, aqueous phase optimized structures of the three metallic complexes (Gaussian 09 program) and the d(CGCGAATTCGCG)₂ B-DNA sequence generated by AVOGADRO 1.1.1 package. The DNA binding-affinities were calculated using the equation S1, mentioned below:

$$E_{\text{Binding-affinity}} = E_{\text{Docked pose}} - (E_{\text{DNA}} + E_{\text{Metal-complex}}) \dots\dots (S1)$$
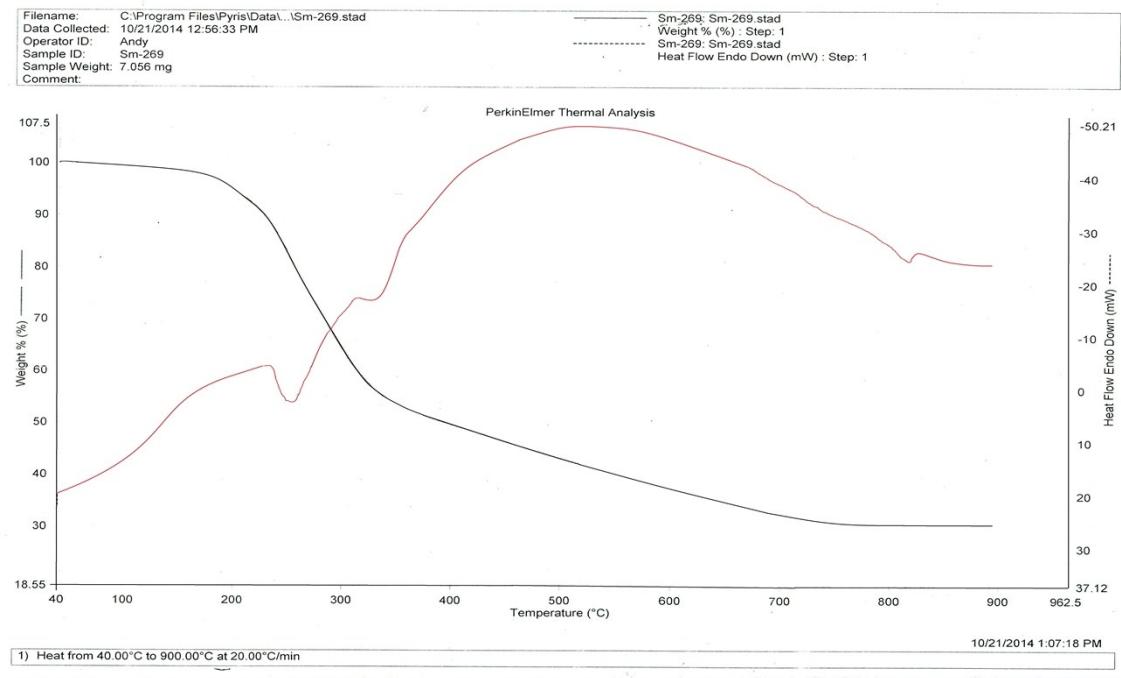
CT-DNA

Fig. S1 Experimental UV-vis spectrum of CT-DNA in aqueous phase
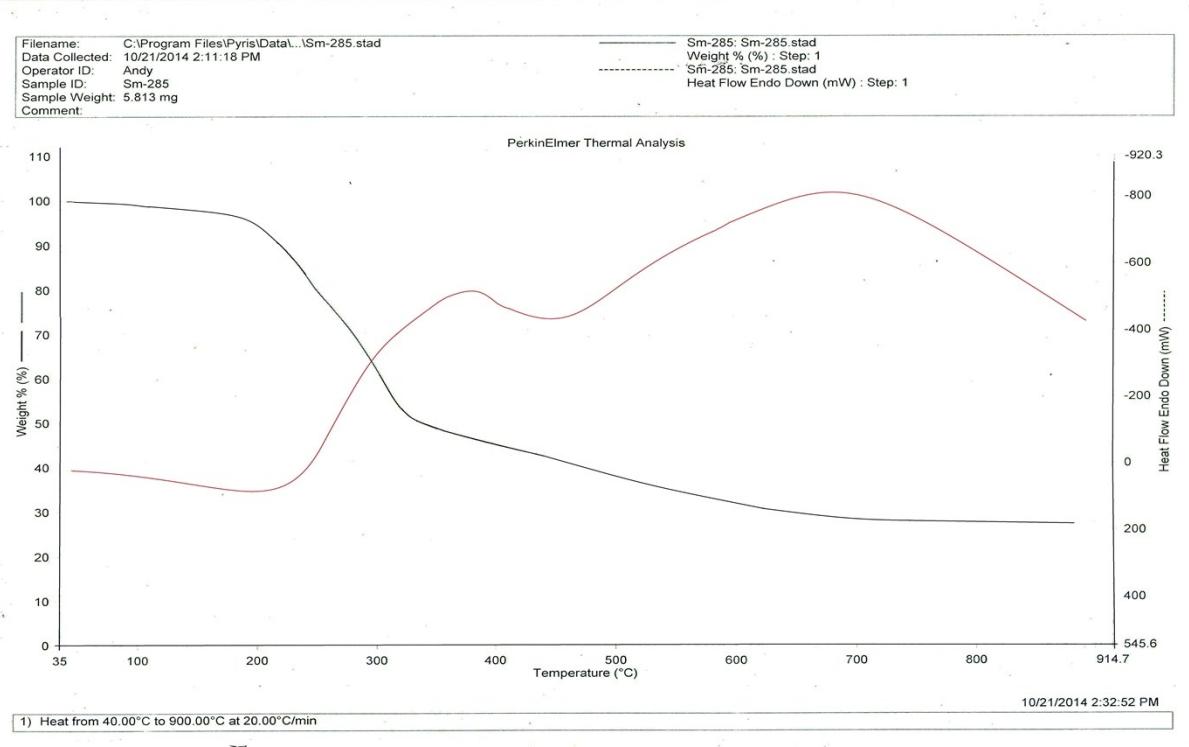
TG/DTA curve for Pt(Ura)(GV) (Solid state technique)

Fig. S2 TG/DTA curves of the metal complexes prepared in solid state
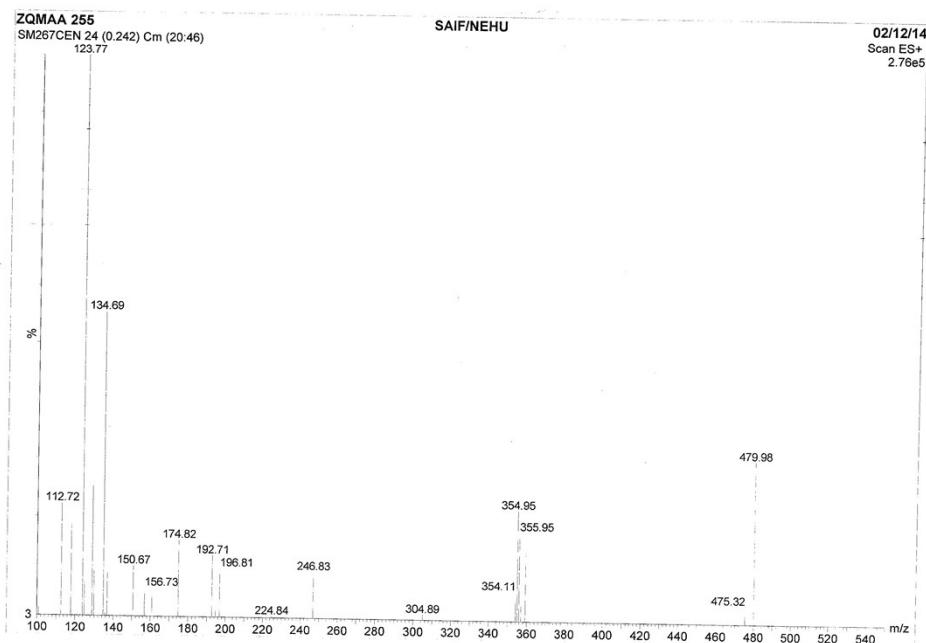
TG/DTA curve for Pt(Ura)(AG) (Solid state technique)
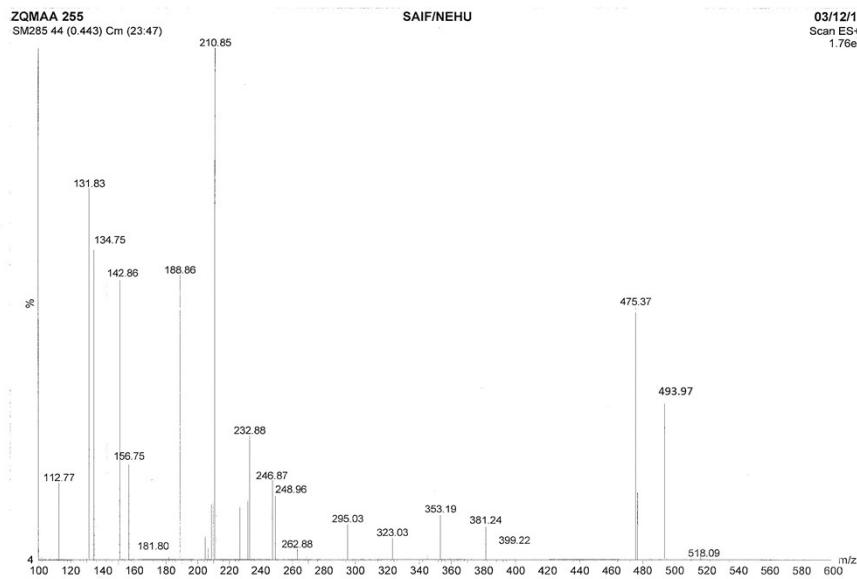
TG/DTA curve for Pt(Ura)(GL) (Solid state technique)

