Electronic Supplementary Information

to the manuscript:

Ligand binding to G-quadruplex DNA: new insights from ultraviolet resonance Raman spectroscopy

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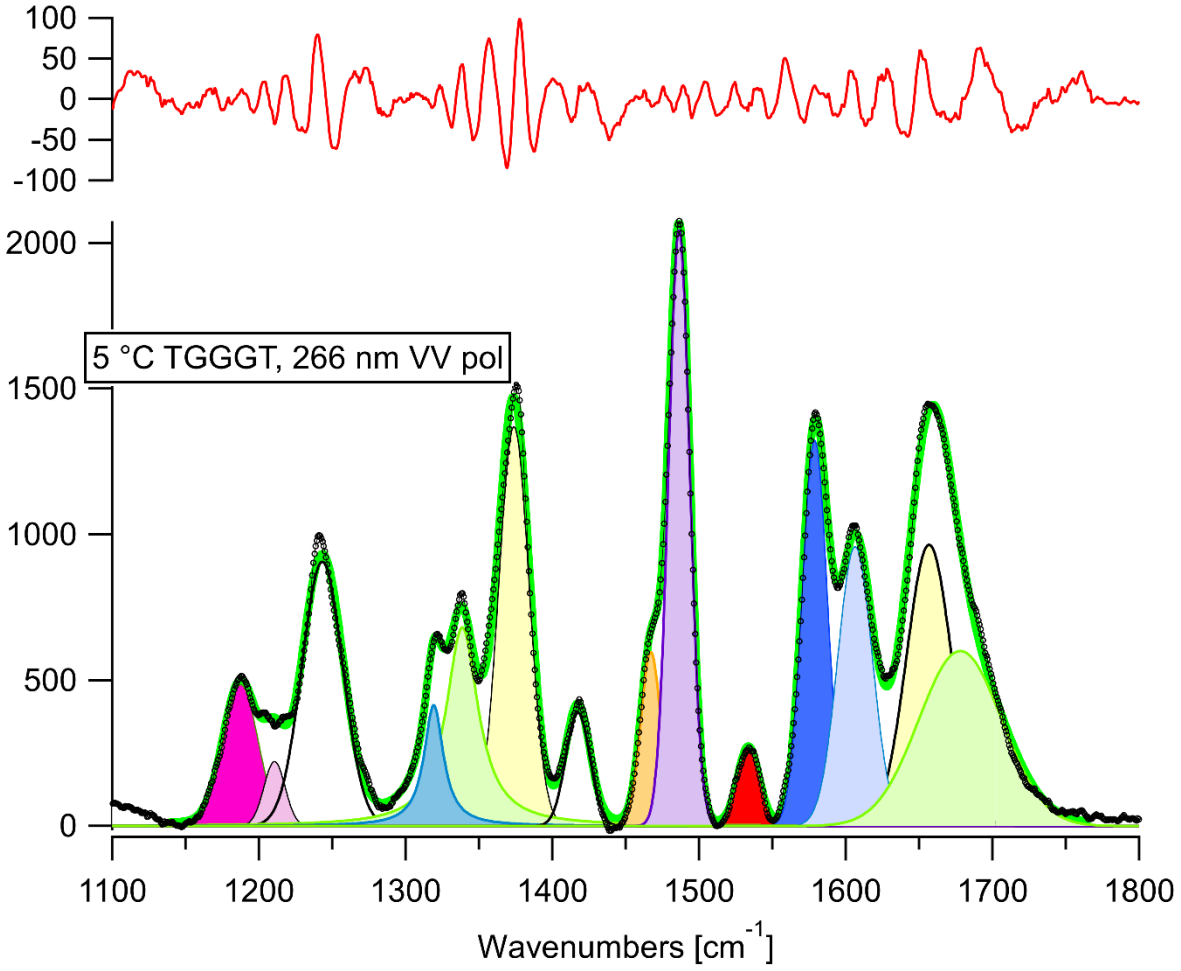

Fig. S1. VV polarized Ultraviolet Resonant Raman spectra at 5 °C and λ = 266 nm for TG_3T G4 solution (dotted line). The spectrum represents the average of 16 spectra of 15 minutes duration each. Data fitting with gaussians (green line). Vibrational assignment and wavenumbers for the position of the maxima of the bands are indicated in Table S1.

Table S1. Intensity, FWHM and position for the VV polarized UVRR bands from data fitting and corresponding vibrational assignment for TG_3T.

	Intensity	FWHM	position	assignment
1	485±7	28.0±1.0	1187.6±0.5	dT
2	222±17	17.0±1.5	1210.6±0.6	dT
3	907±6	32.7±0.4	1243.2±0.14	dT (NH def, CN str)
4	415±20	16.1±1.1	1319.1±0.4	dG (C2' endo/syn)
5	681±11	26.6±1.3	1338.6±0.3	dG (C2' endo/anti)
6	1370±8	24.3±0.2	1373.81±0.08	dT (C5-CH3 def)
7	390±8	19.3±0.5	1417.38±0.19	C2'H_2 scissor
8	597.5±9.6	16.1±05	1467.05±0.24	dG
9	2044±9	17.0±0.2	1486.4±0.1	dG N7 Hoogsteen bond
10	261±9	16.9±0.7	1533.59±0.26	dG
11	1323±10	20.05±0.22	1578.75±0.11	dG (NH def), N2-H, H-bond
12	958±7	27.7±0.5	1606.3±0.2	dG (NH def), N1-H, H-bond
13	965±6	36.0±0.3	1656.75±0.12	dT (C=O str) O4 H-bond
14	600±17	66.7±0.7	1678.0±0.5	dG (C=O str) O6 H-bond
				Baseline = 11.8±2
				Slope = 0.0

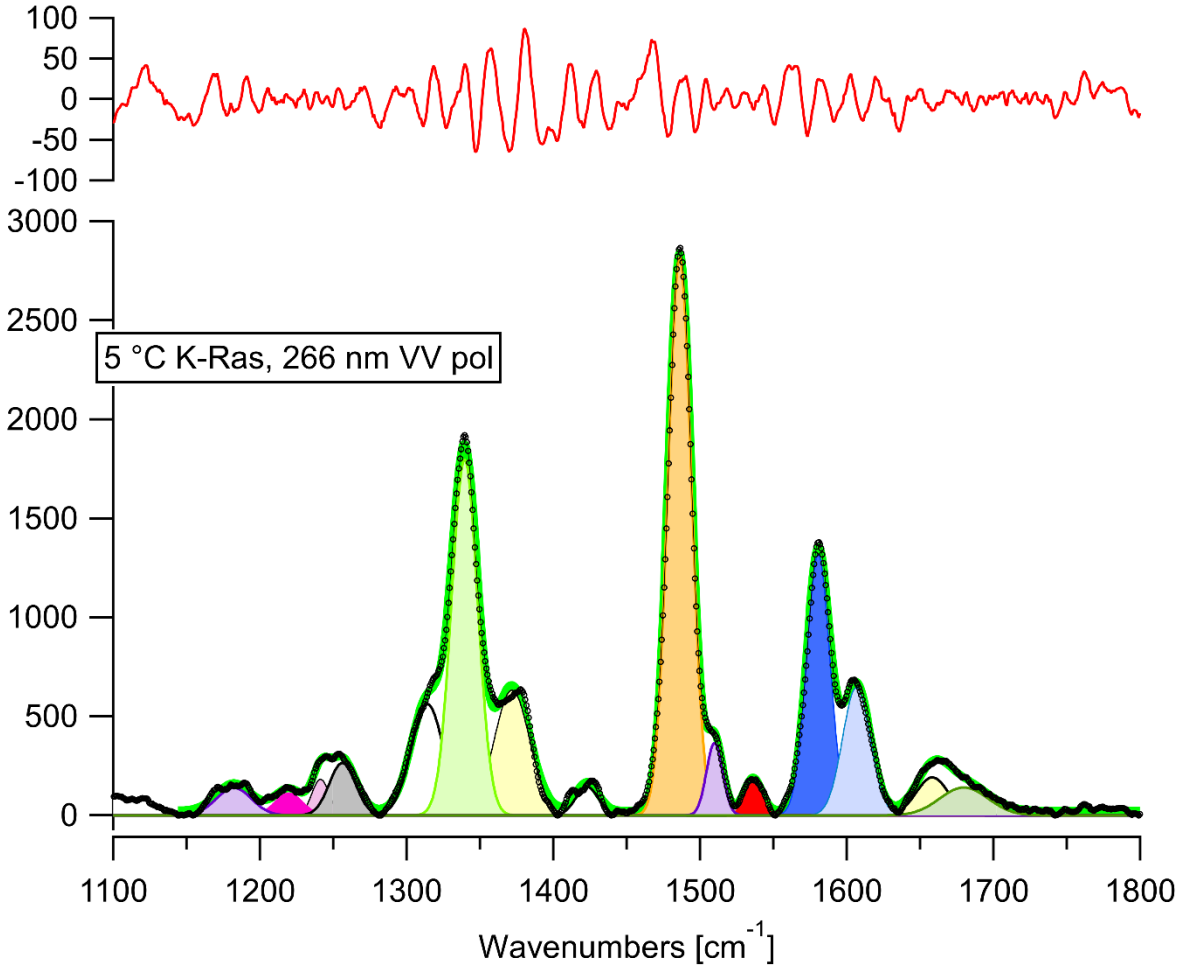

Fig. S2. VV polarized Ultraviolet Resonant Raman spectra at 5 °C and λ = 266 nm for K-Ras G4 solution (dotted line). The spectrum represents the average of 16 spectra of 15 minutes duration each. Data fitting with gaussians (green line). Vibrational assignment and wavenumbers for the position of the maxima of the bands are indicated in Table S2.

Table S2. Intensity, FWHM and position for the VV polarized UVRR bands from data fitting and corresponding vibrational assignment for K-Ras.

