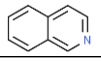
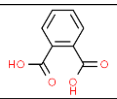
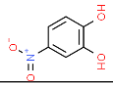
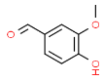
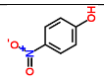
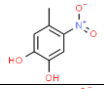
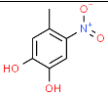
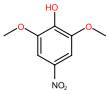
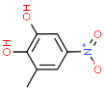
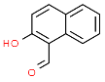
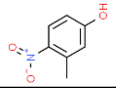
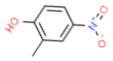
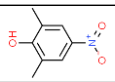
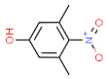
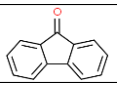
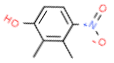
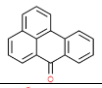
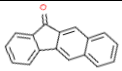
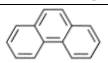
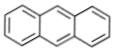
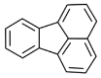
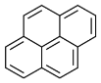
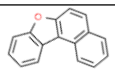
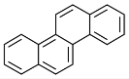
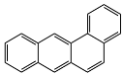
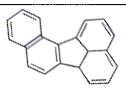
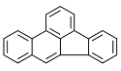
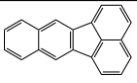
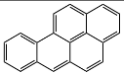
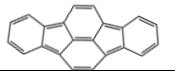
Supplemental Information

Brown Carbon Aerosol in Polluted Urban Air of North China Plain: Day-night Differences in the Chromophores and Optical Properties

Yuquan Gong et al.

Table S1. Retention Times (RTs), Abbreviation, Elemental Formulas, and Assigned Structures of Identified BrC Chromophores. (*) represent tentative structure components.

Peak #	RT (min)	Candidate compound	Abbreviation	m/z &ion. Mech.	Formula	Refernce	Unambiguous/Tentative stucture
1#	1.69	Isoquinoline	ISO	130.065 [M & H]$^+$	C_9H_7N	Banerjee & Zare, 2015	
2#	2.03	Leucoline	LEU	130.065 [M & H]$^+$	C_9H_7N	Banerjee & Zare, 2015	
3#	6.06	Phthalic acid	PA	149.023 [M & H]$^+$	$C_8H_4O_3$	He et al., 2018	
4#	7.21	4-nitrocatechol	4NC	154.014 [M & H]$^-$	$C_6H_5NO_4$	Huang et al. 2020	
5#	7.87	vanillin	VAN	153.054 [M & H]$^+$	$C_8H_8O_3$	Huang et al., 2021	
6#	9.15	p-cis-coumaric acid	PCCA	163.040 [M & H]$^-$	$C_9H_8O_3$	Smith, Kinney, & Anastasio, 2016	
7#	11.48	4-nitrophenol	4NP	139.019 [M & H]$^-$	$C_6H_5NO_3$	Wang et al., 2017	
8#	13.53	4-methyl-5-nitrocatechol	4M5NC	168.030 [M & H]$^-$	$C_7H_7NO_4$	Kitanovski et al., 2012	
9#	13.82	3-methyl-6-nitrocatechol	3M6NC	168.030 [M & H]$^-$	$C_7H_7NO_4$	Lin et al., 2015	
10#	16.06	4-nitrosyringol	4NS	198.040 [M & H]$^-$	$C_8H_9NO_5$	Lin et al., 2017	
11#	18.23	3-methyl-5-nitrocatechol	3M5NC	168.030 [M & H]$^-$	$C_7H_7NO_4$	Wang et al., 2017	
12#	18.72	1-Formyl-2-naphthol	1F2N	171.045 [M & H]$^-$	$C_{11}H_8O_2$	Rao et al., 2003 (*)	
13#	19.43	3-methyl-4-nitrophenol	3M4NP	152.035 [M & H]$^-$	$C_7H_7NO_3$	Wang et al., 2017	
14#	20.06	1,2-acenaphthylenedione	1,2ACE	183.044 [M & H]$^+$	$C_{12}H_6O_2$	Bandowe et al., 2014	

