

## Annex 1 – FTIR spectroscopy

The frequencies of bands obtained for the non-irradiated BG1189 solution in the recorded FTIR spectrum were compared with the theoretical frequencies calculated with Gaussian 09 and GaussView 5.0.

Table S1. Experimental and calculated vibration frequencies for BG1189.

Observed frequencies (cm <sup>-1</sup> )	Calculated frequencies (cm <sup>-1</sup> )	Assigned vibrations
-	3729	O-H stretching
3152, 3138, 3129, 3122	3146, 3129, 3116, 3111	CH <sub>2</sub> asymmetrical stretching
3088, 3045, 3033, 3017	3086, 3082, 3070, 3058	CH <sub>2</sub> symmetrical stretching
2977, 2962	2939, 2931	C-H stretching from CH <sub>3</sub> groups
1716	1731	C=O stretching
1677, 1660	1652, 1629	C-C stretching and C-N stretching from quinazoline radical
1616	1617	C-C ring stretching; N-O stretching; O-H deformation
1561	1574	C-C ring stretching; N-O stretching; O-H deformation; C-H deformation
1533	1522	C-H deformation
1477	1504	C-C ring stretching; N-O stretching; O-H deformation; C-H deformation
1437	1428	C-H deformation; CH <sub>2</sub> wagging
1401, 1382	1410, 1407	C-H deformation, C-N stretching
1370	1381	C-C ring stretching; C-H deformation; O-H deformation
1351	1331	N-O stretching; O-H deformation
1310	1324	C-H deformation
1246	1300	C-N ring stretching; C-H deformation from CH <sub>3</sub> groups; C-H deformation; O-H deformation
1214	1262	C-C ring stretching; C-N ring stretching; C-H deformation; O-H deformation
1163	1217	C-C ring stretching; C-N stretching; O-H deformation; C-H deformation
1138	1199	CH <sub>2</sub> wagging from CH <sub>3</sub> groups; C-H deformation
1078	1161	C-N ring stretching; C-H deformation; CH <sub>2</sub> wagging from CH <sub>3</sub> groups
1011	1118	CH <sub>2</sub> wagging from CH <sub>3</sub> groups; C-H deformation; C-C ring stretching; C-N stretching; N-O stretching; O-H deformation
962, 942	1019, 999	C-C ring stretching; C-N ring stretching; C-H deformation; O-H deformation; N-O stretching; CH <sub>2</sub> wagging from CH <sub>3</sub> groups
919	910	C-C ring stretching; C-N ring stretching; C-H deformation; N-O stretching; CH <sub>2</sub> rocking
906	901	CH <sub>2</sub> rocking
890	872	CH <sub>2</sub> twisting; CH <sub>2</sub> rocking
863	852	C-N stretching; CH <sub>2</sub> rocking
832	803	C-C ring stretching; C-N ring stretching; C-H deformation; O-H deformation; C=O deformation
779	792	C-C ring deformation; C-N ring deformation; C-H deformation; C=O deformation; CH <sub>2</sub> rocking
744	744	C-C ring stretching; C-N ring stretching; C-H deformation; O-H deformation; CH <sub>2</sub> rocking
683, 605	688, 572	C-C ring deformation; C-N ring deformation; N-O deformation; O-H deformation; CH <sub>2</sub> rocking
533, 504	553, 511	C-C ring deformation; C-N ring deformation; N-O deformation; O-H deformation; C-H deformation; CH <sub>2</sub> wagging