	Intensity	FWHM	position	assignment
1	141±6	28.5±1.8	1182.2±0.7	dT
2	114±7	21.9±3.3	1219.7±1.1	dT
3	183±41	13.9±2.2	1241±1	dT (NH def, CN str)
4	265.4±16	21.1±2.2	1256.2±1.5	dT (NH def, CN str)
5	563 ±7	25.8±0.7	1314.1±0.4	dA (C8-N9, C2-N3 purine rings vibration)
6	1797.0±11	20.93±0.24	1339.5±0.1	dA (C5-N7, N7-C8 imidazole ring vibration)
7	633±6	28.4±0.5	1371.8±0.2	dT (C5-CH3 def)
8	145±7	18.1±1.1	1422.9±0.4	dA (N1C6, C6N), C2'H_2 scissor
9	2819±7	18.74±0.07	1486.11±0.025	dG N7 Hoogsteen bond
10	366±9	12.9±0.4	1509.83±0.17	dA
11	169±8	13.9±0.8	1537.11±0.33	dG
12	1317±7	18.67±0.17	1580.42±0.08	dG (NH def), N2-H, H-bond
13	646±7	22.1±0.4	1606.51±0.17	dG (NH def), N1-H, H-bond
14	191±85	25.7±3.6	1657.3±1.8	dT (C=O str) O4 H-bond
15	142±40	41±12	1677±11	dG (C=O str) O6 H-bond
				Baseline = 22.7±.1.9
				Slope = 0.0

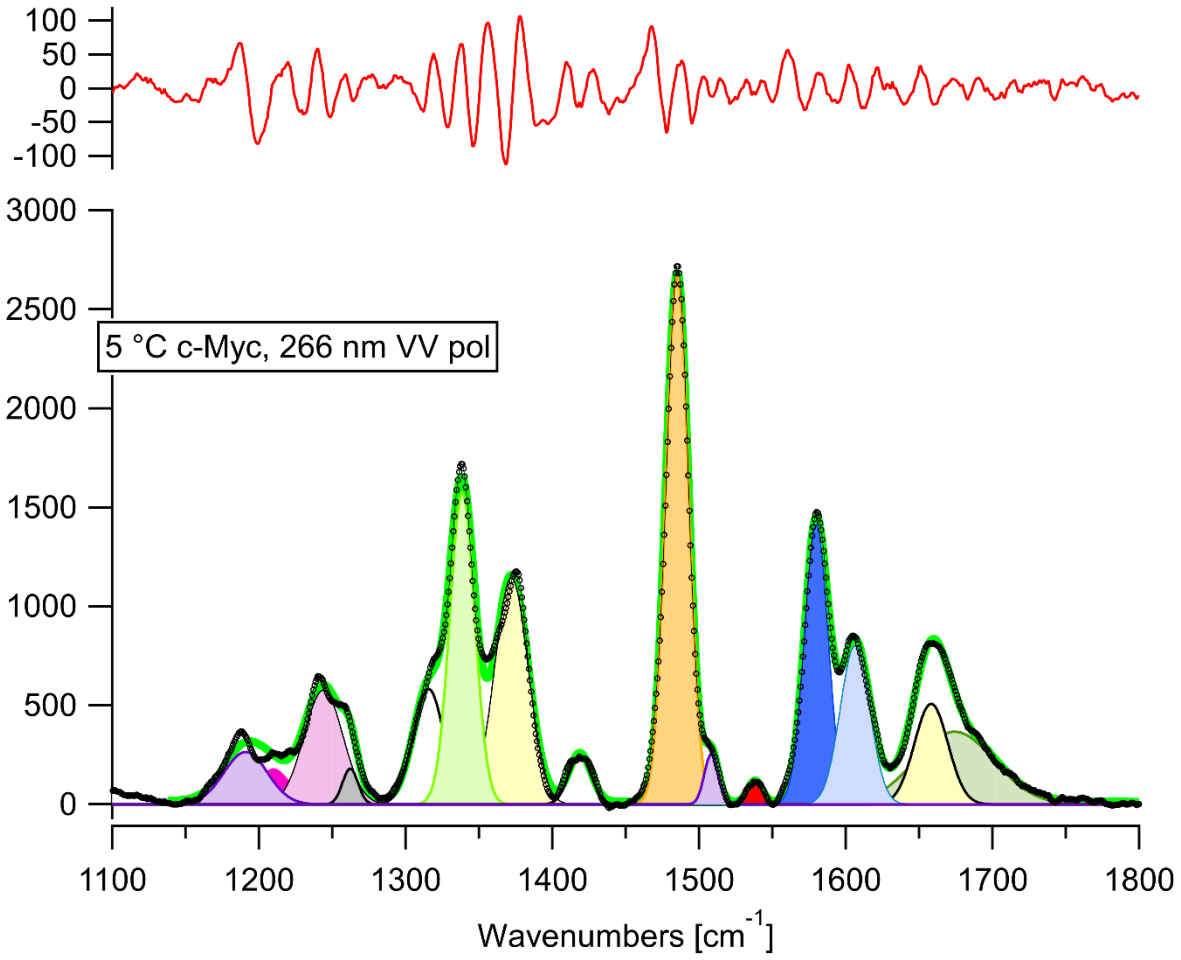

Fig. S3. VV polarized Ultraviolet Resonant Raman spectra at 5 °C and λ = 266 nm for c-Myc G4 solution (dotted line). The spectrum represents the average of 16 spectra of 15 minutes duration each. Data fitting with gaussians (green line). Vibrational assignment and wavenumbers for the position of the maxima of the bands are indicated in Table S3.

Table S3. Intensity, FWHM and position for the VV polarized UVRR bands from data fitting and corresponding vibrational assignment for c-Myc.

	Intensity	FWHM	position	assignment
1	265±78	34.9±1.2	1191.0±0.5	dT
2	180±20	29.6±0.1	1210±3	dT
3	577.0±8	31.0 ±0.7	1244.2±0.4	dT (NH def, CN str)
4	181±14	13 ±1	1262.2±0.4	dT (NH def, CN str)
5	583±12	24.4±1.0	1315.7±0.6	dA (C8-N9, C2-N3 purine rings vibration)
6	1571±18	20.1±0.3	1338.61±0.17	dA (C5-N7, N7-C8 imidazole ring vibration)
7	1143±8	26.9±0.3	1372.07±0.11	dT (C5-CH3 def)
8	246±10	17.8±0.8	1418.8±0.3	dA (N1C6, C6N), C2'H_2 scissor
9	2672±10	18.22±0.09	1486.07±0.03	dG N7 Hoogsteen bond
10	253±12	11.1±0.7	1508.24±0.28	dA
11	107±12	10.8±1.4	1538.1±0.6	dG
12	1413±10	19.04±0.23	1579.81±11	dG (NH def), N2-H, H-bond
13	801±9	23.7±0.7	1606.26±0.21	dG (NH def), N1-H, H-bond
14	508±30	27.0±1.3	1658.2±0.3	dT (C=O str) O4 H-bond
15	367±22	63.4±2.0	1674.3±1.9	dG (C=O str) O6 H-bond
				Baseline = 13.8±2.5
				Slope = 0.0

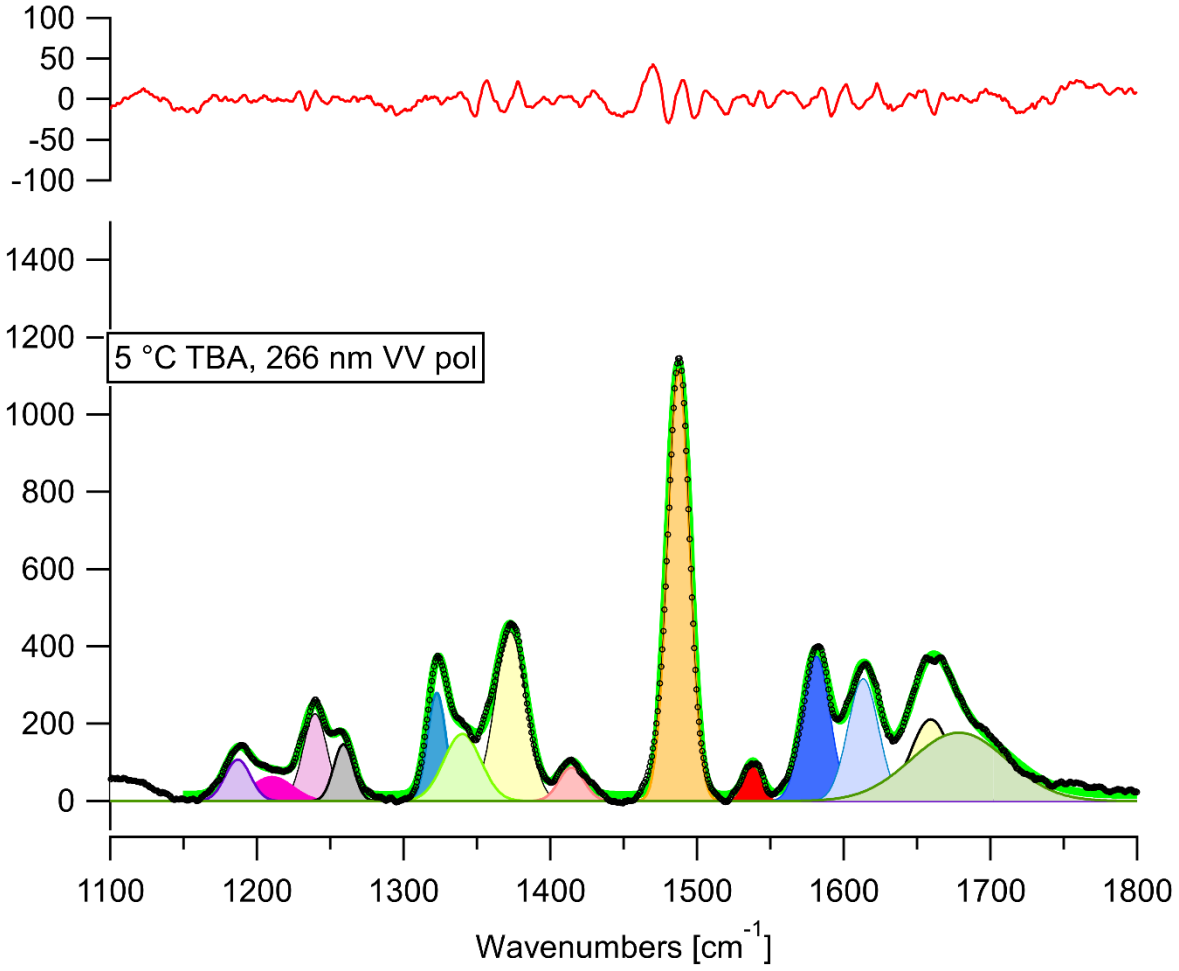

Fig. S4. VV polarized Ultraviolet Resonant Raman spectra at 5 °C and λ = 266 nm for TBA G4 solution (dotted line). The spectrum represents the average of 16 spectra of 15 minutes duration each. Data fitting with gaussians (green line). Vibrational assignment and wavenumbers for the position of the maxima of the bands are indicated in Table S4.

Table S4. Intensity, FWHM and position for the VV polarized UVRR bands from data fitting and corresponding vibrational assignment for TBA.