Fig. S2 Continued…
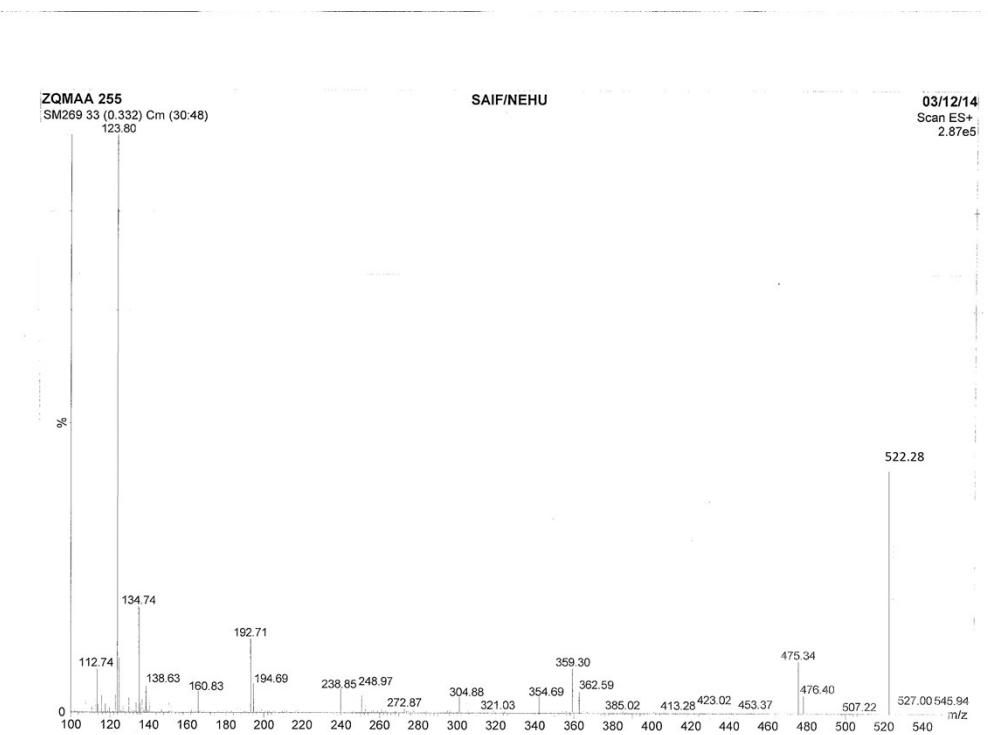
Mass spectrum of the complex Pt(Ura)(GV) in DMSO solution
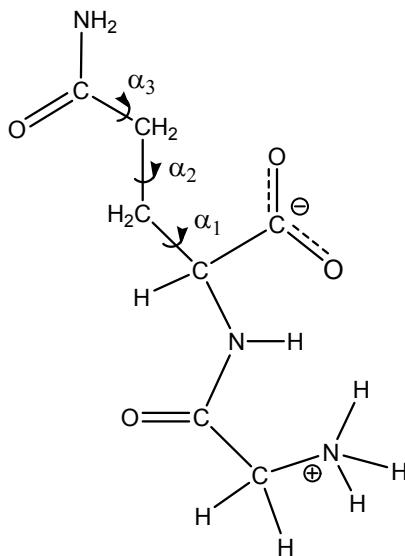
Mass spectrum of the complex Pt(Ura)(GL) in DMSO solution

Fig. S3 Mass spectrum of the metal complexes prepared by solid state technique

ZQMAA 255
SM269 33 (0.332) Cm (30:48)

SAIF/NEHU

03/12/14
Scan ES+
2.87e5
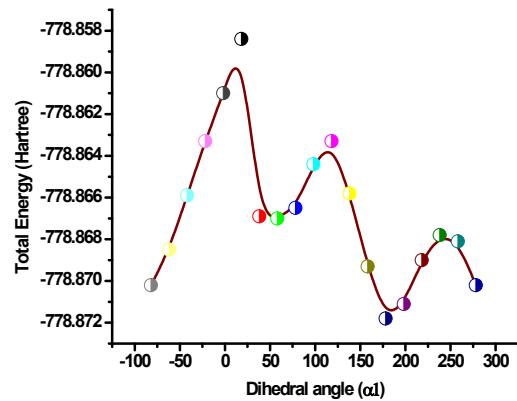
Mass spectrum of the complex Pt(Ura)(AG) in DMSO solution.
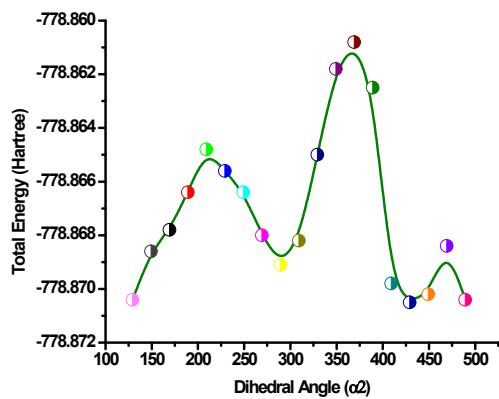
Fig. S3 Continued…..
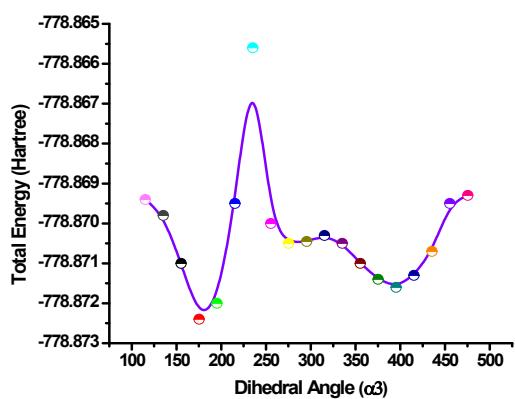
Zwitterion *l*-alanyl-*l*-glutamine