477	483	C–C ring deformation; C–N ring deformation; N–O deformation; O–H deformation; CH <sub>2</sub> wagging
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The FTIR spectrum of the unirradiated BG1189 evidenced bands between 3200 cm<sup>-1</sup> and 2950 cm<sup>-1</sup> that can be assigned to symmetrical and asymmetrical stretching vibrations of C–H bonds. The strongest vibration is the one of the C=O bond and is responsible for the band with the maximum at 1716 cm<sup>-1</sup>. C–C and C–N stretching vibrations from quinazoline radical are responsible for the absorption bands with maxima at 1677 cm<sup>-1</sup> and 1661 cm<sup>-1</sup>. C–C stretching from the aromatic rings, N–O stretching and deformation vibrations contribute to the appearance of the peaks at 1616 cm<sup>-1</sup>, 1561 cm<sup>-1</sup> and 1477 cm<sup>-1</sup>, respectively. C–H deformation also contribute to the last two peaks. The peak observed at 1533 cm<sup>-1</sup> is due to C–H bending vibrations and the one at 1437 cm<sup>-1</sup> is due to C–H bending and CH<sub>2</sub> wagging vibrations. Strong C–N stretching vibrations along with C–H deformation vibrations give rise to a high intensity absorbance band with maximum at 1401 cm<sup>-1</sup> and a weaker one with maximum at 1382 cm<sup>-1</sup>. N–O stretching and deformation vibrations are responsible for the peak at 1351 cm<sup>-1</sup>. A weak absorption band due to C–H deformation vibrations is observed in the IR spectrum with the peak at 1310 cm<sup>-1</sup>. C–N ring stretching vibrations, C–H deformation vibrations from CH<sub>3</sub> groups, C–H deformation and O–H deformation vibrations give rise to the peak at 1246 cm<sup>-1</sup>. C–C and C–N ring stretching vibrations and O–H deformation vibrations are responsible for the appearance of the IR band with maximum at 1214 cm<sup>-1</sup>. The peak at 1181 cm<sup>-1</sup> is due to similar vibrations as the previous one, except C–N stretching vibrations that are not originating from the aromatic ring but from the substituents bonded to the quinazoline radical. CH<sub>2</sub> wagging vibrations from CH<sub>3</sub> groups and C–H deformation vibrations give rise to the absorption band with maximum at 1138 cm<sup>-1</sup>. Along with the vibrations responsible for the previous peak, C–N ring stretching vibrations also contribute for the appearance of the 1078 cm<sup>-1</sup> peak. The peak at 1011 cm<sup>-1</sup> is due to CH<sub>2</sub> wagging vibrations from CH<sub>3</sub> groups, C–H deformation, C–C ring stretching, C–N stretching, N–O stretching, O–H deformation vibrations. The same vibrations are responsible for the 962 cm<sup>-1</sup> and 942 cm<sup>-1</sup> peaks, except that the C–N stretching vibrations originate in the quinazoline radical. The absorption band with maximum at 919 cm<sup>-1</sup> is due to C–C and C–N ring stretching, C–H deformation, N–O stretching and rocking vibrations. The peak at 906 cm<sup>-1</sup> appears due to CH<sub>2</sub> rocking vibrations. These vibrations together with the CH<sub>2</sub> twisting vibrations contribute to the appearance of the absorption band with the peak at 890 cm<sup>-1</sup>. The peak at 863 cm<sup>-1</sup> appears due to C–C stretching and CH<sub>2</sub> rocking vibrations and the one at 832 cm<sup>-1</sup> is due to C–C ring and C–N ring stretching vibrations and C–H deformation and C=O deformation vibrations. C–C and C–N ring deformation, C–H and C=O deformation and CH<sub>2</sub> rocking vibrations give rise to the peak at 779 cm<sup>-1</sup>. The peak at 744 cm<sup>-1</sup> appears due to C–C and C–N ring stretching vibrations, C–H and O–H deformation vibrations and CH<sub>2</sub> rocking vibrations. The absorption bands with maxima at 683 cm<sup>-1</sup> and 604 cm<sup>-1</sup> originate from the C–C and C–N ring deformation, N–O and O–H deformation and CH<sub>2</sub> rocking vibrations. C–C and C–N ring deformation, N–O, O–H and C–H deformation and CH<sub>2</sub> wagging vibrations contribute to the formation of the peaks at 533 cm<sup>-1</sup> and 504 cm<sup>-1</sup>; the same vibrations, except C–H deformation, give rise to the peak 477 cm<sup>-1</sup>.

A comparison between the experimental IR frequencies and the calculated ones, along with an assignment of the vibrations responsible for each absorption band in the FTIR spectrum of the BG1190 solution, is given in Table S2.

Table S2. Experimental and calculated frequencies for BG1190.

Observed frequencies (cm <sup>-1</sup> )	Calculated frequencies (cm <sup>-1</sup> )	Assigned vibrations
-	3729	O–H stretching
3084, 3024, 2964, 2928	3160, 3122, 3104, 3098	CH <sub>2</sub> asymmetrical stretching
2872, 2857, 2840	3060, 3046, 3033	CH <sub>2</sub> symmetrical stretching
1685	1731	C=O stretching
1657	1652	C–C and C–N stretching and C–H deformation from quinazoline ring
1615	1616	C–C ring stretching; C–N deformation; N–O stretching and O–H deformation
1574	1574	C–C ring stretching; C–N deformation; N–O stretching; O–H deformation; C–H deformation from quinazoline ring
1524	1474	CH <sub>2</sub> scissoring; C–N and C–C ring stretching; C–H deformation from quinazoline ring; N–O stretching and O–H deformation
1474, 1457	1468, 1437	C–C stretching and C–H deformation from quinazoline ring; CH <sub>2</sub> scissoring