	Intensity	FWHM	position	assignment
1	107.0±46	20.5±3.0	1187.0±1.7	dT
2	64±6	34±26	1210±6	dT
3	226±20	19.1±1.7	1239.6±0.5	dT (NH def, CN str)
4	147±7	15.6±0.9	1258.9±0.6	dT (NH def, CN str)
5	280±24	14.7±0.7	1322.57±0.15	dG (C2' endo/syn)
6	174±6	29.8±3.3	1340±1.4	dG (C2' endo/anti)
7	438±4	24.7±0.4	1372.75±0.19	dT (C5-CH3 def)
8	87±3	20.1±0.9	1414.4±0.4	C2'H_2 scissor
9	1117.0±3.4	17.69±0.05	1487.37±0.03	dG N7 Hoogsteen bond
10	87±4	13.5±0.7	1537.94±0.29	dG
11	375±3	21.79±0.29	1581.35±0.12	dG (NH def), N2-H, H-bond
12	316±13	24.6±0.8	1613.21±0.25	dG (NH def), N1-H, H-bond
13	211±28	32.2±2.3	1659.2±0.6	dT (C=O str) O4 H-bond
14	177±16	77 ±5	1678±5	dG (C=O str) O6 H-bond
				Baseline = 16.3±0.9
				Slope = 0.0

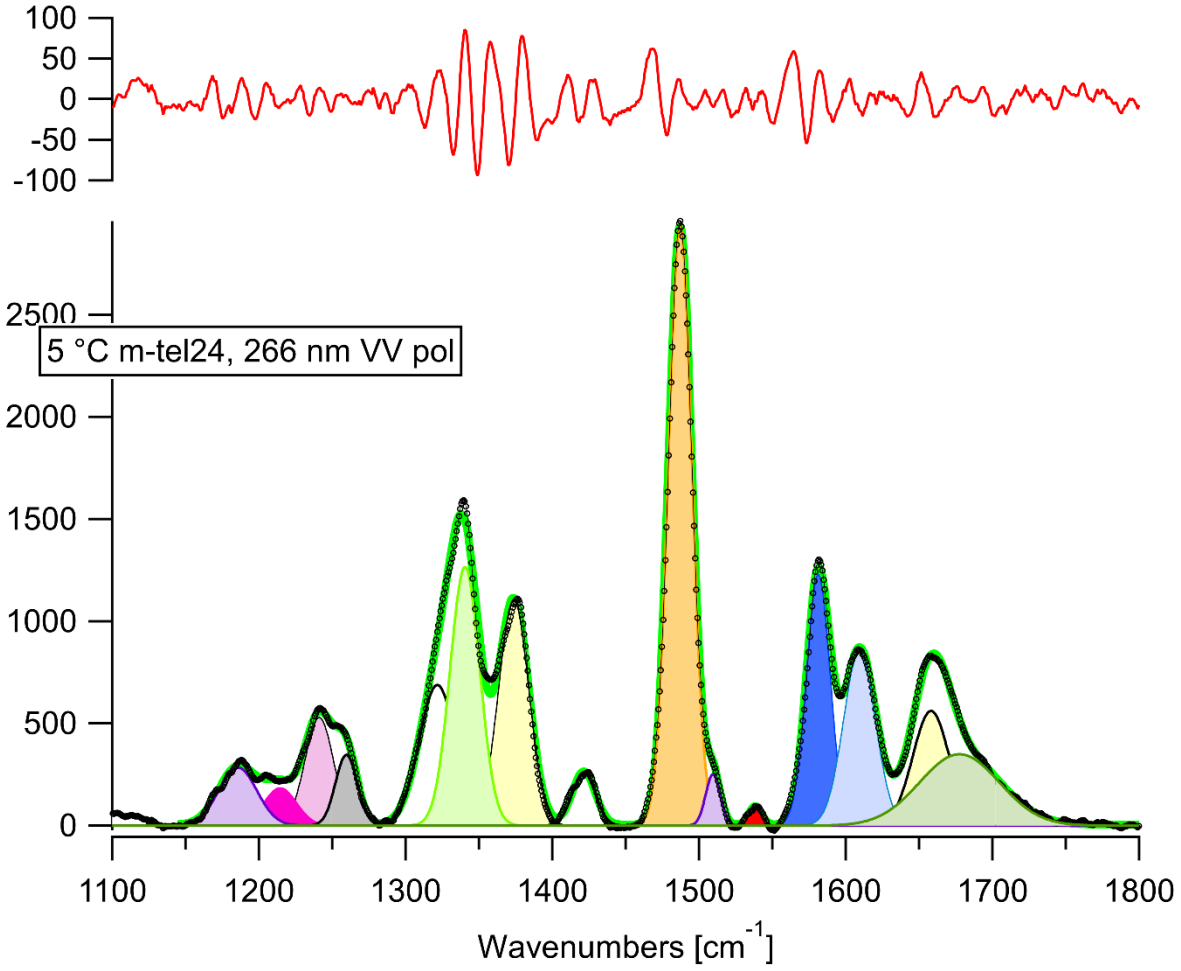

Fig. S5. VV polarized Ultraviolet Resonant Raman spectra at 5 °C and λ = 266 nm for m-tel24 G4 solution (dotted line). The reported spectrum represents the average of 16 spectra of 15 minutes duration each. Data fitting with gaussians (green line). Vibrational assignment and wavenumbers for the position of the maxima of the bands are indicated in Table S5.

Table S5. Intensity, FWHM and position for the VV polarized UVRR bands from data fitting and corresponding vibrational assignment for m-tel24.

	Intensity	FWHM	position	assignment
1	284±18	30.6±2.5	1185.6 ±1.9	dT
2	185 ±28	26±9	1215.5 ±2.5	dT
3	529±36	22.8±3.5	1241.1 ±0.8	dT (NH def, CN str)
4	346±58	17.5±1.3	1259.6±1.3	dT (NH def, CN str)
5	688±73	29.3±2.0	1319.6±0.6	dA (C8-N9, C2-N3 purine rings vibration)
6	1266±109	24.9±0.8	1340.44±0.63	dA (C5-N7, N7-C8 imidazole ring vibration)
7	1105±7	24.20±0.26	1373.64±0.11	dT (C5-CH3 def)
8	261±7	18.4±0.6	1421.39±0.24	dA (N1C6, C6N), C2'H_2 scissor
9	2930±7	18.92±0.06	1487.08±0.025	dG N7 Hoogsteen bond
10	251±9	11.7±0.6	1509.46±0.24	dA
11	92±10	10.0±1.2	1538.6±0.5	dG
12	1229±8	18.95±0.20	1581.21±0.09	dG (NH def), N2-H, H-bond
13	851±11	25.6±0.6	1609.3±0.2	dG (NH def), N1-H, H-bond
14	562±48	29.4±1.4	1658.2±0.3	dT (C=O str) O4 H-bond
15	350±27	66±3	1677.5±3.4	dG (C=O str) O6 H-bond
				Baseline = -1.3±2.2
				Slope = 0.0

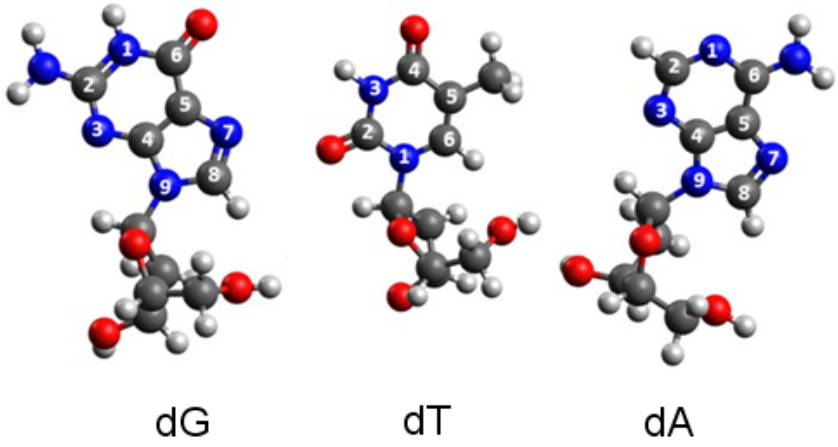

Fig. S6. Structures and numbering convention for the deoxyguanosine (dG), deoxythymidine (dT), and deoxyadenosine (dA).