Rotation about α_1
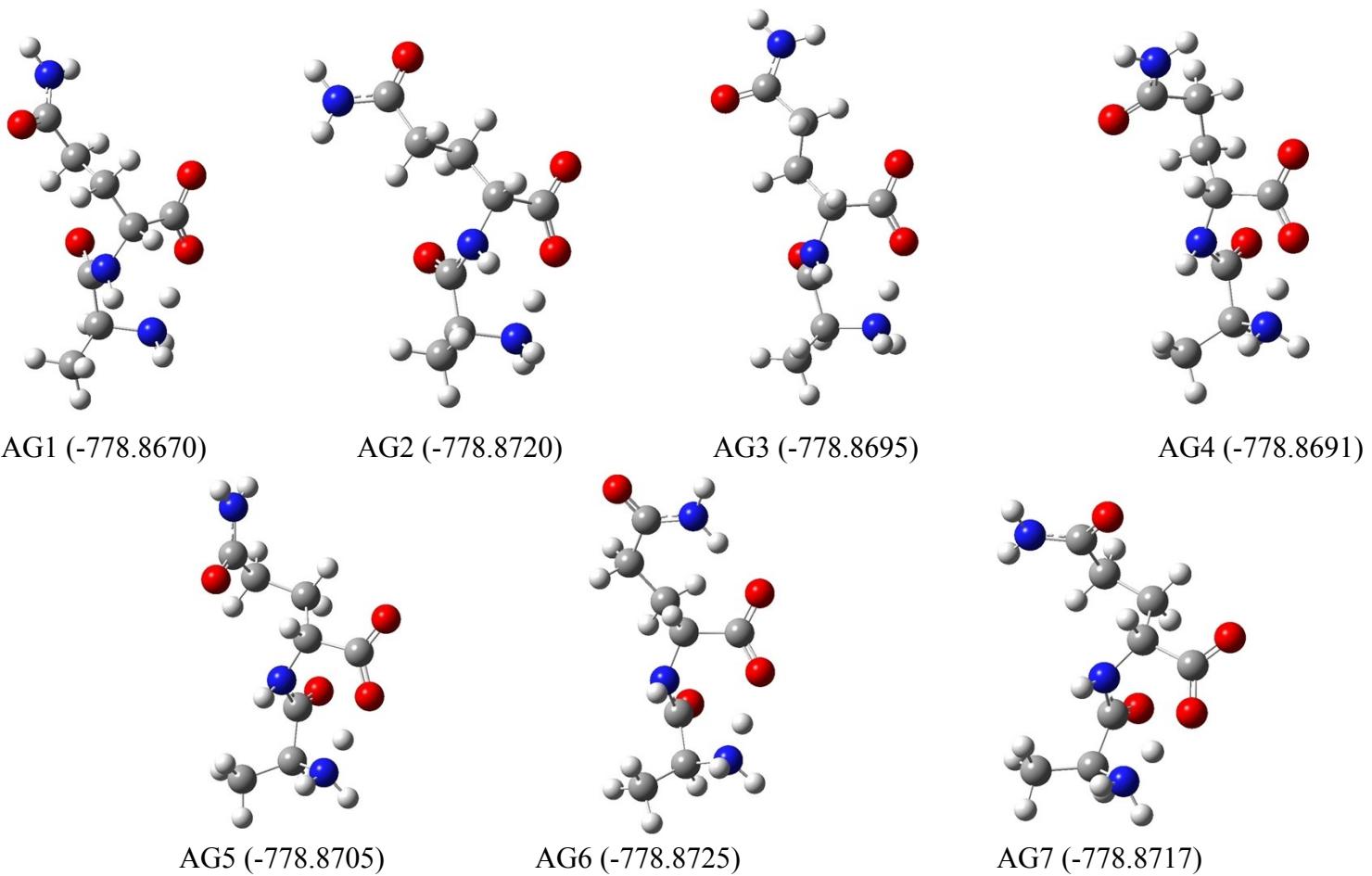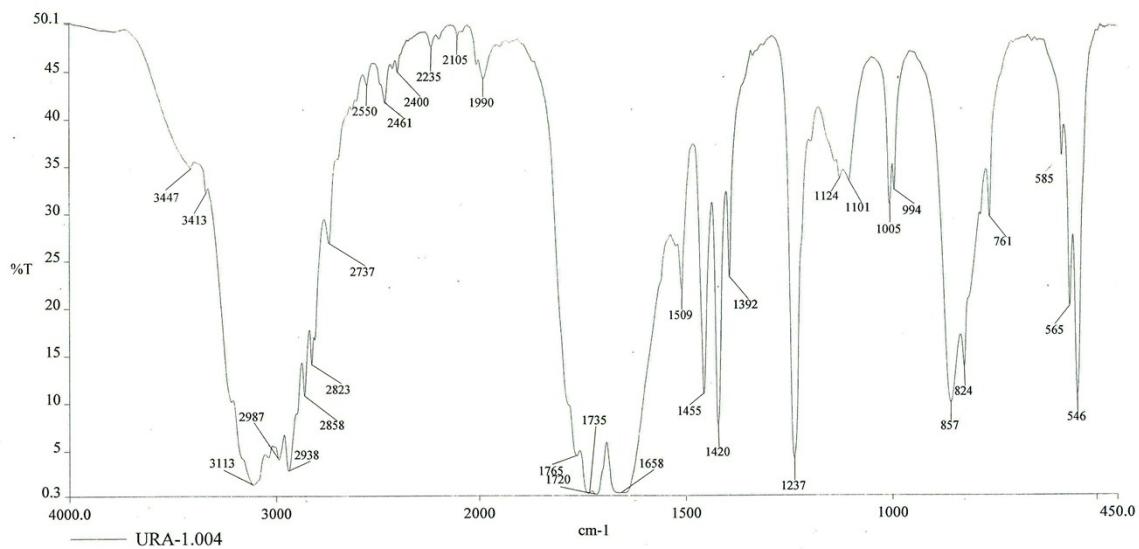
Rotation about α_2

Rotation about α_3

Fig. S4 The potential energy surfaces corresponding to the three dihedrals α_1, α_2 and α_3 of zwitterion *l*-alanyl-*l*-glutamine at B3PW91/6-31++G(d,p) level in the aqueous phase.

AG1 (-778.8670)   AG2 (-778.8720)   AG3 (-778.8695)   AG4 (-778.8691)

AG5 (-778.8705)   AG6 (-778.8725)   AG7 (-778.8717)
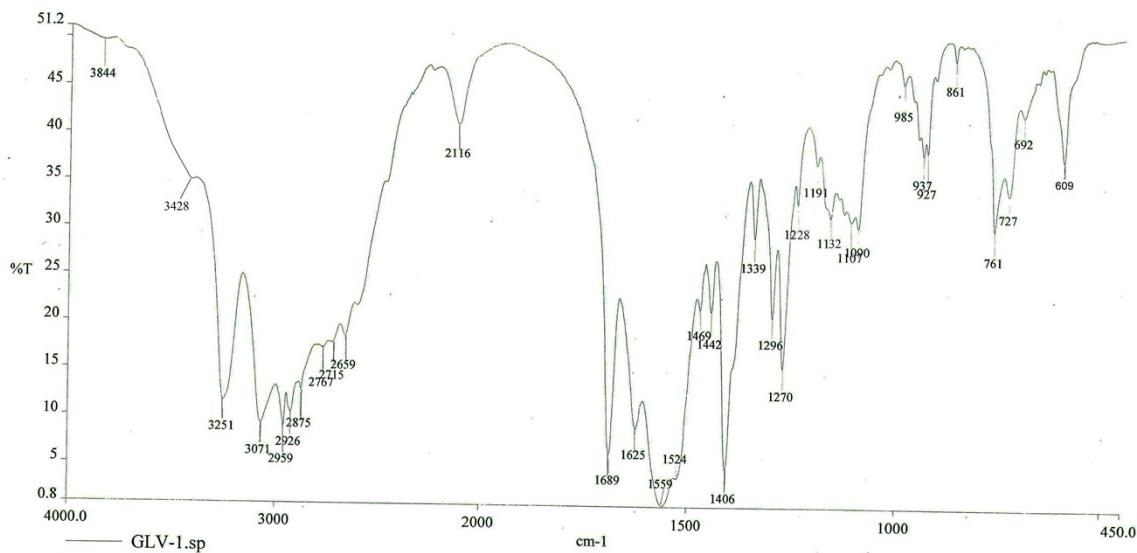
Fig. S5 B3PW91/6-31++G(d,p) level optimized structures of the seven possible conformers of zwitterion *l*-alanyl-*l*-glutamine corresponding to the three dihedrals α_1, α_2 and α_3 in aqueous phase (energy in Hartree)

Experimental FT-IR spectra of Uracil
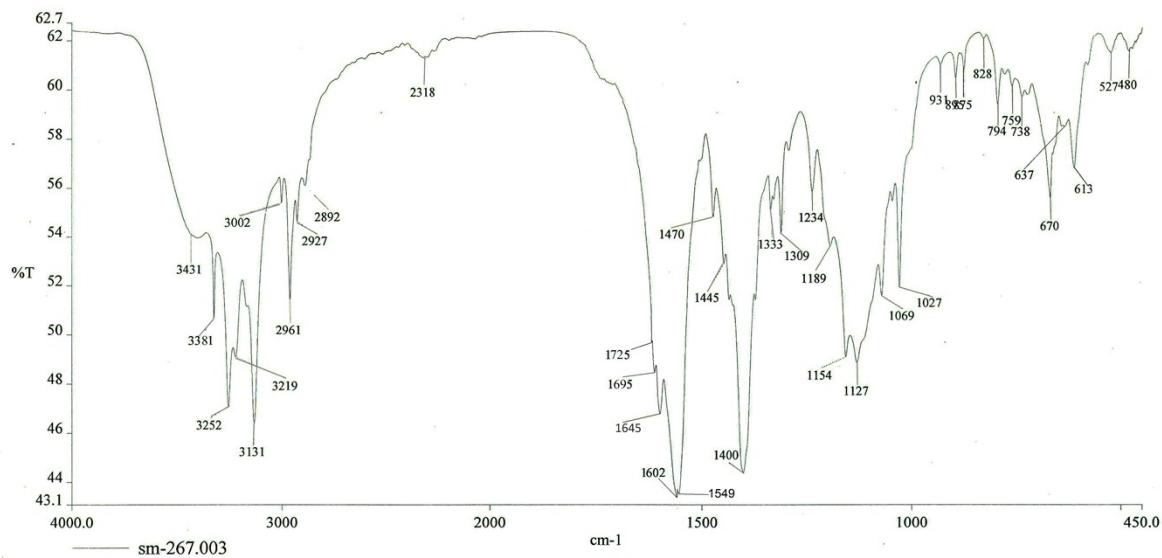
Experimental FT-IR spectra of GV