1428	1424	C-H deformation from quinazoline ring; CH <sub>2</sub> wagging
1409	1401	C-N stretching and C-H deformation from quinazoline ring; CH <sub>2</sub> twisting
1399	1381	C-C stretching and C-H deformation from quinazoline ring; CH <sub>2</sub> wagging;
1376	1377, 1362	CH <sub>2</sub> wagging
1345	1334, 1329	N-O stretching and O-H deformation; CH <sub>2</sub> twisting
1311	1300	C-C, C-N and C-H deformation from quinazoline ring; C-C and C-N stretching from quinazoline ring; N-O and O-H deformation
1271	1277, 1270	C-C and C-N stretching from quinazoline ring; N-O stretching; C-H deformation from quinazoline ring; CH <sub>2</sub> twisting
-	1247	C-C, C-N and C-H deformation from quinazoline ring; C-N stretching; CH <sub>2</sub> twisting
1235	1222	C-C, C-N and C-H deformation from quinazoline ring; C-N stretching; CH <sub>2</sub> twisting; N-O stretching
-	1213	C-C, C-N and C-H deformation from quinazoline ring; C-N stretching; CH <sub>2</sub> rocking; N-O stretching
1167	1142	C-C, C-N and C-H deformation from quinazoline ring; C-N stretching from quinazoline ring; CH <sub>2</sub> twisting
1126	1113	C-C, C-N and C-H deformation from quinazoline ring; N-O deformation; CH <sub>2</sub> rocking
1081	1082	C-C and C-N deformation; CH <sub>2</sub> twisting from radical ring
1020	1023	C-H deformation from quinazoline ring; C-C and C-N deformation and CH <sub>2</sub> rocking from radical ring
1009	1000	NO <sub>2</sub> stretching; C-C, C-N and C-H stretching from quinazoline ring
941	947	C-H deformation from quinazoline ring; CH <sub>2</sub> rocking
915	906	C-C and C-N stretching from quinazoline ring; NO <sub>2</sub> stretching; CH <sub>2</sub> rocking
899	902	C-H deformation from quinazoline ring
-	877	C-C and C-N deformation from radical ring; CH <sub>2</sub> deformation
851	851	C-C, C-N and C-H ring deformation
827, 792, 779, 750	816, 802, 792, 767	C-C and C-N ring deformation; CH <sub>2</sub> rocking
729	745	C-C and C-H ring stretching; NO <sub>2</sub> deformation; CH <sub>2</sub> rocking
695	689	C-C and C-N ring deformation; NO <sub>2</sub> deformation; CH <sub>2</sub> rocking
627	571	NO <sub>2</sub> scissoring; C-C and C-N ring deformation; CH <sub>2</sub> wagging
551	555, 542	C-C and C-N ring deformation; CH <sub>2</sub> wagging and rocking
503	506	N-O deformation
480	484	C-C ring deformation; N-O deformation; CH <sub>2</sub> wagging
465, 453, 418	414, 412	C-N ring deformation; N-O deformation; CH <sub>2</sub> wagging

The FTIR spectrum of the BG1190 solution, showed in Figure 9, presents absorption bands with peaks at 3084 cm<sup>-1</sup>, 3022 cm<sup>-1</sup>, 2964 cm<sup>-1</sup> and 2928 cm<sup>-1</sup>, which can be assigned to CH<sub>2</sub> asymmetrical stretching vibrations. CH<sub>2</sub> symmetrical stretching vibrations are responsible for the appearance of the IR absorption bands with maxima at 2872 cm<sup>-1</sup>, 2857 cm<sup>-1</sup> and 2840 cm<sup>-1</sup>. A strong absorption is observed at 1685 cm<sup>-1</sup> originating from C=O stretching vibrations. C-C and C-N stretching vibrations and C-H deformation vibrations from quinazoline ring give rise to the peak at 1657 cm<sup>-1</sup>. The peak at 1615 cm<sup>-1</sup> is due to C-C ring stretching, C-N deformation, C-N stretching and O-H deformation vibrations. These four types of vibrations along with C-H deformation vibrations from the quinazoline ring are responsible for the peak at 1574 cm<sup>-1</sup>. The peak at 1524 cm<sup>-1</sup> appears due to CH<sub>2</sub> scissoring vibrations, C-N and C-N stretching vibrations, C-H deformation vibrations from quinazoline ring, N-O stretching and O-H deformation vibrations. C-N stretching vibrations and C-H deformation vibrations from quinazoline ring, along with CH<sub>2</sub> scissoring vibrations lead to formation of the absorption bands with maxima at 1474 cm<sup>-1</sup> and 1457 cm<sup>-1</sup>. C-H deformation vibrations from quinazoline ring superimposed with CH<sub>2</sub> wagging vibrations are responsible for the appearance of the peak at 1428 cm<sup>-1</sup>. The peak at 1409 cm<sup>-1</sup> originates from C-N stretching, and C-H deformation vibrations from quinazoline ring and CH<sub>2</sub> twisting vibrations. The absorption band with the maximum at 1399 cm<sup>-1</sup> appears due to C-C stretching and C-H deformation vibrations from quinazoline ring and CH<sub>2</sub> wagging vibrations.