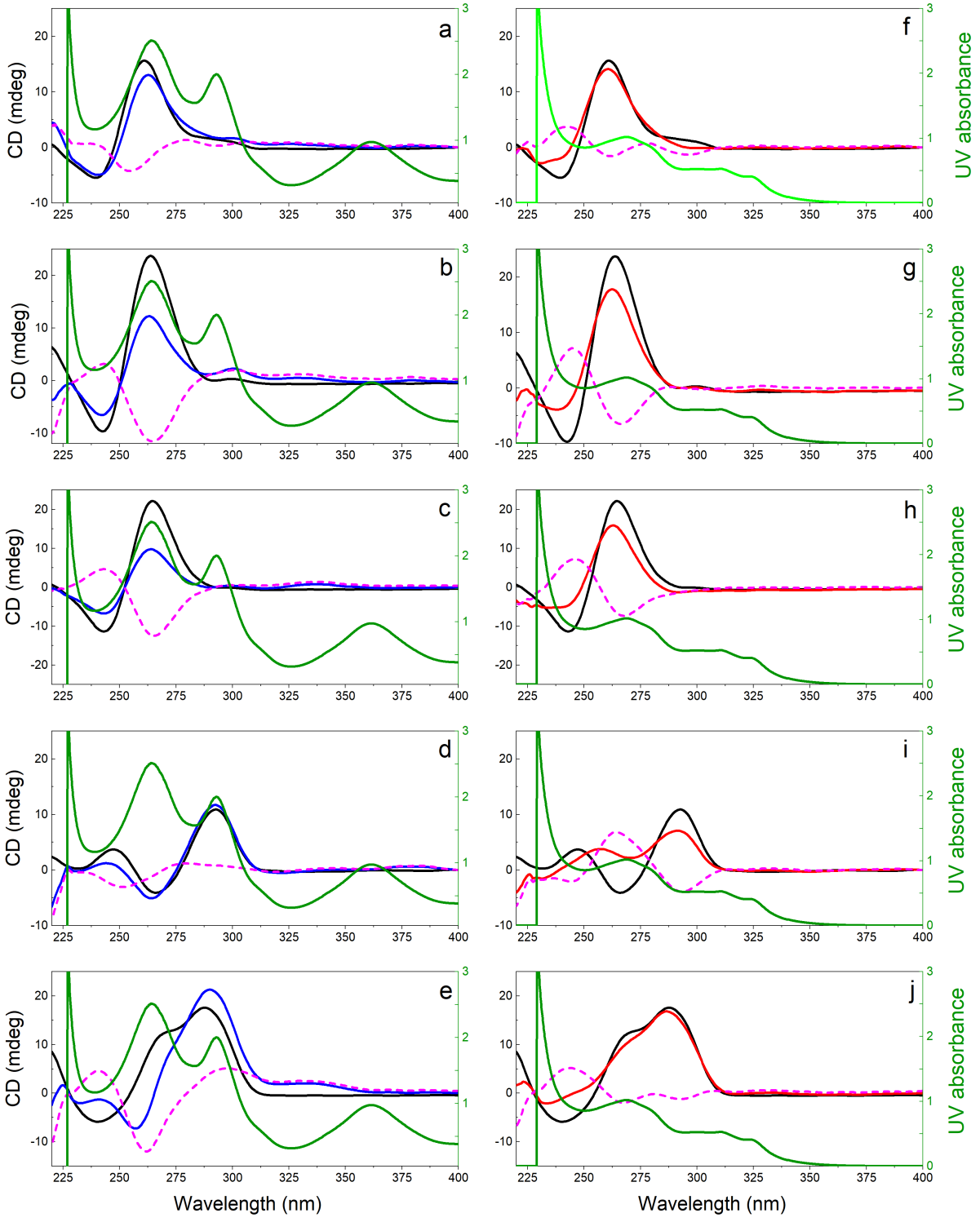

Fig. S7. (a-e) CD spectra of (a) TG_3T, (b) K-Ras, (c) c-Myc, (d) TBA, and (e) m-tel24 G4s in the absence (black line) and presence of B19 (blue line), along with their relative CD difference spectra (dashed magenta line) and UV-VIS absorbance spectra of B19 (green line, right axis). (f-j) CD spectra of (f) TG_3T, (g) K-Ras, (h) c-Myc, (i) TBA, and (j) m-tel24 G4s in the absence (black line) and presence of PDS (red line), along with their relative CD difference spectra (dashed magenta line) and UV-VIS absorbance spectra of PDS (green line, right axis).

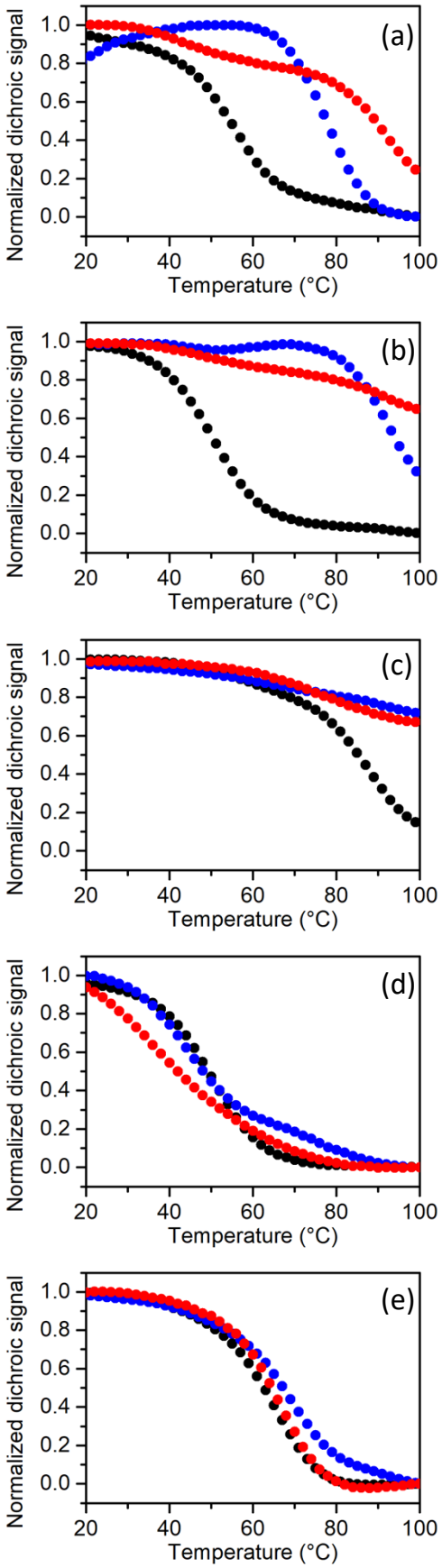

Fig. S8. CD melting curves of (a) TG_3T, (b) K-Ras, (c) c-Myc, (d) TBA, and (e) m-tel24 G4s in the absence (black circles) and presence of of 5 mol. equiv. of B19 (blue circles) or PDS (red circles). Each curve has been normalized for its maximum intensity value.

NCE and anisotropic and isotropic spectra

Polarized VV and HV UVRR spectra with different acquisition times (see Fig. S9 caption) were collected al λ = 266 nm. The measurements were made by rotating the linear polarization of the incoming beam (V is the polarization parallel to the laser beam and H is the polarization perpendicular to the laser beam) by inserting a half-wave plate along the path between laser and sample and by selecting the vertical polarization of the scattered radiation by a polarizer in the beam path between the sample and the spectrometer. In this way, the scattered light from the sample polarized parallel (I_{VV}) and perpendicular (I_{HV}) with respect to the incident radiation was collected. Isotropic and anisotropic Raman intensity profiles were obtained according to the relations:

$$I_{iso} = I_{VV} - 4/3\ I_{HV} \quad \text{and} \quad I_{aniso} = I_{HV}$$

The non-coincidence effect, NCE, is defined as the difference of the position of the maxima of the isotropic and anisotropic Raman components:

$$\Delta\nu_{NCE} = \nu_{aniso} - \nu_{iso}$$

Fig. S9 shows anisotropic and isotropic spectra at 5 °C for TG_3T, TG_3T/B19, and B19 solutions.

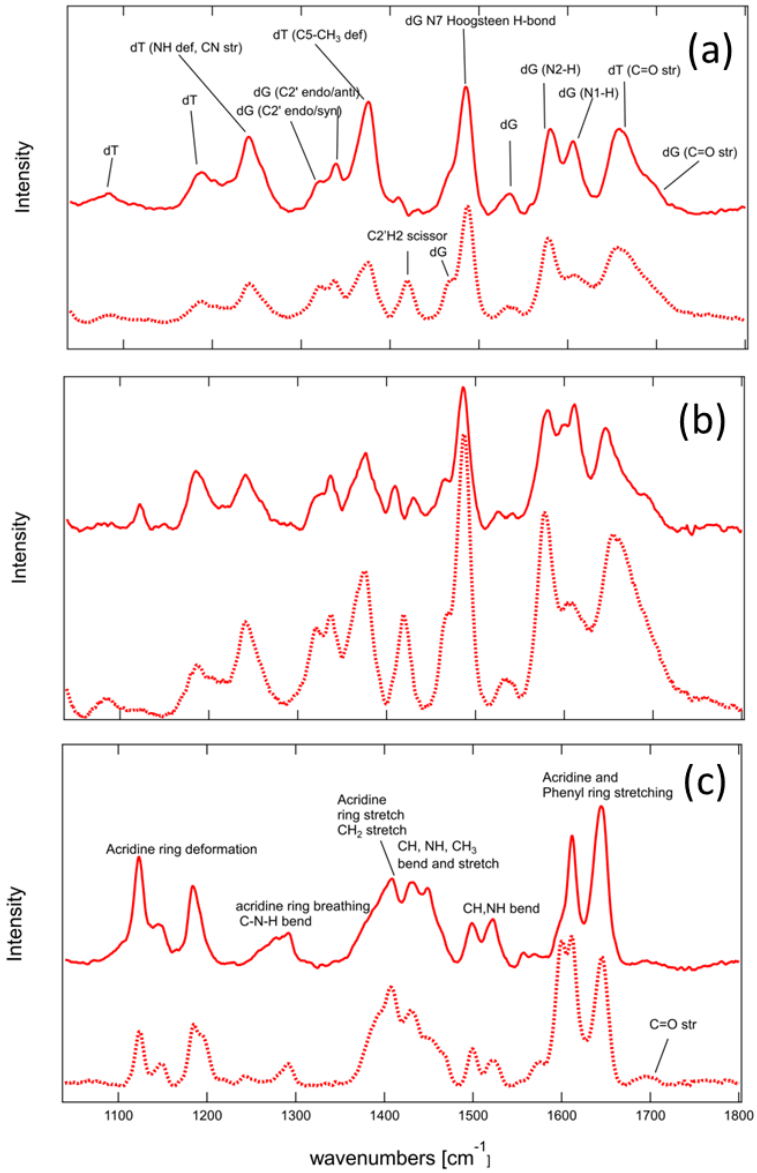

Fig. S9. Reduced anisotropic (dotted line) and isotropic (solid line) UVRR spectra at 5 °C and λ = 266 nm for (a) TG_3T; (b) TG_3T/B19 and (c) B19 solutions. The anisotropic spectrum $I_{aniso} = I_{HV}$ is the average of 32 spectra of 15 min each. The isotropic spectrum $I_{iso} = I_{VV} - 4/3\ I_{HV}$ has been calculated from the reduced spectra where I_{VV} is the average of 16 spectra of 15 min each. Vibrational assignments of wavenumbers for TG_3T and B19 are showed in Tables 2 and 3.

Quantum chemical computations

Raman activities (S_i) were converted to relative Raman Intensities (I_i) using the following relationship derived from the theory of Raman scattering[1]:

$$I_i = \frac{A(\nu_0 - \nu_i)^4 S_i}{\nu_i \left[1 - \exp\left(-\frac{hc\nu_i}{kT}\right)\right]} \quad [1]$$

where ν_0 is the excitation frequency (in cm^{-1} units), ν_i is he vibrational wavenumber of the *i*th normal mode, h is the Planck constant, c is the speed of light, k is the Boltzmann constant and A is a common normalization factor for all peak intensities.

Molecular optimization and Harmonic frequencies have been calculated with the density functional theory employing B3LYP exchange-correlation function and the 6-311G(2d,2p).

Tables S6 and S7 report the PDB files with the coordinates of the molecular optimization for BRACO-19 (B19) and Pyridostatin (PDS), respectively.

Tables S8 and S9 report the simulated harmonic frequencies, Raman activity (RA) and intensity for the ground state molecular structure of B19 and PDS, respectively.

[1] V. Krishnakumar, G. Keresztury, T. Sundius and R. Ramasamy, Simulation of IR and Raman spectra based on scaled DFT force fields: a case study of 2-(methylthio)benzonitrile, with emphasis on band assignment, *Journal of Molecular Structure*, 2004, **702**, 9–21.

Table S6. PDB with the coordinates of the molecular optimization of BRACO-19 (B19).