Fig. S6 Experimental FT-IR spectra of the ligands and their ternary complexes with Pt(II)
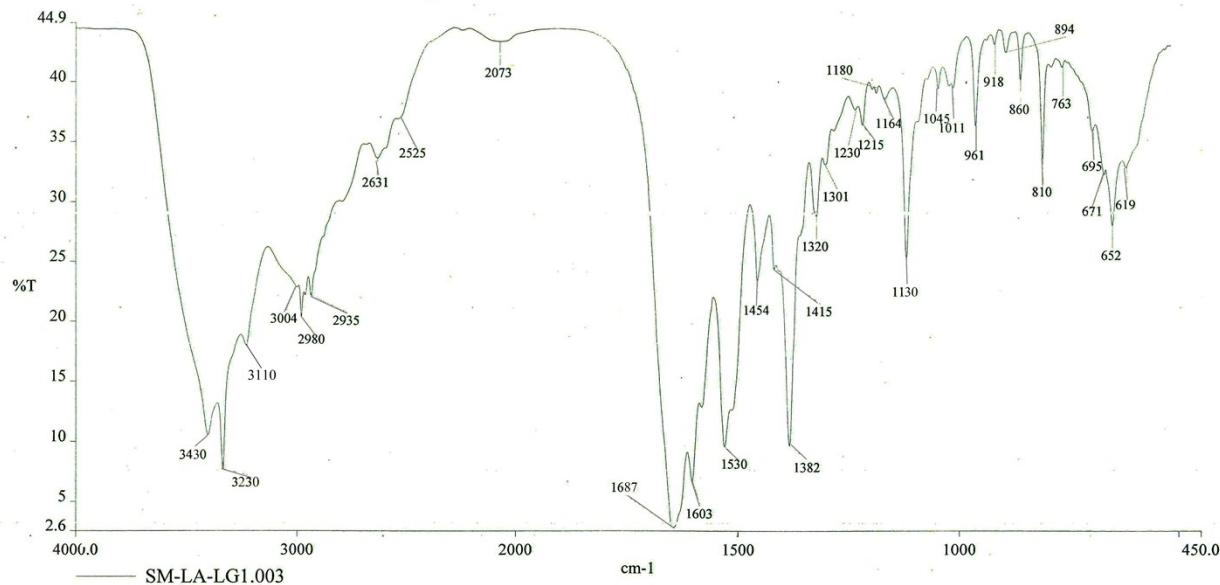
Experimental FT-IR spectra for Pt(Ura)(GV) complex (solid state technique)

Experimental FT-IR spectra for Pt(Ura)(GV) complex (solution method)

Fig. S6 Continued….

Experimental FT-IR spectra for AG

Experimental FT-IR spectra for Pt(Ura)(AG) complex (solid state technique)

Fig. S6 Continued….

Experimental FT-IR spectra for Pt(Ura)(AG) complex (solution method)

Experimental FT-IR spectra for GL

Fig. S6 Continued….
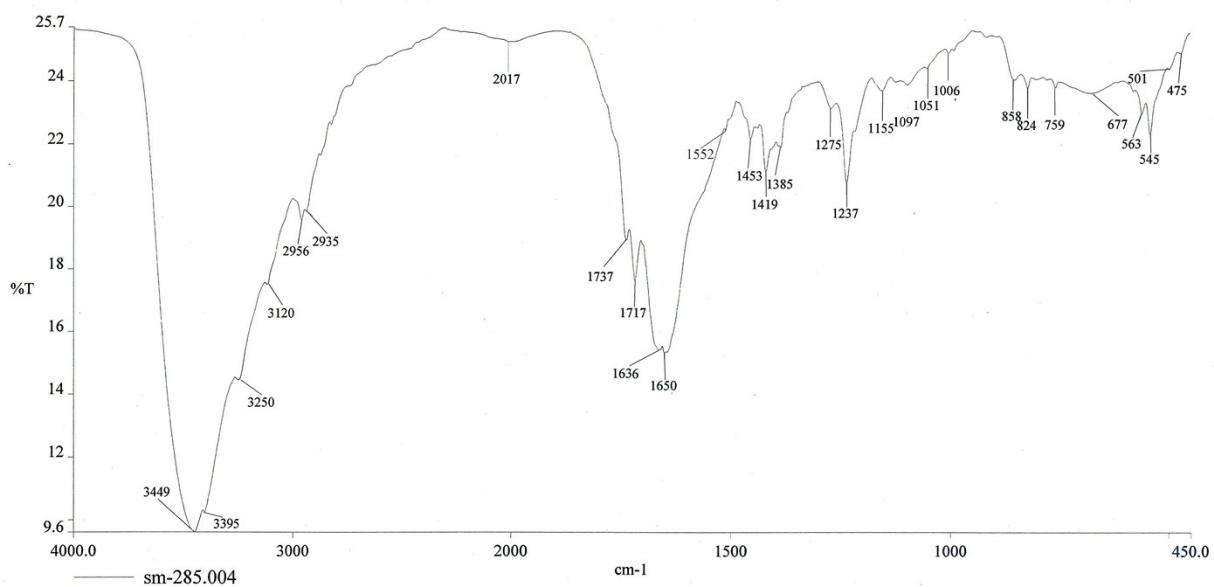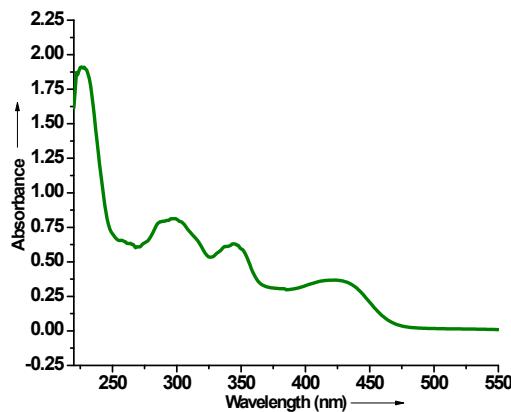
Experimental FT-IR spectra for Pt(Ura)(GL) complex (solid state technique)

Date: Thursday, October 16, 2014
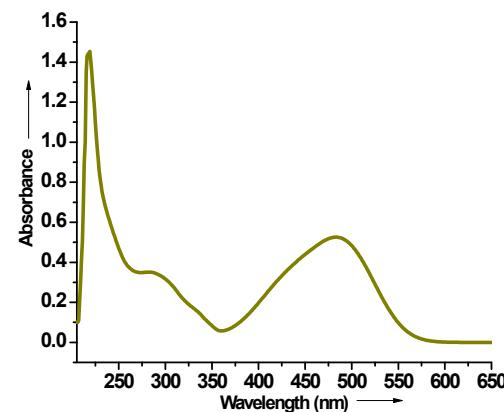
Experimental FT-IR spectra for Pt(Ura)(GL) complex (solution method)
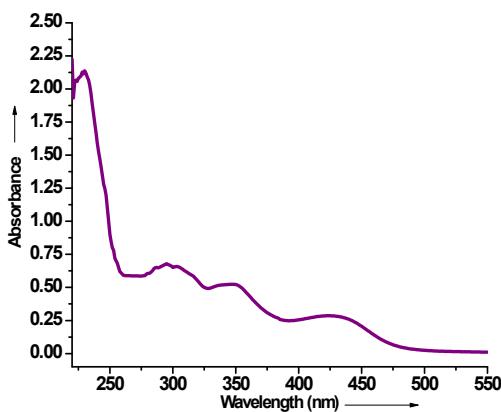
Fig. S6 Continued….
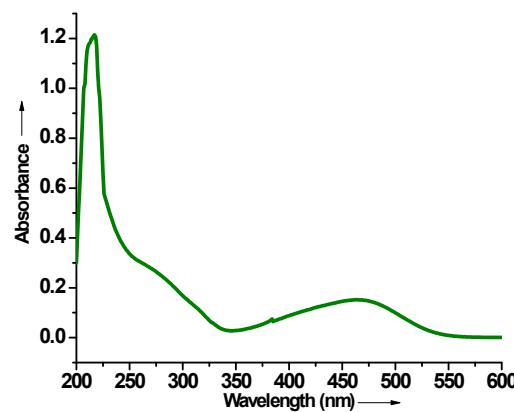
Pt(Ura)(GV) (solid state technique)
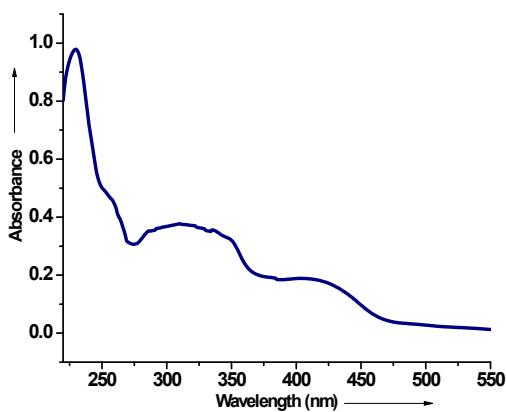
Pt(Ura)(GV) (solution method)
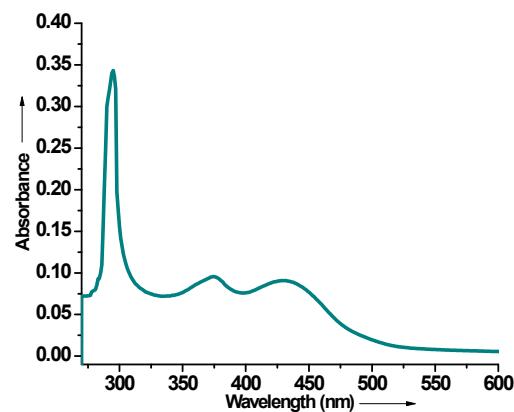
Pt(Ura)(AG) (solid state technique)