Last type of vibrations is also responsible for the peak at  $1376\text{ cm}^{-1}$ . A strong absorption band with the maximum at  $1345\text{ cm}^{-1}$  assigned to N–O stretching, O–H deformation and  $\text{CH}_2$  twisting vibrations. C–C, C–N and C–H deformation vibrations from quinazoline ring, C–C and C–N stretching vibrations from quinazoline ring, along with N–O and O–H deformation vibrations are responsible for the appearance of the shoulder at  $1311\text{ cm}^{-1}$ . The peak observed at  $1235\text{ cm}^{-1}$  appears due to C–C, C–N and C–H deformation vibrations from quinazoline ring, C–N and N–O stretching vibrations, together with  $\text{CH}_2$  twisting vibrations. C–C, C–N and C–H deformation vibrations and C–N stretching vibrations from quinazoline ring along with  $\text{CH}_2$  twisting give rise to the peak at  $1167\text{ cm}^{-1}$ . IR band with maximum at  $1126\text{ cm}^{-1}$  appears due to C–C, C–N and C–H deformation vibrations from quinazoline ring, N–O deformation and  $\text{CH}_2$  rocking vibrations. C–C and C–N deformation vibrations together with  $\text{CH}_2$  twisting vibrations from the aromatic rings are responsible for the peak at  $1081\text{ cm}^{-1}$ . The peak at  $1020\text{ cm}^{-1}$  originates from the superposition of the following vibrations: C–H deformation and  $\text{CH}_2$  rocking vibrations from quinazoline ring along with C–C and C–N deformation vibrations. The absorption band with the maximum at  $1009\text{ cm}^{-1}$  is due to  $\text{NO}_2$  stretching vibrations in combination with C–C, C–N and C–H stretching vibrations from quinazoline ring. C–H deformation vibrations from the aromatic rings and  $\text{CH}_2$  rocking vibrations lead to formation of the absorption band with maximum at  $941\text{ cm}^{-1}$ . The peak at  $915\text{ cm}^{-1}$  appears due to C–C and C–N stretching vibrations from quinazoline ring,  $\text{NO}_2$  bending vibrations and  $\text{CH}_2$  rocking vibrations. C–H deformation vibrations from the quinazoline radical are responsible for the bands at  $899\text{ cm}^{-1}$  and C–C, C–N and C–H deformation vibrations, from the quinazoline ring as well, give rise to the peak at  $851\text{ cm}^{-1}$ . C–N ring deformation vibrations along with  $\text{CH}_2$  rocking vibrations lead to the formation of consecutive absorption bands with maxima at  $827\text{ cm}^{-1}$ ,  $792\text{ cm}^{-1}$ ,  $779\text{ cm}^{-1}$  and  $750\text{ cm}^{-1}$ . The peak at  $729\text{ cm}^{-1}$  originates from C–C and C–H quinazoline ring stretching vibrations and  $\text{NO}_2$  deformation vibrations along with  $\text{CH}_2$  rocking vibrations. The peak at  $695\text{ cm}^{-1}$  appears due to C–C and C–N deformation vibrations from the aromatic radical,  $\text{NO}_2$  deformation and  $\text{CH}_2$  rocking vibrations.  $\text{NO}_2$  scissoring vibrations, C–C and C–N deformation vibrations from the quinazoline ring along with  $\text{CH}_2$  wagging vibrations give rise to an absorption band with maximum at  $625\text{ cm}^{-1}$ . The peak at  $551\text{ cm}^{-1}$  is due to C–C and C–N deformation vibrations from the quinazoline radical together with  $\text{CH}_2$  wagging and rocking vibrations. N–O deformation vibrations are responsible for the appearance of the absorption band with maximum at  $500\text{ cm}^{-1}$  and C–C ring deformation vibrations, N–O deformation vibrations along with  $\text{CH}_2$  wagging vibrations. C–N deformation vibrations from the quinazoline ring, N–O deformation vibrations and  $\text{CH}_2$  wagging vibrations give rise to absorption bands with maxima at  $460\text{ cm}^{-1}$ ,  $453\text{ cm}^{-1}$  and  $418\text{ cm}^{-1}$ .