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HETATM   77 C         0      11.210  -3.628   0.846                C
HETATM   78 N         0      -4.197  -1.540  -0.670                N
HETATM   79 C         0      -1.081   1.318  -0.870                C
HETATM   80 H         0       7.423  -0.692   1.483                H
HETATM   81 C         0       7.839  -2.287   0.116                C
HETATM   82 C         0       2.428   2.649  -0.670                C
HETATM   83 H         0      -8.702  -8.041   1.217                H
HETATM   84 C         0      -0.027   2.256  -0.922                C
HETATM   85 H         0      -9.974  -6.023   1.103                H
HETATM   86 C         0      -1.644   4.272   0.649                C
HETATM   87 H         0      -4.644   9.159   1.151                H
END
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Table S7. PDB with the coordinates of the molecular optimization of Pyridostatin (PDS).

```
TITLE     PDS freq b3lyp optimized structure
REMARK   1 File created by GaussView 6.0.16
HETATM    1  O        0     -6.565  -2.036   0.155                O
HETATM    2  O        0      7.153  -0.761  -0.363                O
HETATM    3  O        0     -0.285   5.762  -0.123                O
HETATM    4  O        0     -3.540   1.852   0.013                O
HETATM    5  O        0      3.461   2.506  -0.224                O
HETATM    6  N        0      0.008   1.632  -0.108                N
HETATM    7  N        0     -2.416  -2.241  -0.022                N
HETATM    8  N        0      3.108  -1.723  -0.164                N
HETATM    9  N        0     -2.160   0.013  -0.028                N
HETATM   10  N        0      2.439   0.446  -0.183                N
HETATM   11  N        0     -2.556   8.640  -0.069                N
HETATM   12  N        0     -9.473   0.193   0.277                N
HETATM   13  N        0      8.781   0.512   1.717                N
HETATM   14  C        0     -4.603  -3.332   0.068                C
HETATM   15  C        0      5.460  -2.386  -0.248                C
HETATM   16  C        0     -3.182  -3.366   0.008                C
HETATM   17  C        0      4.070  -2.684  -0.183                C
HETATM   18  C        0     -1.189   2.216  -0.072                C
HETATM   19  C        0      1.082   2.434  -0.149                C
HETATM   20  C        0     -3.034  -1.083   0.007                C
HETATM   21  C        0     -5.217  -2.043   0.098                C
HETATM   22  C        0      3.499  -0.471  -0.208                C
HETATM   23  C        0      5.826  -1.006  -0.293                C
HETATM   24  C        0     -2.429   1.347  -0.024                C
HETATM   25  C        0      2.460   1.807  -0.190                C
HETATM   26  C        0     -4.438  -0.912   0.069                C
HETATM   27  C        0      4.847  -0.042  -0.271                C
HETATM   28  C        0     -0.257   4.417  -0.117                C
HETATM   29  C        0     -1.381   3.595  -0.075                C
HETATM   30  C        0      1.003   3.815  -0.155                C
HETATM   31  C        0     -5.332  -4.540   0.096                C
HETATM   32  C        0      6.401  -3.438  -0.270                C
HETATM   33  C        0     -2.537  -4.624  -0.023                C
HETATM   34  C        0      3.671  -4.041  -0.138                C
HETATM   35  C        0     -4.675  -5.746   0.065                C
HETATM   36  C        0      5.982  -4.745  -0.224                C
HETATM   37  C        0     -3.268  -5.785   0.005                C
HETATM   38  C        0      4.606  -5.045  -0.157                C
HETATM   39  C        0     -7.248  -0.778   0.184                C
HETATM   40  C        0      7.637   0.593  -0.441                C
HETATM   41  C        0     -1.553   6.429  -0.083                C
HETATM   42  C        0     -8.738  -1.073   0.233                C
HETATM   43  C        0      7.772   1.228   0.932                C
HETATM   44  C        0     -1.278   7.924  -0.100                C
HETATM   45  H        0     -6.949  -0.201   1.061                H
HETATM   46  H        0     -6.995  -0.201  -0.710                H
HETATM   47  H        0     -1.183  -0.241  -0.065                H
HETATM   48  H        0     -6.410  -4.497   0.142                H
HETATM   49  H        0     -1.457  -4.632  -0.069                H
HETATM   50  H        0     -2.391   3.966  -0.046                H
HETATM   51  H        0      8.622   0.497  -0.892                H
HETATM   52  H        0      6.998   1.183  -1.098                H
HETATM   53  H        0      1.525   0.017  -0.144                H
HETATM   54  H        0      7.452  -3.195  -0.327                H
HETATM   55  H        0      2.612  -4.250  -0.088                H
HETATM   56  H        0      1.905   4.405  -0.188                H
HETATM   57  H        0     -4.842   0.083   0.092                H
HETATM   58  H        0      5.051   1.012  -0.290                H
HETATM   59  H        0     -2.160   6.150  -0.945                H
HETATM   60  H        0     -2.090   6.144   0.826                H
HETATM   61  H        0     -5.238  -6.669   0.086                H
HETATM   62  H        0      6.707  -5.547  -0.242                H
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HETATM   63  H         0     -2.761  -6.741  -0.019               H
HETATM   64  H         0      4.287  -6.079  -0.122               H
HETATM   65  H         0     -9.499   0.618  -0.643               H
HETATM   66  H         0    -10.435   0.029   0.541               H
HETATM   67  H         0     -8.951  -1.630   1.146               H
HETATM   68  H         0     -8.999  -1.725  -0.611               H
HETATM   69  H         0      8.866   0.931   2.635               H
HETATM   70  H         0      8.470  -0.441   1.870               H
HETATM   71  H         0      6.786   1.282   1.409               H
HETATM   72  H         0      8.112   2.255   0.783               H
HETATM   73  H         0     -2.424   9.602  -0.349               H
HETATM   74  H         0     -0.763   8.169  -1.029               H
HETATM   75  H         0     -0.595   8.169   0.722               H
HETATM   76  H         0     -2.925   8.666   0.874               H
END
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Table S8. Simulated Raman activity (RA) and intensity (T = 5 °C, λ = 266 nm) for the ground state molecular structure of B19. Vibrational modes with RA >10 are highlighted in red.

Mode	frequency	infrared	Raman Activity	Depolar P	Depolar U	Raman Intensity
1	8.52	0.3563	1.1293	0.7185	0.8362	116507.42
2	9.51	0.2515	2.2243	0.732	0.8453	184660.06
3	14.49	0.3074	3.6442	0.7483	0.856	132010.89
4	17.83	0.757	0.6598	0.739	0.8499	15921.99
5	19.76	0.1144	2.0285	0.7405	0.8509	40054.05
6	20.38	0.3284	0.9199	0.6554	0.7918	17102.90
7	24.88	0.8999	7.6245	0.5617	0.7193	96218.85
8	29.04	1.741	1.6195	0.7153	0.834	15161.82
9	34.91	1.4453	1.7447	0.6872	0.8146	11472.64
10	39.39	0.3713	8.4516	0.6242	0.7686	44149.84
11	54.2	2.2851	3.3542	0.544	0.7046	9604.23
12	59.79	0.8554	1.4786	0.3581	0.5273	3527.65
13	60.47	5.3356	1.6383	0.7309	0.8445	3827.68
14	63.01	1.7347	1.2414	0.7406	0.8509	2688.05
15	64.13	0.061	0.449	0.7496	0.8569	941.17
16	73.7	1.0437	2.3574	0.5536	0.7127	3830.22
17	79.27	1.2877	1.1225	0.341	0.5086	1598.00
18	83.73	0.258	0.6732	0.4171	0.5886	868.31
19	89.81	0.3201	0.5043	0.5912	0.7431	573.70