Pt(Ura)(AG) (solution method)
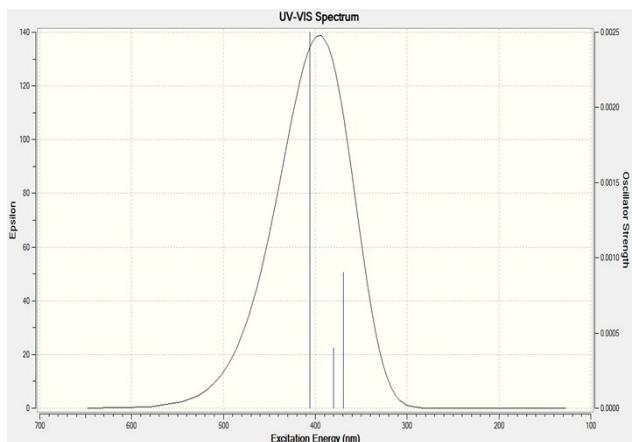
Pt(Ura)(GL) (solid state technique)
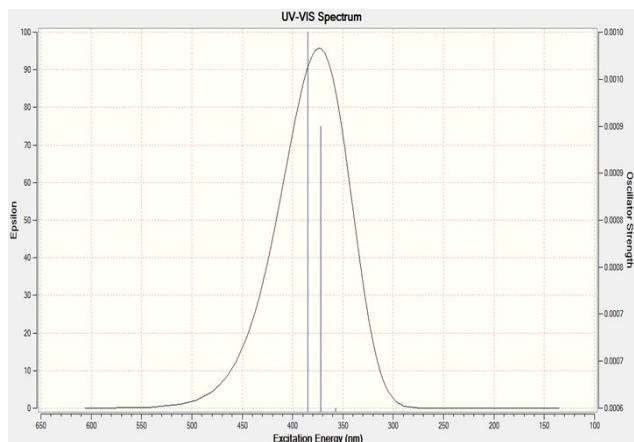
Pt(Ura)(GL) (solution method)
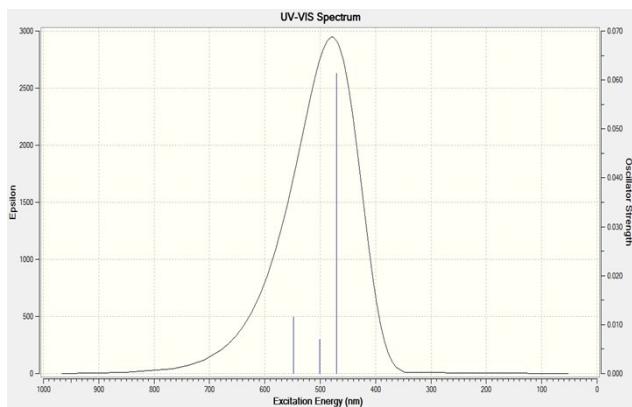
Fig. S7 Experimental UV-vis spectra of the synthesized complexes in deionized water.
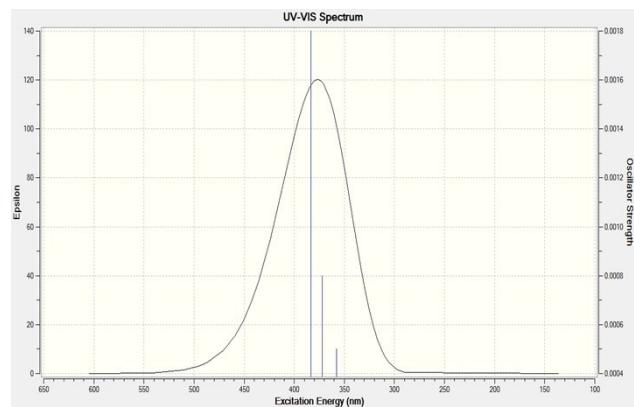
UV-vis spectra of Pt(Ura)(GV) in aqueous phase
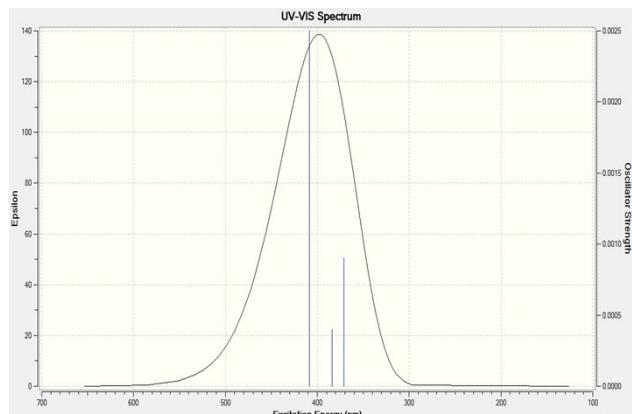
UV-vis spectra of Pt(Ura)(GV) in gas phase
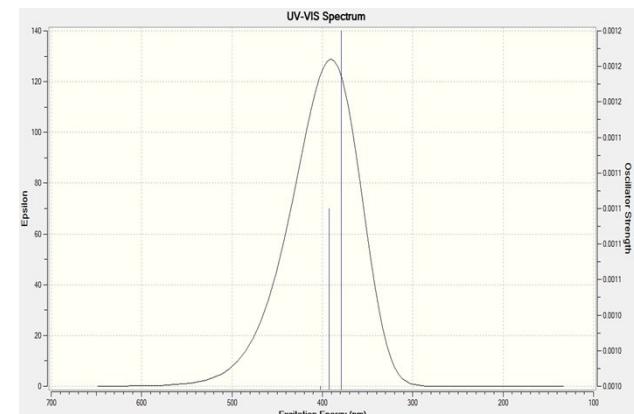
UV-vis spectra for Pt(Ura)(AG) in aqueous phase

UV-vis spectra for Pt(Ura)(AG) in gas phase

UV-vis spectra for Pt(Ura)(GL) in aqueous phase

UV-vis spectra for Pt(Ura)(GL) in gas phase

Fig. S8 Theoretical UV-vis spectra of the complexes in gas and aqueous phases

► Cartesian coordinates of the optimized structures of the ligands their metal complexes in gas and aqueous phases using the B3PW91 level of theory

Uracil- gas phase

```
-------------------------------------------------------------------
    1          7          0        1.174268     0.983918     0.000004
    2          6          0        1.216779    -0.404842     0.000025
    3          7          0       -0.034940    -0.985084     0.000005
    4          6          0       -1.288273    -0.345363     0.000016
    5          6          0       -1.201736     1.108262     0.000015
    6          6          0        0.008782     1.707049     0.000007
    7          1          0        0.129318     2.785200    -0.000006
    8          1          0       -2.121369     1.677028     0.000009
    9          8          0       -2.314807    -1.005361    -0.000011
   10          1          0       -0.047714    -1.998131    -0.000020
   11          8          0        2.261799    -1.030361    -0.000040
   12          1          0        2.075225     1.439209    -0.000016
-------------------------------------------------------------------
```

Uracil- aqueous phase

```
-------------------------------------------------------------------
    1          7          0        1.176489     0.979917     0.000017
    2          6          0        1.209982    -0.399286     0.000016
    3          7          0       -0.038803    -0.981720     0.000030
    4          6          0       -1.281832    -0.336865     0.000137
    5          6          0       -1.197750     1.107613     0.000026
    6          6          0        0.017002     1.705428     0.000016
    7          1          0        0.142207     2.781842    -0.000032
    8          1          0       -2.111471     1.685934    -0.000038
    9          8          0       -2.316214    -1.004017    -0.000087
   10          1          0       -0.051474    -1.995459    -0.000040
   11          8          0        2.253599    -1.042004    -0.000083
   12          1          0        2.073455     1.447131    -0.000023
-------------------------------------------------------------------
```

Gly-Val- aqueous phase

```
-------------------------------------------------------------------
    1          8          0       -0.945449     1.846987    -0.122710
    2          6          0        0.293803     1.549203     0.017787
    3          8          0        1.144769     2.296656     0.528083
    4          6          0        0.774154     0.175233    -0.565321
    5          1          0        1.132664     0.401711    -1.578090
    6          7          0       -3.105192     0.423022    -0.206282
    7          6          0       -2.701011    -1.023542    -0.167420
    8          1          0       -2.854429    -1.455553    -1.157125
    9          1          0       -3.303623    -1.559531     0.563403
   10          6          0       -1.231379    -0.993602     0.244873
   11          8          0       -0.898076    -1.084314     1.424802
   12          7          0       -0.387592    -0.690796    -0.769426
   13          1          0       -0.802468    -0.634435    -1.689319
   14          1          0       -3.724920     0.624965    -0.990112
   15          1          0       -3.601186     0.687355     0.644733
   16          6          0        1.949054    -0.490070     0.193656
   17          1          0        1.758660    -0.383375     1.267792
   18          6          0        2.058281    -1.982534    -0.130890
```

```
    19              6              0          3.273633      0.205714     -0.140144
    20              1              0          1.168854     -2.537597      0.177762
    21              1              0          2.202612     -2.142808     -1.206662
    22              1              0          2.922808     -2.412063      0.387316
    23              1              0          3.224610      1.274149      0.076459
    24              1              0          4.089956     -0.234152      0.443703
    25              1              0          3.519226      0.075932     -1.202545
    26              1              0         -2.192442      1.052779     -0.263996
    ------------------------------------------------------------------------
```

