Supplementary Information for

Comprehensive Molecular Characterization of Atmospheric Brown Carbon by High Resolution Mass Spectrometry with Electrospray and Atmospheric Pressure Photoionization

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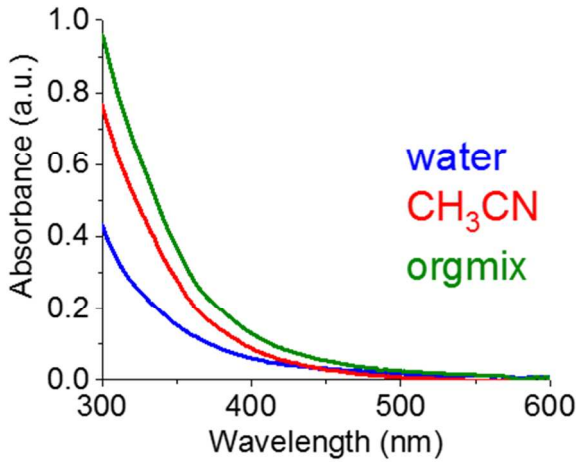
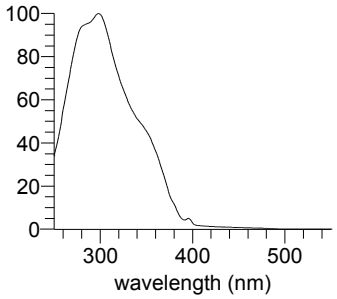
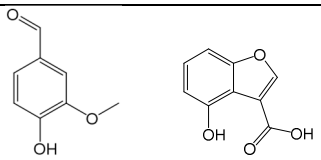
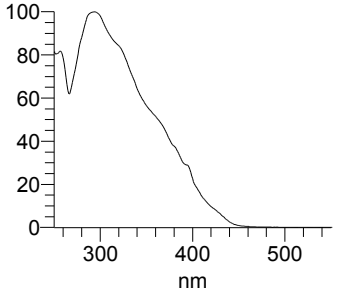
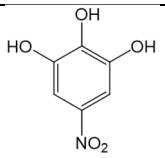
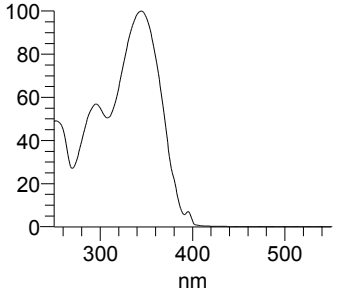
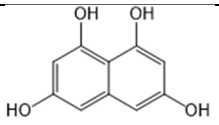
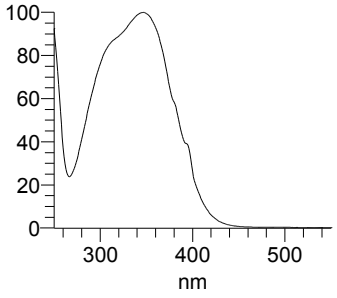
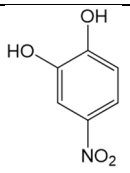
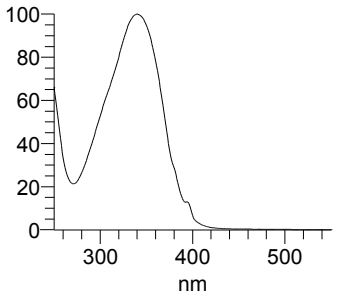
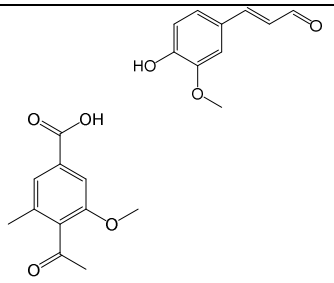
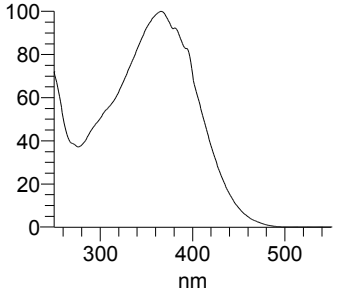
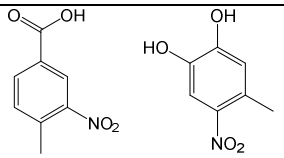