20	101.53	1.1834	1.0729	0.4516	0.6223	982.09
21	106.77	2.3731	1.4377	0.6491	0.7872	1204.85
22	113.8	2.1919	0.3476	0.7413	0.8514	260.69
23	122.34	0.3571	1.1166	0.6991	0.8229	739.15
24	130.19	2.1037	1.971	0.0892	0.1638	1173.22
25	135.25	6.8601	1.3337	0.1836	0.3102	744.17
26	141.28	6.8373	5.2885	0.436	0.6073	2741.78
27	176.58	0.2863	1.0407	0.711	0.8311	373.69
28	184.04	1.3297	0.7966	0.2565	0.4083	267.64
29	186.51	0.8803	1.4726	0.0877	0.1612	484.33
30	203.72	0.7813	1.5354	0.6721	0.8039	439.18
31	206.95	5.7307	0.2895	0.5819	0.7357	80.80
32	217.03	14.5311	4.8464	0.4136	0.5852	1256.22
33	222.66	4.4111	3.155	0.7477	0.8556	786.15
34	241.28	4.4498	2.0654	0.1936	0.3245	455.42
35	261.01	1.3765	9.0506	0.5969	0.7476	1774.55
36	263.75	0.8062	1.5134	0.7242	0.84	292.19
37	275.12	15.3098	7.5981	0.4903	0.658	1378.81
38	287.15	1.7219	0.7912	0.7473	0.8554	134.93
39	313.64	2.6826	2.0671	0.4334	0.6047	310.78
40	338.35	2.5642	17.7425	0.4384	0.6096	2399.44
41	348.62	0.4254	1.122	0.4846	0.6528	145.62
42	355.54	23.762	8.9078	0.2915	0.4514	1125.41
43	364.68	0.4238	1.8296	0.1621	0.2789	223.31
44	368.66	6.7427	1.8405	0.1092	0.1968	221.37
45	373.92	19.3266	12.5996	0.2516	0.4021	1486.78
46	381.51	2.5217	0.3086	0.6189	0.7646	35.45
47	400.17	17.1373	11.4665	0.1747	0.2975	1236.09
48	411.34	12.9523	3.6425	0.1284	0.2275	378.70
49	419.78	3.6957	2.0233	0.5889	0.7413	204.84
50	428.96	0.4351	9.767	0.3657	0.5355	961.43
51	448.72	12.8325	0.6628	0.7179	0.8358	61.57
52	463.61	56.074	231.0581	0.2485	0.398	20588.15
53	465.94	29.5863	27.7473	0.6303	0.7732	2456.72
54	483.48	4.0784	3.7162	0.4201	0.5917	314.04
55	486.22	39.8487	83.4994	0.2669	0.4213	7006.41
56	498.82	22.1972	4.141	0.3913	0.5625	336.54
57	512.25	14.9572	4.8602	0.5049	0.671	382.17
58	515.51	40.2199	5.5895	0.422	0.5935	436.09
59	522.8	19.7774	17.4869	0.5555	0.7142	1340.88

60	533.4	0.4904	1.1738	0.5898	0.742	87.81
61	558.58	4.3965	4.5827	0.2818	0.4397	324.10
62	580.39	9.633	3.4283	0.6835	0.812	231.50
63	590.77	7.8046	11.5017	0.1056	0.191	760.33
64	601.32	0.049	1.0483	0.1404	0.2462	67.85
65	608.39	0.9719	3.2964	0.2233	0.3651	210.40
66	612.52	11.8936	22.5646	0.2881	0.4474	1428.66
67	636.49	18.0551	13.0121	0.3654	0.5352	787.23
68	644.52	4.2672	5.1917	0.1202	0.2145	309.49
69	651.99	1.0388	1.3603	0.7492	0.8566	80.00
70	652.04	0.5132	1.7186	0.7476	0.8556	101.06
71	654.01	6.222	3.8108	0.75	0.8571	223.30
72	658.38	0.3791	18.3561	0.2563	0.4081	1067.23
73	668.66	17.3525	6.7985	0.1439	0.2516	388.16
74	677.5	7.8711	16.9653	0.1354	0.2386	953.87
75	717.8	6.7403	10.2874	0.2438	0.392	540.83
76	723.9	3.0973	16.2528	0.0526	0.0999	846.12
77	733.11	7.157	5.3453	0.3764	0.547	274.24
78	738.16	4.8988	63.4672	0.1519	0.2638	3230.52
79	750.8	1.5147	19.814	0.7087	0.8295	989.01
80	757.27	0.9667	4.829	0.2334	0.3785	238.67
81	779.01	28.493	5.2657	0.3076	0.4705	251.93
82	782.05	0.9416	10.7357	0.3507	0.5193	511.36
83	782.48	10.9866	3.0816	0.6959	0.8207	146.69
84	787.28	1.7207	7.3675	0.7489	0.8564	348.26
85	801.81	4.7194	5.6168	0.5678	0.7243	260.00
86	807.59	3.2288	1.2883	0.4091	0.5807	59.15
87	809.6	1.0767	2.9525	0.23	0.374	135.17
88	823.19	6.245	3.801	0.2109	0.3484	170.74
89	825.74	20.536	5.8675	0.1186	0.212	262.64
90	833.84	19.4411	2.3488	0.1398	0.2453	103.97
91	850.55	11.9705	13.3043	0.7425	0.8522	575.78
92	865.56	1.4413	10.2752	0.6431	0.7828	435.93
93	869.28	0.1572	1.2305	0.7453	0.8541	51.95
94	870.59	8.6242	6.7852	0.5209	0.685	285.98
95	889.95	26.4944	6.5282	0.4438	0.6147	268.36
96	890.09	3.2445	40.4438	0.1914	0.3212	1662.24
97	904.07	6.9781	9.3068	0.0448	0.0857	375.80
98	904.25	7.3409	7.7889	0.0563	0.1066	314.44
99	933.09	4.633	33.9061	0.2687	0.4236	1320.93
100	937.73	7.644	3.122	0.5704	0.7264	120.95
101	939	16.2568	2.0938	0.6567	0.7928	80.99
102	945.44	1.6531	37.8612	0.1925	0.3228	1453.20
103	948.63	3.3734	11.2259	0.4306	0.602	429.24
104	956.24	2.9795	11.9169	0.4589	0.6291	451.55
105	958.29	0.4904	1.0075	0.5578	0.7161	38.08
106	959.56	5.9333	10.746	0.4547	0.6251	405.59
107	962.36	46.1614	11.3265	0.1888	0.3177	426.09
108	964.64	0.364	0.6117	0.5521	0.7115	22.95
109	969.09	2.8739	3.9616	0.2385	0.3851	147.86
110	971.01	7.016	4.2951	0.3475	0.5158	159.95
111	977.94	2.9129	4.2579	0.3735	0.5438	157.29
112	978	4.2474	1.117	0.7232	0.8394	41.26
113	981.17	5.5951	24.2108	0.2204	0.3612	891.03
114	1012.56	21.2957	0.1619	0.6321	0.7746	5.75
115	1024.53	0.3783	0.5579	0.3585	0.5278	19.55
116	1048.49	18.5694	4.0074	0.6411	0.7813	136.80
117	1048.61	17.1615	3.608	0.7455	0.8542	123.15
118	1062	22.2363	8.8903	0.207	0.343	299.12
119	1062.12	19.9189	6.8042	0.3259	0.4916	228.90
120	1067.49	11.1847	11.5149	0.3154	0.4795	385.16
121	1068.05	8.4468	13.638	0.2593	0.4118	455.91
122	1080.17	21.2636	0.0418	0.6477	0.7862	1.38

123	1109.81	54.9487	110.341	0.1009	0.1833	3531.49
124	1124.35	0.2641	1.0357	0.7392	0.85	32.66
125	1124.6	0.7572	1.1611	0.6057	0.7544	36.61
126	1135.47	0.5216	2.3073	0.7443	0.8534	71.95
127	1139.28	5.4615	1.2432	0.736	0.848	38.62
128	1139.66	9.8125	1.0467	0.7401	0.8506	32.50
129	1149.01	65.9779	44.231	0.3905	0.5616	1360.84
130	1153.42	2.3067	6.1472	0.7351	0.8473	188.31
131	1156.81	75.9835	15.1935	0.363	0.5327	463.87
132	1157.85	320.4409	3.4248	0.7312	0.8447	104.45
133	1159.55	79.2737	8.9161	0.3531	0.5219	271.48
134	1177.64	0.406	44.6364	0.335	0.5019	1335.36
135	1188.81	24.5803	2.439	0.6527	0.7898	72.18
136	1194.66	53.8642	15.0443	0.3126	0.4763	442.77
137	1203.78	124.5345	78.2001	0.4827	0.6511	2281.60
138	1210.58	4.5532	9.4918	0.5901	0.7422	275.16
139	1210.95	0.4391	16.7608	0.1689	0.289	485.72
140	1217.52	12.956	263.3501	0.1413	0.2476	7584.67
141	1219.41	358.6973	95.3237	0.7498	0.857	2740.53
142	1227.03	19.1172	36.9074	0.4141	0.5857	1053.55
143	1228.81	5.7111	7.6312	0.674	0.8053	217.48
144	1231.27	124.7912	97.96	0.2271	0.3701	2785.33
145	1237.37	15.7408	20.5047	0.4101	0.5817	579.73
146	1242.07	2.2843	4.3871	0.435	0.6062	123.50
147	1242.2	10.6108	4.5653	0.6618	0.7965	128.50
148	1254.05	33.8555	10.1941	0.6349	0.7767	283.83
149	1267.03	94.735	19.7803	0.5244	0.688	544.28
150	1267.82	3.157	15.7661	0.2398	0.3869	433.52
151	1269.85	131.0723	90.1389	0.6083	0.7564	2473.99
152	1276.11	118.8634	263.5321	0.206	0.3416	7192.33
153	1277.9	20.4198	3.9885	0.448	0.6188	108.68
154	1278.16	20.2947	24.6942	0.7267	0.8417	672.71
155	1287.37	101.8485	261.4741	0.1896	0.3187	7064.57
156	1295.86	3.4471	11.6815	0.7493	0.8567	313.24
157	1311.3	47.7584	14.1901	0.443	0.614	375.36
158	1312.15	10.1232	37.1267	0.2633	0.4168	981.36
159	1325.57	12.8085	74.2048	0.1539	0.2668	1938.60
160	1326.9	8.5055	12.8005	0.2958	0.4565	334.03
161	1327.62	14.3561	12.6528	0.1926	0.323	329.97
162	1332.5	16.6957	2.8615	0.2693	0.4243	74.31
163	1332.7	3.6642	2.4694	0.4589	0.6291	64.12
164	1344.82	8.0507	22.8566	0.6495	0.7875	587.29
165	1349.92	4.1307	8.8822	0.2396	0.3866	227.23
166	1353.69	14.376	34.621	0.7493	0.8567	882.85
167	1359.77	7.4138	11.755	0.674	0.8053	298.21
168	1365.73	309.7527	248.1281	0.1751	0.298	6263.02
169	1366.74	21.6962	14.9164	0.725	0.8406	376.18
170	1367.18	49.6334	14.9566	0.7359	0.8478	377.06
171	1386.13	26.0194	865.0162	0.1996	0.3328	21462.86
172	1390.71	38.2692	70.37	0.6778	0.8079	1739.37
173	1391.08	13.4991	13.8455	0.326	0.4917	342.12
174	1393.62	43.4671	165.789	0.6899	0.8165	4087.99
175	1426.51	21.6096	30.2527	0.3599	0.5293	726.06
176	1426.81	36.3166	25.0406	0.6004	0.7503	600.83
177	1439.04	240.7756	852.4819	0.2573	0.4093	20252.68
178	1450.31	256.4216	684.0557	0.2281	0.3714	16104.57
179	1458.18	59.2587	104.4468	0.2164	0.3558	2443.53