Gly-Val- gas phase
```
    ------------------------------------------------------------------------
     1              8              0         -0.712487      2.095465     -0.129427
     2              6              0          0.514791      1.570918      0.033947
     3              8              0          1.386603      2.220293      0.557844
     4              6              0          0.767130      0.162590     -0.563745
     5              1              0          1.125568      0.354282     -1.585488
     6              7              0         -3.226462      0.391891     -0.344421
     7              6              0         -2.783632     -0.987596     -0.086161
     8              1              0         -2.899065     -1.573174     -1.004976
     9              1              0         -3.324769     -1.494496      0.719706
    10              6              0         -1.313685     -0.879894      0.311699
    11              8              0         -0.940114     -0.944660      1.473015
    12              7              0         -0.489330     -0.559557     -0.732337
    13              1              0         -0.921493     -0.502657     -1.643212
    14              1              0         -4.048445      0.417346     -0.938510
    15              1              0         -3.472929      0.852193      0.527638
    16              6              0          1.884634     -0.623197      0.169602
    17              1              0          1.716721     -0.508845      1.245512
    18              6              0          1.832047     -2.113290     -0.174064
    19              6              0          3.264000     -0.053582     -0.181688
    20              1              0          0.906816     -2.582849      0.167633
    21              1              0          1.925512     -2.278910     -1.255010
    22              1              0          2.666996     -2.629977      0.310560
    23              1              0          3.337705      1.006811      0.063813
    24              1              0          4.040905     -0.590013      0.373334
    25              1              0          3.477088     -0.183164     -1.251637
    26              1              0         -1.383782      1.462636     -0.461046
    ------------------------------------------------------------------------
```

Gly-Leu- aqueous phase
```
    ------------------------------------------------------------------------
     1              8              0          1.487840      1.768224      0.013508
     2              6              0          0.228251      1.538315     -0.021450
     3              8              0         -0.632684      2.346836     -0.410509
     4              6              0         -0.288451      0.168653      0.520916
     5              1              0         -0.698501      0.394190      1.511734
     6              7              0          3.588940      0.258740      0.171556
     7              6              0          3.139432     -1.174446      0.210630
     8              1              0          3.273577     -1.555420      1.223796
     9              1              0          3.729033     -1.768254     -0.485165
    10              6              0          1.673130     -1.124778     -0.213986
    11              8              0          1.345975     -1.284411     -1.387399
    12              7              0          0.834647     -0.733080      0.777765
    13              1              0          1.258465     -0.621140      1.689289
    14              1              0          4.211313      0.483724      0.947022
    15              1              0          4.098827      0.456783     -0.689146
```

```
        16              6              0        -1.405256     -0.461834     -0.332885
        17              1              0        -1.226405     -0.229090     -1.386847
        18              1              0        -1.328968     -1.552134     -0.236714
        19              6              0        -2.831449     -0.034192      0.052964
        20              1              0        -2.842498      1.061099      0.120668
        21              6              0        -3.815591     -0.453128     -1.042862
        22              6              0        -3.264641     -0.612621      1.403803
        23              1              0        -4.839290     -0.153823     -0.791265
        24              1              0        -3.558484      0.002414     -2.005794
        25              1              0        -3.811308     -1.542718     -1.176672
        26              1              0        -3.290130     -1.709269      1.365780
        27              1              0        -2.592840     -0.324898      2.220193
        28              1              0        -4.268340     -0.264666      1.672247
        29              1              0         2.698849      0.922575      0.188047
-------------------------------------------------------------------------

Gly-Leu- gas phase
-------------------------------------------------------------------------
         1              8              0         1.331278      2.009238     -0.002235
         2              6              0         0.065685      1.571113     -0.100843
         3              8              0        -0.789995      2.271446     -0.586793
         4              6              0        -0.272800      0.192987      0.512872
         5              1              0        -0.667357      0.430920      1.508756
         6              7              0         3.718050      0.147873      0.307916
         7              6              0         3.193430     -1.223252      0.194681
         8              1              0         3.259655     -1.709292      1.174265
         9              1              0         3.712443     -1.847443     -0.540144
        10              6              0         1.740042     -1.059408     -0.242836
        11              8              0         1.389061     -1.187417     -1.405380
        12              7              0         0.922196     -0.606517      0.758767
        13              1              0         1.355521     -0.489264      1.663882
        14              1              0         4.530004      0.191233      0.914727
        15              1              0         4.007250      0.490073     -0.604435
        16              6              0        -1.367740     -0.551593     -0.273055
        17              1              0        -1.170858     -0.440506     -1.342274
        18              1              0        -1.260751     -1.619634     -0.045172
        19              6              0        -2.807476     -0.112419      0.044911
        20              1              0        -2.854645      0.978439     -0.056149
        21              6              0        -3.765620     -0.724376     -0.980801
        22              6              0        -3.235458     -0.495843      1.464852
        23              1              0        -4.799529     -0.419255     -0.785368
        24              1              0        -3.510201     -0.410953     -1.998514
        25              1              0        -3.731035     -1.821103     -0.948563
        26              1              0        -3.209494     -1.584688      1.601630
        27              1              0        -2.598923     -0.048154      2.237308
        28              1              0        -4.258727     -0.160346      1.665404
        29              1              0         1.971806      1.341093      0.324441
-------------------------------------------------------------------------
Ala-Gln-aqueous phase
-------------------------------------------------------------------------
         1              8              0        -1.047882      1.967115     -0.239945
         2              6              0         0.088838      1.399086     -0.314636
         3              8              0         1.181496      1.959126     -0.081298
         4              6              0         0.131899     -0.084872     -0.799420
         5              1              0         0.299257     -0.033504     -1.881834
         6              7              0        -3.464945      0.998006      0.081234
         7              6              0        -3.335862     -0.457297      0.492509
```

```
    8            1            0        -3.698630    -0.537872    1.517141
    9            6            0        -1.819877    -0.698420    0.548467
   10            8            0        -1.236930    -0.751568    1.628240
   11            7            0        -1.189031    -0.693781   -0.652166
   12            1            0        -1.774971    -0.628881   -1.473160
   13            1            0        -4.042823     1.106361   -0.753558
   14            1            0        -3.903683     1.551063    0.817759
   15            6            0         1.265760    -0.921009   -0.183063
   16            1            0         1.339182    -0.693320    0.883226
   17            6            0        -4.139586    -1.370614   -0.419078
   18            1            0        -4.011850    -2.407009   -0.097305
   19            1            0        -5.203021    -1.124605   -0.353789
   20            1            0        -3.837390    -1.300158   -1.468553
   21            1            0         0.973136    -1.972214   -0.255396
   22            6            0         2.633733    -0.730520   -0.885605
   23            1            0         2.912677    -1.630590   -1.437312
   24            1            0         2.572499     0.090462   -1.608917
   25            6            0         3.774978    -0.413892    0.068010
   26            8            0         4.734845    -1.180843    0.233085
   27            7            0         3.657476     0.767010    0.704161
   28            1            0         2.824818     1.338171    0.544078
   29            1            0         4.348035     1.036550    1.388880
   30            1            0        -2.473264     1.421498   -0.117617
        ----------------------------------------------------------------
```