Peak #	RT (min)	Candidate compound	Abbreviation	m/z &ion. Mech.	Formula	Refernce	Unambiguous/Tentative stucture
15#	20.53	1,8-naphthalic anhydride	1,8NA	199.038[M & H]$^+$	$C_{12}H_6O_3$	Bandowe et al., 2014	
16#	21.95	2-methyl-4-nitrophenol	2M4NP	152.035 [M & H]$^-$	$C_7H_7NO_3$	Yuan et al., 2020	
17#	26.08	2,6-Dimethyl-4-nitrophenol	2,6D4NP	166.051 [M & H]$^-$	$C_8H_9NO_3$	Yuan et al., 2020	
18#	26.39	3,5-Dimethyl-4-nitrophenol	3,5D4NP	166.051 [M & H]$^-$	$C_8H_9NO_3$	Fischer & Mathivanan, 1988 (*)	
19#	27.12	9-fluorenone	9FLU	181.064 [M & H]$^+$	$C_{13}H_8O$	Huang et al. 2020	
20#	28.21	2,3-Dimethyl-4-nitrophenol	2,3D4NP	166.051 [M & H]$^-$	$C_8H_9NO_3$	Fischer & Mathivanan, 1988 (*)	
21#	36.93	Benzanthrone	BEN	231.079 [M & H]$^+$	$C_{17}H_{10}O$	Huang et al. 2020	
22#	38.41	Benzo[b]fluoren-11-one	BbF11O	231.080 [M & H]$^+$	$C_{17}H_{10}O$	Yuan et al., 2020	
23#	39.27	Phenanthrene	PHE	178.23 [M & H]$^+$	$C_{14}H_{10}$	Ho et al., 2009	
24#	39.88	Anthracene	ANT	178.22[M & H]$^+$	$C_{14}H_{10}$	Alcanzare, 2006	
25#	41.23	Fluoranthene	FLU	202.25[M & H]$^+$	$C_{16}H_{10}$	Lee & Lane, 2010	
26#	41.7	Pyrene	PYR	202.25[M & H]$^+$	$C_{16}H_{10}$	Ho et al., 2009	
27#	42.48	Benzo[b]naphtho[1,2-d]furan	BbN[1,2d]F	218.25[M & H]$^+$	$C_{16}H_{10}O$	Standards	
28#	43.46	Chrysene	CHR	228.28[M & H]$^+$	$C_{18}H_{12}$	Bandowe et al., 2014	
29#	43.63	Benzo(a)anthracene	BaA	240.36[M & H]$^+$	$C_{18}H_{12}$	Huang et al. 2020	
30#	44.94	Benzo(j)fluoranthen	BjF	252.31[M & H]$^+$	$C_{20}H_{12}$	Standards	
31#	45.23	Benzo(e)pyrene	BeP	252.31[M & H]$^+$	$C_{20}H_{12}$	Ho et al., 2009 (*)	
32#	45.29	Benzo(b)fluoranthene	BbF	252.31[M & H]$^+$	$C_{20}H_{12}$	Yuan et al., 2020	
33#	45.46	Benzo(k)fluoranthene	BkF	252.31[M & H]$^+$	$C_{20}H_{12}$	Standards	
34#	45.79	Benzo(a)pyrene	BaP	252.31[M & H]$^+$	$C_{20}H_{12}$	Ho et al., 2009	
35#	46.73	Indeno[1,2,3-cd]fluoranthene	I[1,2,3cd]F	276.33[M & H]$^+$	$C_{22}H_{12}$	Alcanzare, 2006 (*)	

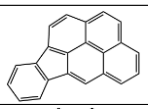
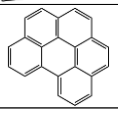
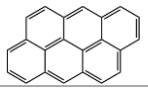
Peak #	RT (min)	Candidate compound	Abbreviation	m/z &ion. Mech.	Formula	Refernce	Unambiguous/Tentative stucture
36#	47.43	Indeno(1,2,3-cd)pyrene	I[1,2,3cd]P	276.33[M & H]$^+$	$C_{22}H_{12}$	Standards	
37#	47.53	Benzo(g,h,i)perylene	B(g,h,i)P	276.33[M & H]$^+$	$C_{22}H_{12}$	Alcanzare, 2006	
38#	48.25	Anthanthrene	ANTHA	276.33[M & H]$^+$	$C_{22}H_{12}$	Standards (*)	

Table S2. Average (± standard deviation) values Abs_{365nm}, $MAE_{365nm,}$ and AAE of WS-BrC and WIS-BrC, as well as concentrations of WSOC and WISOC, measured organic species in the PM 2.5 aerosols from the urban. [a] represents the determination of the HULIS extraction solution. Here $\mathbf{Abs_{365,\ MS\text{-}BrC}}$ is the light absorption coefficient of methanol-soluble BrC at 365 nm.