180	1460.25	174.8828	127.8946	0.2718	0.4274	2987.15
181	1475.63	6.5772	11.4674	0.5807	0.7348	264.59
182	1476.68	0.0564	9.193	0.5298	0.6927	211.93
183	1480.83	55.6089	58.8107	0.4565	0.6268	1351.38
184	1491.25	2.9837	7.4958	0.5049	0.671	170.84
185	1492.48	31.9021	14.0629	0.6336	0.7757	320.20

186	1496.68	1.4723	13.2856	0.75	0.8571	301.51
187	1496.83	1.2722	13.6757	0.749	0.8565	310.33
188	1498.38	20.7561	27.1338	0.7292	0.8434	614.98
189	1504.56	270.3767	114.2248	0.1751	0.2981	2576.44
190	1505.95	0.6219	6.054	0.3125	0.4762	136.41
191	1506.09	8.5612	3.8597	0.6602	0.7954	86.96
192	1514.56	5.6049	6.534	0.5061	0.672	146.24
193	1514.67	5.3254	5.5976	0.5532	0.7123	125.27
194	1515.62	2.3899	7.3887	0.7167	0.835	165.24
195	1515.71	1.7188	6.5061	0.7413	0.8515	145.49
196	1520.02	53.7621	86.6492	0.2044	0.3394	1931.21
197	1520.27	47.5641	108.1569	0.1093	0.1971	2410.10
198	1526.65	645.9187	340.4157	0.6473	0.7859	7548.51
199	1535.18	1.9122	7.2247	0.6431	0.7828	159.16
200	1535.35	2.2135	4.8882	0.7287	0.8431	107.67
201	1535.71	36.8609	27.2177	0.4134	0.5849	599.37
202	1555.35	271.1073	43.2405	0.5416	0.7026	938.11
203	1557.04	412.3974	540.8927	0.1578	0.2726	11719.86
204	1569.66	727.237	51.3032	0.7471	0.8552	1101.12
205	1592.84	310.6236	423.7586	0.6095	0.7574	8939.53
206	1600.67	20.7557	8.8056	0.7349	0.8472	184.69
207	1611.34	33.5708	3.9924	0.7495	0.8568	83.08
208	1656.82	184.865	166.1472	0.6137	0.7606	3345.60
209	1660.53	20.8164	1374.6274	0.3669	0.5368	27606.72
210	1675.43	42.922	291.9723	0.5138	0.6788	5801.86
211	1762.01	14.4701	101.6256	0.7127	0.8322	1901.68
212	1763.47	233.5744	197.0126	0.1398	0.2453	3682.96
213	2890.39	44.8101	38.3342	0.4807	0.6493	384.73
214	2890.96	45.3778	40.3408	0.4745	0.6436	404.76
215	2900.51	35.732	33.9026	0.337	0.5042	338.67
216	2900.64	29.9549	31.1129	0.3779	0.5485	310.79
217	2912.25	132.3042	238.3307	0.0904	0.1658	2368.02
218	2912.6	157.9694	179.9055	0.0962	0.1754	1787.23
219	2963.01	75.2867	133.7478	0.6147	0.7613	1298.50
220	2970.47	137.324	280.9864	0.1041	0.1886	2718.78
221	3028.62	10.1952	168.897	0.0847	0.1561	1592.11
222	3028.76	11.4012	215.3993	0.0735	0.1369	2030.33
223	3056.88	7.8877	58.9875	0.7347	0.8471	549.10
224	3056.98	7.9614	59.9038	0.7359	0.8479	557.61
225	3058.24	30.9934	98.9472	0.482	0.6504	920.53
226	3060.49	32.3504	72.4292	0.2093	0.3462	673.15
227	3060.6	23.8221	13.3841	0.4899	0.6576	124.39
228	3060.83	21.5087	10.9918	0.5201	0.6843	102.14
229	3065.42	38.9672	95.1988	0.4923	0.6598	882.85
230	3065.61	34.8487	104.1603	0.4823	0.6507	965.87
231	3069.36	69.0629	26.0559	0.3619	0.5314	241.21
232	3069.48	83.1899	31.9626	0.2466	0.3957	295.88
233	3077.04	23.0935	278.0761	0.0273	0.0532	2565.61
234	3077.18	21.9672	317.2124	0.0276	0.0538	2926.51
235	3089.03	1.1266	79.723	0.6845	0.8127	731.67
236	3089.22	1.1619	81.2639	0.6837	0.8121	745.75
237	3099.64	13.4959	36.5876	0.1143	0.2052	334.23
238	3099.73	13.7431	41.5993	0.1063	0.1922	380.00
239	3110.63	58.314	118.1238	0.7454	0.8541	1073.88
240	3110.79	60.8316	119.784	0.7418	0.8518	1088.90
241	3116.29	2.5141	2.0452	0.6865	0.8141	18.55
242	3127.34	48.2515	251.4489	0.4492	0.62	2269.35
243	3153.06	11.5933	115.4683	0.4883	0.6562	1030.53
244	3154.16	18.3604	110.9824	0.3396	0.5071	990.02
245	3163.09	14.198	82.6233	0.4355	0.6068	734.20
246	3179.06	24.061	165.9121	0.1766	0.3002	1464.19
247	3188.94	9.7431	27.0789	0.5862	0.7391	237.96
248	3213.98	15.372	91.9571	0.3659	0.5358	799.46

249	3215.46	8.2593	109.4233	0.145	0.2533	950.70
250	3216.17	6.0063	140.9776	0.203	0.3374	1224.49
251	3262.96	2.0479	12.1472	0.4831	0.6515	103.43
252	3263.23	14.5339	80.2589	0.2288	0.3723	683.30
253	3612.99	19.1912	535.8201	0.2115	0.3492	3954.82
254	3625.88	19.2937	213.8095	0.2077	0.344	1570.11
255	3626.62	20.1287	265.102	0.2036	0.3383	1946.20

Table S9. Simulated Raman activity (RA) and intensity (T = 5 °C, λ = 266 nm) for the ground state molecular structure of PDS. Vibrational modes with RA >10 are highlighted in red.

Mode	Frequency	Infrared	Raman Activity	Depolar P	Depolar U	Raman Intensity
1	4.33	0.0391	1.1668	0.75	0.8571	461003.43
2	9	0.1576	1.7492	0.7498	0.857	161927.16
3	16.83	0.7057	1.5307	0.7498	0.857	41351.38
4	17.36	0.1717	0.9333	0.7361	0.848	23729.22
5	27.61	0.4656	0.4424	0.734	0.8466	4565.22
6	33.98	0.2058	0.6751	0.7399	0.8505	4674.55
7	40.3	0.8961	0.5816	0.7148	0.8337	2909.20
8	43.65	0.2784	2.7447	0.7361	0.848	11801.76
9	45.63	0.2339	3.1595	0.7496	0.8569	12493.84
10	50.9	0.4264	2.1984	0.6924	0.8183	7079.04
11	58.79	0.1327	3.5492	0.75	0.8571	8736.57
12	63.07	1.8071	0.9437	0.749	0.8565	2039.84
13	70.77	2.4272	1.1834	0.7494	0.8567	2070.39
14	78.63	0.1553	1.5419	0.7179	0.8358	2227.47
15	83.68	1.1747	0.317	0.7448	0.8537	409.31
16	84.51	4.4695	0.4571	0.7492	0.8566	579.84
17	103.36	1.0532	0.1907	0.7163	0.8347	169.16
18	112.81	4.3235	1.5322	0.7357	0.8478	1166.66
19	118.41	2.3942	2.6603	0.7278	0.8425	1862.77
20	126.89	2.3743	1.8603	0.7493	0.8567	1156.84
21	140.67	2.6603	0.4981	0.7428	0.8524	260.12
22	142.73	4.9502	1.4818	0.7489	0.8565	755.18
23	152.9	3.9253	0.371	0.4814	0.6499	168.59
24	163.62	1.2642	0.7673	0.7488	0.8564	311.85
25	174.58	2.5889	0.4794	0.7482	0.856	175.34
26	183.78	3.9407	2.5167	0.4794	0.6481	847.46
27	188.31	2.7682	0.5823	0.6466	0.7853	188.60
28	190	1.4401	0.5377	0.7499	0.8571	171.70
29	196.73	3.1423	1.9513	0.7215	0.8382	589.66
30	212.99	7.6342	2.9194	0.661	0.7959	779.08
31	216.6	46.279	1.1969	0.5154	0.6802	311.20
32	219.68	26.032	0.77	0.492	0.6595	195.89
33	234.95	2.8047	2.339	0.4426	0.6136	536.91
34	238.35	9.8368	2.545	0.3893	0.5604	571.62
35	244.3	14.9837	1.304	0.2693	0.4244	282.19
36	252.06	36.4156	1.3253	0.6653	0.799	273.68
37	259.6	4.7449	0.43	0.7277	0.8424	84.99
38	271.69	11.6958	0.7461	0.1728	0.2947	137.90
39	280.41	9.8396	1.0807	0.5673	0.7239	190.75
40	310.71	3.1724	0.9429	0.554	0.713	143.66
41	318.36	0.8741	1.7233	0.1084	0.1956	253.70
42	329.78	0.1374	0.3917	0.6088	0.7569	54.89
43	332.4	1.7657	0.7644	0.6831	0.8117	105.95
44	347.69	5.0942	8.8061	0.1975	0.3298	1147.07
45	376.75	27.0179	0.4977	0.743	0.8526	58.14
46	391.02	1.2385	2.25	0.1656	0.2842	250.10
47	424.23	8.3672	5.5671	0.1046	0.1894	555.95
48	437.05	5.1504	6.4611	0.1389	0.244	620.83
49	446.02	1.7553	0.2303	0.5366	0.6985	21.56
50	446.65	2.8516	0.6638	0.7198	0.837	62.03
51	475.62	25.5142	1.6216	0.5501	0.7098	139.89
52	503.02	3.5613	2.4238	0.6052	0.7541	194.94
53	504.39	5.5551	0.855	0.2115	0.3491	68.53
54	505.4	0.066	0.0757	0.6955	0.8204	6.05
55	513.71	13.544	1.7937	0.7378	0.8491	140.55
56	521.61	0.7894	9.3482	0.36	0.5294	718.83
57	531.27	9.9294	2.7315	0.1277	0.2265	205.35
58	551.28	1.4184	0.0101	0.3673	0.5372	0.73
59	552.31	0.0331	0.0135	0.1258	0.2236	0.97

60	562.47	12.5215	10.1671	0.1081	0.1951	713.02
61	586.69	10.1918	2.5739	0.7499	0.8571	171.57
62	592.23	5.6556	2.6979	0.2068	0.3427	177.82
63	600.23	16.0475	0.1301	0.7429	0.8525	8.44
64	622.55	18.1689	1.2996	0.3567	0.5258	80.71
65	624.87	10.4954	3.3254	0.6455	0.7846	205.62
66	635.33	3.6718	6.0393	0.6809	0.8101	366.16
67	662.22	3.3445	0.7877	0.7499	0.8571	45.49
68	662.92	4.3806	0.6415	0.7499	0.8571	37.00
69	687.72	28.007	10.7933	0.1211	0.216	596.35
70	692.19	0.2473	0.5571	0.6623	0.7968	30.55
71	694.17	21.1467	12.8744	0.107	0.1933	703.64
72	702.27	12.0383	0.0162	0.7064	0.828	0.87
73	717.4	0.5378	1.5088	0.7457	0.8543	79.37
74	724.6	0.125	3.5743	0.75	0.8571	185.87
75	751.96	85.6731	0.7857	0.75	0.8571	39.15
76	770.82	0.117	16.1239	0.669	0.8017	780.85
77	780.57	23.9922	0.1501	0.7286	0.843	7.16
78	782.01	65.0489	0.4273	0.7236	0.8396	20.35