Ala-Gln-gas phase

```
        ----------------------------------------------------------------
    1            8            0        -0.996896     2.164445   -0.314916
    2            6            0         0.147465     1.473506   -0.314937
    3            8            0         1.186871     2.011645   -0.000845
    4            6            0         0.103638     0.012520   -0.820652
    5            1            0         0.256818     0.086549   -1.906266
    6            7            0        -3.641132     0.838543    0.151708
    7            6            0        -3.367640    -0.568545    0.515292
    8            1            0        -3.706099    -0.804766    1.530911
    9            6            0        -1.836105    -0.642231    0.564969
   10            8            0        -1.223659    -0.618329    1.621414
   11            7            0        -1.222628    -0.566812   -0.657770
   12            1            0        -1.831125    -0.517301   -1.462091
   13            1            0        -4.548923     0.935546   -0.294025
   14            1            0        -3.652374     1.424311    0.982560
   15            6            0         1.243591    -0.833618   -0.235200
   16            1            0         1.301379    -0.645689    0.839280
   17            6            0        -4.033239    -1.525015   -0.467358
   18            1            0        -3.728395    -2.556982   -0.274081
   19            1            0        -5.122255    -1.471838   -0.363391
   20            1            0        -3.792959    -1.287066   -1.510220
   21            1            0         0.967177    -1.885212   -0.351110
   22            6            0         2.601155    -0.570358   -0.927471
   23            1            0         2.825948    -1.356018   -1.652378
   24            1            0         2.572131     0.385963   -1.460919
   25            6            0         3.761672    -0.524670    0.058099
   26            8            0         4.579511    -1.432070    0.162101
   27            7            0         3.805432     0.607073    0.808938
   28            1            0         3.079751     1.308676    0.731956
   29            1            0         4.503464     0.678544    1.532524
   30            1            0        -1.806073     1.618601   -0.441361
```

```
------------------------------------------------------------------------

Pt(Ura)(AG)-gas phase
------------------------------------------------------------------------
     1          8           0      -0.494082     0.351884    -1.262593
     2          6           0      -1.501555    -0.270090    -0.682952
     3          8           0      -1.468872    -1.348931    -0.119335
     4          6           0      -2.786052     0.606753    -0.752940
     5          1           0      -3.080123     0.690815    -1.806372
     6          7           0       0.573571     2.590011    -0.333212
     7          6           0      -0.420557     3.104992     0.666112
     8          1           0       0.068955     3.059842     1.641315
     9          6           0      -1.587334     2.107281     0.765586
    10          8           0      -1.733751     1.444651     1.778206
    11          7           0      -2.381940     1.970332    -0.348497
    12          1           0      -2.098887     2.533046    -1.138774
    13          1           0       0.176752     2.658127    -1.272818
    14          1           0       1.388444     3.203540    -0.316709
    15         78           0       1.248098     0.603792    -0.263802
    16          7           0       3.339905    -3.189051     0.059503
    17          6           0       4.354127    -2.655534     0.785676
    18          1           0       5.132025    -3.345145     1.097501
    19          6           0       4.382140    -1.327947     1.092574
    20          1           0       5.178747    -0.871288     1.662672
    21          6           0       3.277023    -0.572001     0.611238
    22          8           0       3.081294     0.695300     0.753485
    23          7           0       2.265850    -1.141493    -0.080929
    24          6           0       2.240686    -2.461776    -0.461243
    25          8           0       1.417669    -3.009504    -1.162576
    26          1           0       3.338998    -4.169529    -0.186931
    27          6           0      -3.950635     0.038029     0.052304
    28          1           0      -3.590994    -0.199719     1.056121
    29          6           0      -0.837148     4.537675     0.343992
    30          1           0      -1.548724     4.898561     1.092131
    31          1           0       0.029289     5.208205     0.354662
    32          1           0      -1.315693     4.620888    -0.638795
    33          1           0      -4.706253     0.821918     0.164076
    34          6           0      -4.574802    -1.202422    -0.627001
    35          1           0      -5.501743    -0.943109    -1.143377
    36          1           0      -3.882048    -1.611805    -1.372785
    37          6           0      -4.907861    -2.321766     0.352707
    38          8           0      -6.060642    -2.666996     0.596612
    39          7           0      -3.819333    -2.901441     0.919110
    40          1           0      -2.885575    -2.558290     0.715891
    41          1           0      -3.962285    -3.620706     1.610260
------------------------------------------------------------------------


Pt(Ura)(AG)-aqueous phase
------------------------------------------------------------------------
     1          8           0      -0.538846     0.225238    -1.239523
     2          6           0      -1.575219    -0.323102    -0.662361
     3          8           0      -1.611456    -1.426868    -0.123323
     4          6           0      -2.819958     0.606927    -0.725628
     5          1           0      -3.098384     0.704303    -1.781157
     6          7           0       0.563347     2.549464    -0.362254
     7          6           0      -0.404132     3.076855     0.656647
     8          1           0       0.111569     3.048170     1.618125
```

```
  9         6         0       -1.543029    2.059333    0.766306
 10         8         0       -1.626425    1.322091    1.745701
 11         7         0       -2.368198    1.942891   -0.313566
 12         1         0       -2.202169    2.580213   -1.080017
 13         1         0        0.163274    2.650877   -1.297077
 14         1         0        1.387244    3.152125   -0.350386
 15        78         0        1.235129    0.571131   -0.268434
 16         7         0        3.569071   -3.100774    0.076764
 17         6         0        4.578241   -2.480639    0.737919
 18         1         0        5.418229   -3.107113    1.015799
 19         6         0        4.522757   -1.146344    1.019570
 20         1         0        5.317783   -0.625446    1.534430
 21         6         0        3.350341   -0.485795    0.579515
 22         8         0        3.069627    0.772345    0.694383
 23         7         0        2.345301   -1.141570   -0.050048
 24         6         0        2.406477   -2.467245   -0.377376
 25         8         0        1.557608   -3.090477   -1.007502
 26         1         0        3.638199   -4.087810   -0.137652
 27         6         0       -4.022763    0.091425    0.063352
 28         1         0       -3.692727   -0.162683    1.073442
 29         6         0       -0.833998    4.503447    0.330067
 30         1         0       -1.530833    4.865999    1.090708
 31         1         0        0.035297    5.167551    0.323567
 32         1         0       -1.323273    4.580203   -0.646675
 33         1         0       -4.737162    0.914216    0.160485
 34         6         0       -4.711567   -1.113531   -0.620369
 35         1         0       -5.633941   -0.804281   -1.115913
 36         1         0       -4.054595   -1.534662   -1.391104
 37         6         0       -5.061666   -2.238056    0.340921
 38         8         0       -6.229925   -2.581721    0.566055
 39         7         0       -3.997584   -2.834404    0.916523
 40         1         0       -3.059138   -2.497170    0.715374
 41         1         0       -4.140555   -3.566468    1.596280
      -----------------------------------------------------------------
```

Pt(Ura)(GL)-gas phase
```
      -----------------------------------------------------------------
  1         8         0        0.705774   -0.177460   -1.151092
  2         6         0        1.573610    0.501398   -0.406816
  3         8         0        1.354153    1.502376    0.240093
  4         6         0        2.958365   -0.208940   -0.416701
  5         1         0        3.357252   -0.149441   -1.435629
  6         7         0       -0.152823   -2.590529   -0.528659
  7         6         0        0.814974   -3.091248    0.492559
  8         1         0        1.292109   -4.010662    0.126630
  9         1         0        0.265831   -3.308862    1.408444
 10         6         0        1.849121   -2.011909    0.830093
 11         8         0        1.854942   -1.492404    1.932223
 12         7         0        2.691879   -1.648882   -0.194317
 13         1         0        2.519899   -2.136544   -1.062815
 14         1         0        0.318114   -2.484151   -1.428602
 15         1         0       -0.885002   -3.287829   -0.655809
 16        78         0       -1.054272   -0.706834   -0.310163
 17         7         0       -3.558351    2.806227    0.190213
 18         6         0       -4.542620    2.112798    0.815548
 19         1         0       -5.403141    2.690519    1.137683
```

```
    20              6             0         -4.443468      0.768301       1.013675
    21              1             0         -5.213238      0.185618       1.499584
    22              6             0         -3.242012      0.171929       0.536896
    23              8             0         -2.923690     -1.076301       0.585271
    24              7             0         -2.263436      0.899684      -0.045558
    25              6             0         -2.367451      2.239895      -0.330878
    26              8             0         -1.586371      2.923077      -0.956924
    27              1             0         -3.651272      3.798054       0.018832
    28              6             0          3.964386      0.383543       0.568138
    29              1             0          3.466912      0.498055       1.534927
    30              1             0          4.772949     -0.347621       0.703980
    31              6             0          4.565933      1.730177       0.131396
    32              1             0          3.734794      2.398384      -0.126865
    33              6             0          5.322790      2.359529       1.304401
    34              6             0          5.486598      1.597770      -1.086384
    35              1             0          5.749667      3.329555       1.025277
    36              1             0          4.659906      2.517646       2.161647
    37              1             0          6.148649      1.714541       1.632537
    38              1             0          6.333395      0.933626      -0.868017
    39              1             0          4.969235      1.199774      -1.966917
    40              1             0          5.896414      2.573114      -1.372038
    ----------------------------------------------------------------------
```