Components	This study		Li et al. (2020)		Huang et al. (2021)		Li et al. (2021)	
	Day	Night	Day	Night	Xi'an	Beijing	Day	Night
WSOC (μg m^{-3})	17.29±14.49	12.90±13.36	22.1±8.0	21.7±10.4	12.4 ± 6.50[a]	6.4 ± 3.80[a]	/	/
WISOC (μg m^{-3})	29.78±22.39	31.07±12.47	21.9±10.1	26.2±17.3	20.80±7.90	16.30±8.90	/	/
$\mathbf{Abs_{365,\ WS\text{-}BrC}}$ **(Mm^{-1})**	46.04±38.91	35.68±35.50	19.2±6.8	19.9±9.5	31.50±16.40[a]	15.00±9.50[a]	/	/
$\mathbf{Abs_{365,\ MS\text{-}BrC}}$ **(Mm^{-1})**	79.86±66.50	82.69±55.84	/	/	/	/	50.0±5.00	75.0±7.50
$\mathbf{Abs_{365,\ WIS\text{-}BrC}}$ **(Mm^{-1})**	27.90±24.80	40.88±23.42	17.2±8.2	26.7±15.8	33.90±16.40	26.10±18.40		
$\mathbf{MAE_{365,\ WS\text{-}BrC}}$ **($m^2g\ C^{-1}$)**	2.58±0.14	2.88±0.24	0.92±0.21	0.94±0.28	1.80 ± 0.30[a]	1.80 ± 0.40[a]	/	/
$\mathbf{MAE_{365,\ WIS\text{-}BrC}}$ **($m^2g\ C^{-1}$)**	1.02±0.49	1.43±0.83	0.85±0.34	1.05±0.28	1.50±0.50	1.50±0.40	1.73±0.64	2.13±0.65
$\mathbf{AAE_{WS\text{-}BrC}}$	5.10±0.28	5.51±0.40	5.14±0.2	5.07±0.72	8.20 ± 1.00	9.40 ± 2.60	/	/
$\mathbf{AAE_{WIS\text{-}BrC}}$	6.36±0.45	6.97±0.80	5.94±0.12	6.15±0.24	5.4 ± 0.20	5.7 ± 0.20	5.16 ±1.15	4.07 ±0.87

Table S3. The identified 38 BrC chromophores are divided into ten subgroups.

Categories	Subgroups	Candidate compound
I	quinolines	Isoquinoline Leucoline
II	2–3-ring OPAHs	1-Formyl-2-naphthol 1,2-acenaphthylenedione 1,8-naphthalic anhydride 9-fluorenone
III	nitrocatechols	4-nitrocatechol 4-methyl-5-nitrocatechol 3-methyl-6-nitrocatechol 3-methyl-5-nitrocatechol
IV	nitrophenols	4-nitrophenol 3-methyl-4-nitrophenol 2-methyl-4-nitrophenol 2,6-Dimethyl-4-nitrophenol 3,5-Dimethyl-4-nitrophenol 2,3-Dimethyl-4-nitrophenol
V	aromatic alcohols and acids	Phthalic acid vanillin p-cis-coumaric acid 4-nitrosyringol
VI	4-ring OPAHs	Benzanthrone Benzo[b]fluoren-11-one Benzo[b]naphtho[1,2-d]furan
VII	3-ring PAHs	Phenanthrene Anthracene
VIII	4-ring PAHs	Fluoranthene Pyrene Chrysene Benzo(a)anthracene
IX	5-ring PAHs	Benzo(j)fluoranthene Benzo(e)pyrene Benzo(b)fluoranthene Benzo(k)fluoranthene Benzo(a)pyrene
X	6-ring PAHs	Indeno[1,2,3-cd]fluoranthene Indeno(1,2,3-cd)pyrene Benzo(g,h,i)perylene Anthanthrene