79	788.88	8.166	75.4257	0.1018	0.1848	3557.03
80	794.69	0.1764	1.4733	0.7474	0.8554	68.90
81	799.33	3.4026	3.3785	0.7494	0.8567	156.95
82	805.3	0.7756	0.5004	0.7336	0.8464	23.05
83	806.26	0.3578	0.4358	0.7465	0.8548	20.05
84	811.87	2.1309	1.8892	0.7133	0.8327	86.22
85	818.96	34.8048	1.2303	0.7128	0.8323	55.59
86	819.45	32.9459	1.0262	0.6619	0.7966	46.34
87	838.92	8.8238	4.7372	0.6389	0.7797	208.26
88	863.71	4.9345	3.6681	0.1945	0.3257	156.00
89	864.73	107.9065	1.3341	0.3932	0.5645	56.66
90	867.12	143.3355	3.077	0.1418	0.2484	130.28
91	875.42	36.7624	4.3165	0.4485	0.6193	180.79
92	889.49	27.9897	1.4726	0.7382	0.8494	60.57
93	890.69	1.6801	1.7044	0.7428	0.8524	70.00
94	891.91	28.4058	0.3382	0.7118	0.8316	13.87
95	892.45	29.7274	1.4647	0.3541	0.523	60.02
96	892.57	16.809	0.884	0.5661	0.7229	36.22
97	905.76	84.1983	21.1114	0.0808	0.1496	850.66
98	907.23	47.3917	3.7254	0.4205	0.5921	149.84
99	923.27	20.6049	0.0196	0.5552	0.714	0.77
100	941.15	4.7304	0.2321	0.7423	0.8521	8.95
101	976.45	43.2255	3.4933	0.7073	0.8286	129.27
102	977.06	0.6966	0.1517	0.75	0.8571	5.61
103	979.63	1.1133	0.2013	0.6746	0.8057	7.42
104	987.75	31.9869	8.1505	0.748	0.8558	297.70
105	999.32	12.5649	2.4578	0.6287	0.772	88.60
106	1000.94	3.6999	6.9435	0.3245	0.49	249.83
107	1002.54	9.5642	1.7378	0.7308	0.8445	62.41
108	1003.41	0.0795	0.072	0.5337	0.6959	2.58
109	1004.39	0.2023	0.1212	0.7485	0.8562	4.34
110	1012.26	16.9014	10.543	0.2373	0.3835	374.54
111	1015.63	4.5991	113.35	0.1151	0.2064	4011.64
112	1017.85	33.1174	26.2271	0.1641	0.282	925.93
113	1025.45	12.1698	3.966	0.1799	0.3049	138.84
114	1045.14	40.3388	49.5175	0.1326	0.2342	1696.54
115	1047.11	4.2649	9.4232	0.3471	0.5153	322.16
116	1062.75	191.5492	19.4353	0.2204	0.3612	653.38
117	1073.65	19.3484	10.5991	0.3101	0.4734	352.23
118	1074.29	3.007	7.061	0.3146	0.4786	234.49
119	1088.06	14.0438	2.9764	0.7143	0.8334	97.43
120	1124.47	64.4222	3.4277	0.4235	0.595	108.08
121	1129.45	6.3489	3.6307	0.5491	0.7089	113.91
122	1129.86	107.5139	3.1504	0.6259	0.7699	98.80

123	1131.49	15.0569	5.3942	0.1855	0.3129	168.89
124	1136.62	127.9679	3.6908	0.3087	0.4718	114.96
125	1139.93	6.7824	1.4061	0.121	0.2159	43.65
126	1151.48	13.7381	11.793	0.7485	0.8562	361.95
127	1165.76	8.5367	15.0059	0.1692	0.2894	454.14
128	1173.35	11.4659	6.2897	0.4844	0.6527	188.95
129	1182.44	28.8008	12.8739	0.4309	0.6023	383.36
130	1186.87	59.6449	9.4432	0.7306	0.8443	280.00
131	1194.23	20.6738	3.4238	0.6504	0.7882	100.81
132	1206.38	61.5371	19.5023	0.5285	0.6915	567.61
133	1207.7	32.4295	8.7951	0.3941	0.5654	255.66
134	1208.53	38.0802	11.411	0.7287	0.8431	331.44
135	1213.59	14.6369	43.9745	0.6843	0.8126	1271.18
136	1218.34	188.8616	321.5191	0.7476	0.8555	9252.86
137	1229.97	27.8748	607.5878	0.1318	0.2329	17296.66
138	1269.3	23.8373	5.8663	0.2168	0.3564	161.09
139	1270.1	23.9261	16.8288	0.1642	0.2821	461.79
140	1293.36	71.6701	54.649	0.2821	0.4401	1468.67
141	1294.14	9.8071	26.7868	0.1621	0.279	719.39
142	1295.85	22.9416	5.7165	0.2366	0.3827	153.29
143	1300.97	0.9857	7.7641	0.1446	0.2526	207.26
144	1301.25	8.1391	3.0123	0.7187	0.8364	80.39
145	1309.39	9.7506	19.5891	0.1593	0.2748	519.05
146	1332.32	4.7142	8.0915	0.7057	0.8274	210.16
147	1334.62	6.9329	9.7801	0.7316	0.845	253.51
148	1348.99	159.8417	110.1005	0.1957	0.3273	2818.90
149	1350.42	12.3211	12.3716	0.7342	0.8467	316.36
150	1356.07	111.0842	6.9833	0.7499	0.8571	177.72
151	1367.24	251.5051	347.4326	0.1571	0.2715	8758.38
152	1376.28	128.5806	34.8272	0.5144	0.6794	871.29
153	1380.88	217.8031	122.7078	0.3781	0.5487	3058.03
154	1389.61	25.2192	374.2959	0.132	0.2332	9260.16
155	1395.48	16.678	109.5365	0.3179	0.4824	2696.76
156	1397.54	7.7013	373.2183	0.2076	0.3438	9172.86
157	1412.66	173.5141	401.5545	0.3255	0.4911	9746.99
158	1422.65	169.8397	359.1292	0.2657	0.4199	8646.22
159	1437.96	6.0528	37.624	0.1827	0.309	894.63
160	1442.71	9.7087	13.1642	0.4368	0.608	311.82
161	1448.31	146.4786	163.617	0.3307	0.4971	3858.19
162	1450.89	172.9295	3.9107	0.3794	0.5501	92.03
163	1461.19	95.2053	199.6749	0.2664	0.4207	4660.19
164	1462.63	122.6442	96.8202	0.5376	0.6992	2257.08
165	1473.5	12.0675	2.4524	0.7052	0.8271	56.68
166	1488.38	199.9745	8.0747	0.232	0.3767	184.45
167	1490.47	29.5773	45.338	0.7146	0.8335	1033.94
168	1506.73	12.5916	12.2615	0.5036	0.6698	276.10
169	1508.43	4.66	10.9499	0.7097	0.8302	246.24
170	1514.38	62.7806	49.2895	0.7005	0.8239	1103.34
171	1514.72	15.3957	30.9063	0.7058	0.8275	691.65
172	1526.13	252.5695	78.5833	0.7057	0.8274	1743.23
173	1527.02	44.3551	1.4024	0.548	0.708	31.09
174	1531.07	459.882	315.9374	0.6488	0.787	6982.03
175	1538.64	333.4848	208.5576	0.1866	0.3145	4582.43
176	1557.94	4.5704	136.8775	0.7412	0.8514	2963.80
177	1564.25	339.5017	277.7978	0.1762	0.2996	5986.63
178	1593	83.5445	222.6704	0.7165	0.8349	4696.86
179	1608.25	44.5718	15.7102	0.6974	0.8218	327.68
180	1611.02	383.7905	63.6944	0.2018	0.3358	1325.82
181	1626.3	516.5511	258.0642	0.7488	0.8563	5312.12
182	1627.59	556.5914	153.6163	0.749	0.8565	3159.15
183	1633.72	10.9581	1077.4983	0.138	0.2426	22060.69
184	1656.81	1.8429	94.5884	0.7153	0.834	1904.68
185	1657.47	22.2245	91.2724	0.2368	0.3829	1837.04

186	1666.84	23.7924	8.6363	0.6039	0.753	172.66
187	1672.27	25.7827	6.3206	0.7421	0.852	125.88
188	1673.24	24.4274	5.7773	0.6673	0.8004	114.98
189	1733.23	190.3977	114.4397	0.7495	0.8568	2184.05
190	1738.38	198.8118	272.673	0.1363	0.2399	5185.48
191	2978.81	48.8215	105.8129	0.1529	0.2652	1019.98
192	2984.29	47.8671	120.7192	0.1462	0.2551	1160.80
193	2988.45	44.5944	110.0335	0.1352	0.2382	1056.07
194	3018.52	18.4077	81.417	0.051	0.097	770.94
195	3018.96	22.0931	134.9976	0.0386	0.0744	1278.05
196	3049.16	11.8876	76.5954	0.6917	0.8178	715.46
197	3065.48	7.2721	53.8555	0.6948	0.8199	499.43
198	3065.83	48.0479	153.8493	0.0607	0.1144	1426.50
199	3067.71	7.6858	57.9841	0.7156	0.8342	537.18
200	3084.55	38.5141	33.3898	0.1386	0.2434	307.05
201	3087.23	38.4714	40.9021	0.1715	0.2927	375.68
202	3120	20.8105	84.6779	0.4767	0.6456	766.68
203	3166.92	4.9153	86.2014	0.7411	0.8513	764.73
204	3167.36	4.2847	75.3537	0.7441	0.8533	668.37
205	3182.51	11.9051	157.6814	0.4544	0.6249	1389.48
206	3182.65	23.8663	301.6645	0.4007	0.5721	2658.10
207	3198.5	12.3839	73.1169	0.3598	0.5292	639.89
208	3199.06	11.0292	159.7419	0.1384	0.2431	1397.67
209	3206.82	12.9233	162.9266	0.1841	0.3109	1420.80
210	3206.91	15.9582	292.3867	0.1576	0.2723	2549.66
211	3229.95	4.5725	77.8754	0.2539	0.405	672.44
212	3241.41	8.0555	53.7461	0.2101	0.3473	461.83
213	3266.81	23.1156	45.8798	0.1311	0.2318	390.01
214	3269.53	23.4847	46.5366	0.1222	0.2178	395.14
215	3496.24	0.3171	116.5757	0.1251	0.2224	901.45
216	3503.17	0.1362	159.0436	0.1202	0.2146	1226.41
217	3506.55	0.1854	180.9179	0.1259	0.2236	1393.18
218	3565.39	1.164	66.7438	0.59	0.7422	502.01
219	3569.46	229.809	121.6813	0.7465	0.8549	913.73
220	3576	1.0541	124.0044	0.5589	0.7171	928.76
221	3579.72	1.566	141.6191	0.5505	0.7101	1059.12
222	3582.2	1.5763	419.2112	0.1251	0.2224	3132.06

Table S10. LE values for BRACO-19 (B19) and Pyridostatin (PDS) on guanine (G), thymine (T) and adenine (A) bases of the investigated G-quadruplexes.

		B19	PDS
TG_3T	G	20.1 ± 2.7	1.1 ± 0.1
	T	2.8 ± 0.6	4.3 ± 0.8
K-Ras	G	5.2 ± 0.6	0.7 ± 0.1
	T	2.0 ± 0.3	4.7 ± 1.0
	A	1.1 ± 0.1	3.0 ± 0.6
c-Myc	G	6.7 ± 0.8	2.6 ± 0.5
	T	1.6 ± 0.2	4.2 ± 0.8
	A	1.3 ± 0.1	2.7 ± 0.5
TBA	G	2.8 ± 0.5	1.1 ± 0.1
	T	3.1 ± 0.6	5.4 ± 0.8
m-tel_{24}	G	5.0 ± 0.6	1.1 ± 0.2
	T	3.4 ± 0.5	2.2 ± 0.4
	A	2.9 ± 0.4	2.2 ± 0.2