Pt(Ura)(GL) - aqueous phase

```
    ----------------------------------------------------------------------
     1              8             0          0.745149     -0.031326      -1.078057
     2              6             0          1.656148      0.572820      -0.345750
     3              8             0          1.510367      1.607479       0.291227
     4              6             0          3.006771     -0.198304      -0.371878
     5              1             0          3.374552     -0.157106      -1.402669
     6              7             0         -0.138880     -2.529581      -0.543460
     7              6             0          0.803833     -3.047177       0.492785
     8              1             0          1.296817     -3.950137       0.115633
     9              1             0          0.233076     -3.293446       1.387135
    10              6             0          1.800540     -1.950005       0.843744
    11              8             0          1.723433     -1.346350       1.911309
    12              7             0          2.685288     -1.616210      -0.138702
    13              1             0          2.646924     -2.178067      -0.978086
    14              1             0          0.341985     -2.464556      -1.441714
    15              1             0         -0.875255     -3.223337      -0.673956
    16             78             0         -1.047645     -0.663598      -0.302062
    17              7             0         -3.798819      2.695122       0.186751
    18              6             0         -4.782087      1.909976       0.694066
    19              1             0         -5.704217      2.415684       0.957064
    20              6             0         -4.602040      0.566173       0.847908
    21              1             0         -5.372151     -0.084579       1.237772
    22              6             0         -3.333103      0.077057       0.451074
    23              8             0         -2.929880     -1.151279       0.468394
    24              7             0         -2.359653      0.894741      -0.019649
    25              6             0         -2.542208      2.234005      -0.222844
    26              8             0         -1.722513      3.004176      -0.714098
    27              1             0         -3.958648      3.687108       0.063736
    28              6             0          4.073040      0.358905       0.572290
    29              1             0          3.608029      0.556760       1.542427
    30              1             0          4.823828     -0.426867       0.729402
    31              6             0          4.779826      1.628792       0.067243
    32              1             0          4.008074      2.344456      -0.246117
```

33	6	0	5.575698	2.268553	1.208892
34	6	0	5.695861	1.350279	-1.129285
35	1	0	6.078605	3.183441	0.875935
36	1	0	4.925283	2.528261	2.051728
37	1	0	6.346686	1.581111	1.580489
38	1	0	6.490394	0.645092	-0.853771
39	1	0	5.156233	0.926786	-1.983575
40	1	0	6.174415	2.273488	-1.474834

Pt(Ura)(GV)- gas phase

1	8	0	0.878166	0.214599	-1.156379
2	6	0	1.596093	1.027598	-0.388740
3	8	0	1.178344	1.912602	0.325549
4	6	0	3.101523	0.630065	-0.462462
5	1	0	3.448459	0.798784	-1.490345
6	7	0	0.549167	-2.344884	-0.620723
7	6	0	1.613519	-2.658869	0.379496
8	1	0	2.267103	-3.448593	-0.015796
9	1	0	1.134206	-3.011411	1.292659
10	6	0	2.406973	-1.398418	0.739079
11	8	0	2.330210	-0.919366	1.857234
12	7	0	3.136731	-0.839746	-0.281651
13	1	0	3.064655	-1.329414	-1.162497
14	1	0	0.976253	-2.114820	-1.519439
15	1	0	-0.019550	-3.177975	-0.765727
16	78	0	-0.726209	-0.702319	-0.335176
17	7	0	-3.898554	2.191277	0.315020
18	6	0	-4.713738	1.282756	0.907203
19	1	0	-5.671786	1.656035	1.254829
20	6	0	-4.338390	-0.019976	1.044204
21	1	0	-4.967272	-0.769421	1.503584
22	6	0	-3.043614	-0.334242	0.542666
23	8	0	-2.472908	-1.490254	0.538731
24	7	0	-2.242028	0.604384	-0.007807
25	6	0	-2.620487	1.906693	-0.228935
26	8	0	-2.000217	2.764689	-0.818873
27	1	0	-4.194363	3.149774	0.190407
28	6	0	4.006565	1.421025	0.492994
29	1	0	3.516341	1.429748	1.472221
30	6	0	5.382997	0.767591	0.632227
31	6	0	4.140177	2.865410	-0.001118
32	1	0	5.313184	-0.239580	1.052054
33	1	0	5.892619	0.696688	-0.337985
34	1	0	6.017452	1.367395	1.293891
35	1	0	3.164524	3.348933	-0.088292
36	1	0	4.746221	3.450314	0.699087
37	1	0	4.640559	2.901259	-0.978557

Pt(Ura)(GV)- aqueous phase

1	8	0	0.900073	0.350103	-1.077335
2	6	0	1.695871	1.068585	-0.315323
3	8	0	1.363683	1.987131	0.421607
4	6	0	3.169577	0.580732	-0.438756

5	1	0	3.473932	0.728891	-1.482170
6	7	0	0.517344	-2.294393	-0.644136
7	6	0	1.563967	-2.662148	0.356426
8	1	0	2.204124	-3.447256	-0.061688
9	1	0	1.070237	-3.039814	1.250763
10	6	0	2.356151	-1.415996	0.732002
11	8	0	2.218749	-0.886343	1.832644
12	7	0	3.120846	-0.880408	-0.260034
13	1	0	3.159185	-1.405771	-1.122266
14	1	0	0.958696	-2.108424	-1.545710
15	1	0	-0.074976	-3.111554	-0.791737
16	78	0	-0.727275	-0.644323	-0.324046
17	7	0	-4.057547	2.107209	0.298296
18	6	0	-4.865822	1.133763	0.787953
19	1	0	-5.863475	1.446056	1.075020
20	6	0	-4.432017	-0.155468	0.895723
21	1	0	-5.059013	-0.952442	1.270193
22	6	0	-3.099337	-0.381844	0.472465
23	8	0	-2.468670	-1.510314	0.445665
24	7	0	-2.306097	0.620997	0.021304
25	6	0	-2.742775	1.906391	-0.137623
26	8	0	-2.091552	2.832179	-0.612645
27	1	0	-4.405487	3.053815	0.209799
28	6	0	4.170355	1.320968	0.463457
29	1	0	3.727180	1.388959	1.463199
30	6	0	5.498069	0.566558	0.563217
31	6	0	4.402121	2.739466	-0.068590
32	1	0	5.369053	-0.425799	1.004229
33	1	0	5.956769	0.439381	-0.425546
34	1	0	6.202577	1.127690	1.186719
35	1	0	3.466469	3.298447	-0.151469
36	1	0	5.069012	3.292721	0.601355
37	1	0	4.876133	2.710348	-1.058331

----

^{W}Pt(Ura)(GV)

1	8	0	0.765367	0.396344	-1.171068
2	6	0	1.652515	1.056917	-0.471854
3	8	0	1.440221	2.003973	0.280021
4	6	0	3.072701	0.460005	-0.678980
5	1	0	3.301391	0.542804	-1.748578
6	7	0	0.252808	-2.256129	-0.593398
7	6	0	1.303853	-2.614013	0.402884
8	1	0	1.864657	-3.482251	0.037611
9	1	0	0.825428	-2.868582	1.347619
10	6	0	2.215483	-1.418473	0.637724
11	8	0	2.217639	-0.844372	1.731873
12	7	0	2.914609	-0.985294	-0.438471
13	1	0	2.786438	-1.525143	-1.292467
14	1	0	0.685352	-2.222999	-1.526351
15	1	0	-0.409833	-3.030930	-0.627866
16	78	0	-0.879959	-0.517327	-0.366192
17	7	0	-4.094473	2.405126	0.077568
18	6	0	-4.954543	1.495510	0.599029
19	1	0	-5.941931	1.865609	0.850192
20	6	0	-4.579116	0.195290	0.779886

```
21          1          0       -5.247873   -0.552872    1.181690
22          6          0       -3.253613   -0.108511    0.392326
23          8          0       -2.668160   -1.265031    0.427295
24          7          0       -2.407942    0.831775   -0.093954
25          6          0       -2.786414    2.122186   -0.315221
26          8          0       -2.079808    2.996666   -0.819152
27          1          0       -4.396098    3.361401   -0.064320
28          6          0        4.197705    1.151502    0.104357
29          1          0        3.858459    1.276503    1.138539
30          6          0        5.476023    0.309820    0.099159
31          6          0        4.470740    2.537831   -0.489738
32          1          0        5.323360   -0.665848    0.569299
33          1          0        5.831337    0.138242   -0.924735
34          1          0        6.270939    0.830542    0.643757
35          1          0        3.572472    3.160557   -0.496802
36          1          0        5.237641    3.057129    0.094693
37          1          0        4.839762    2.453145   -1.520047
38          8          0       -0.021089    4.422189    0.529612
39          1          0       -0.829367    4.117881    0.084080
40          1          0        0.540138    3.627553    0.497286
41          1          0        3.396209   -0.346295    3.085760
42          8          0        3.909166   -0.147939    3.890392
43          1          0        4.824236   -0.079153    3.596991
44          8          0        2.048844   -2.384379   -2.937744
45          1          0        2.339701   -3.239569   -3.277847
46          1          0        1.929421   -1.820235   -3.711979
47          1          0       -3.223708   -2.899206    1.203636
48          8          0       -3.497925   -3.762550    1.559578
49          1          0       -3.202364   -3.762717    2.476744
          ----------------------------------------------------------------
```

REFERENCES

(1) Rappe, A. K., Casewit, C. J.; Colwell, K. S., Goddard III, W. A., Skiff, W. M. UFF, a Full Periodic Table Force Field for Molecular Mechanics and Molecular Dynamics Simulations. *J. Am. Chem. Soc.* **1992**, 114, 10024–10035

(2) Thompson, M. ArgusLab 4.0, Planaria Software LLC, Seattle, http://www.ArgusLab.com.