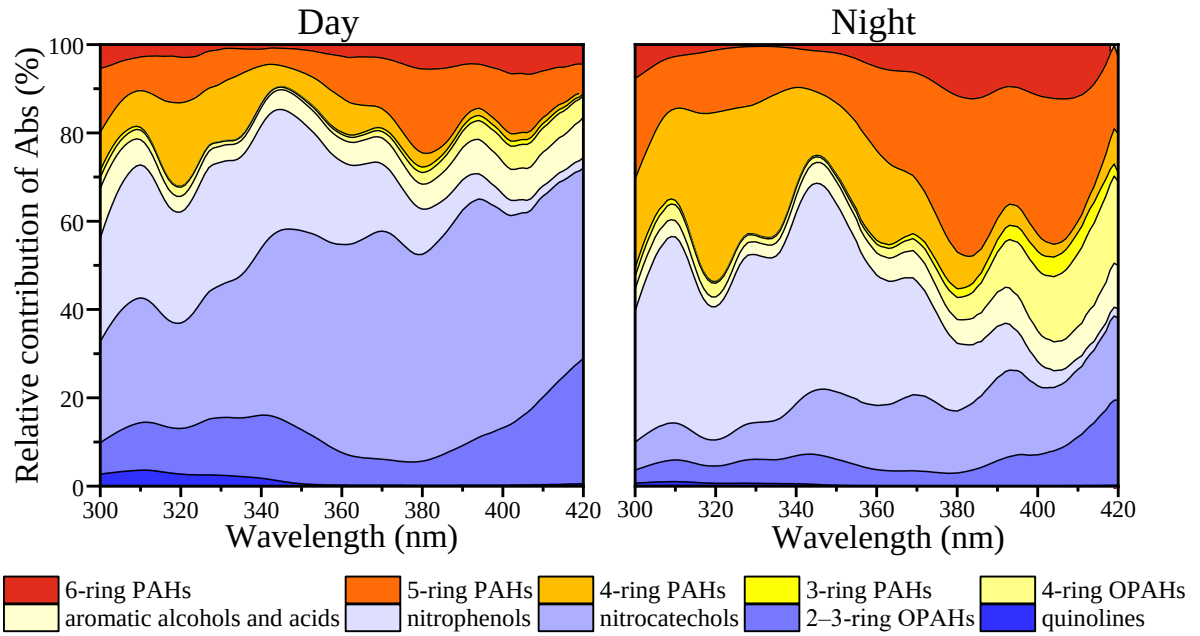


Figure S1. Relative contributions of light absorption of ten BrC subgroups during the day and night.

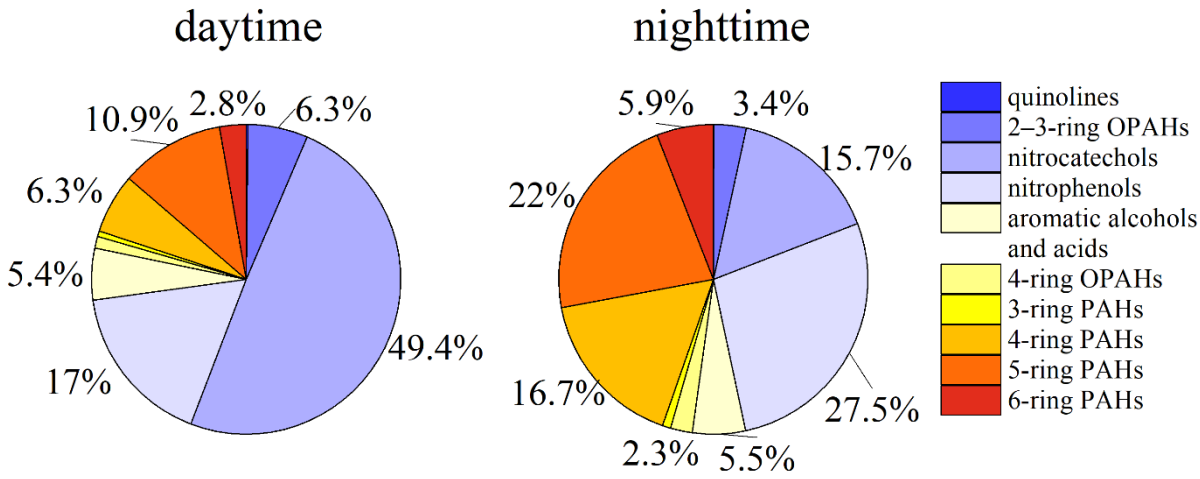


Figure S2. Light-absorbing contributions of ten BrC subgroups at 365nm in the daytime and nighttime.

References

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