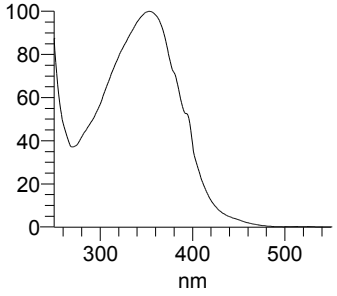
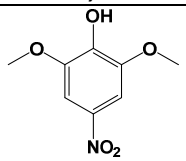
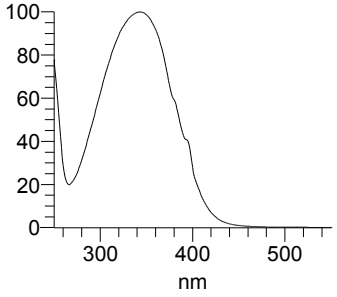
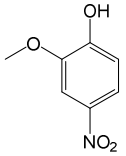
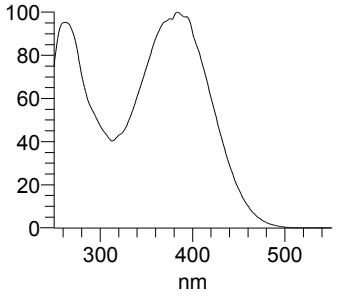
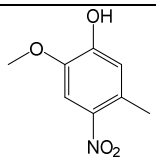
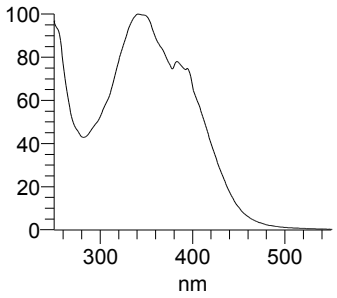
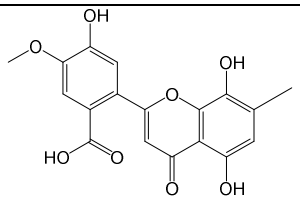
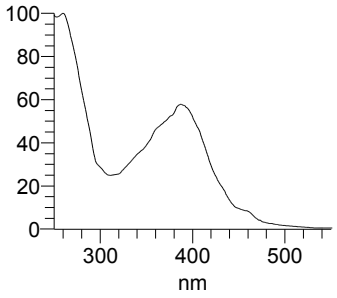
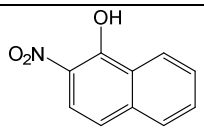
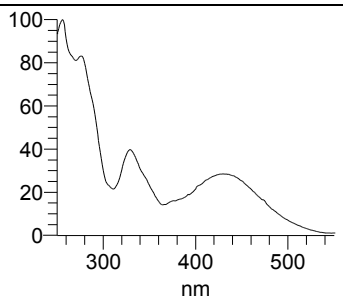
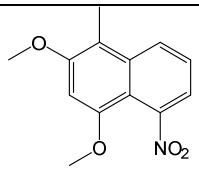
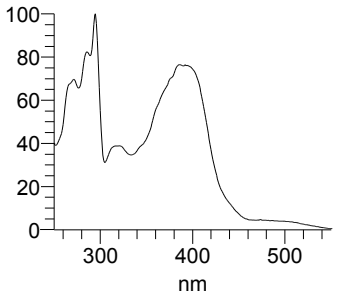
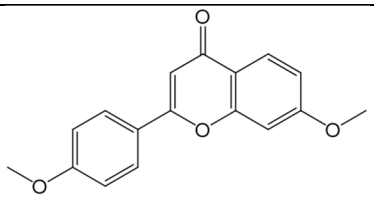
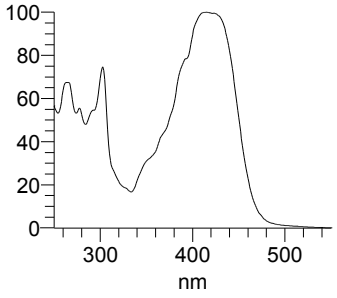
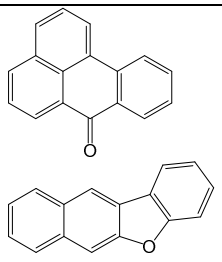


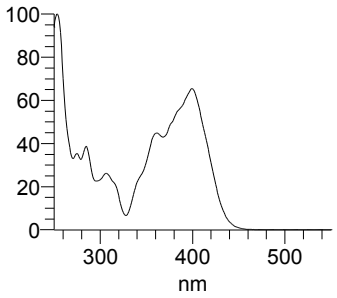
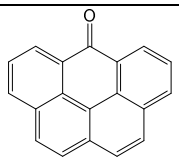
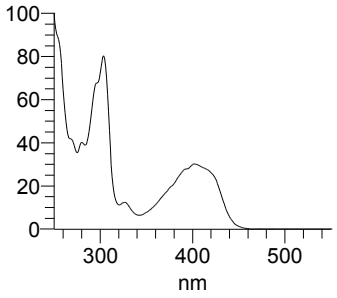
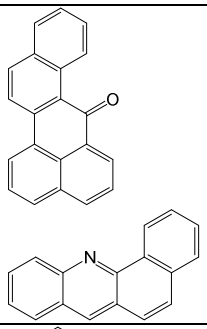
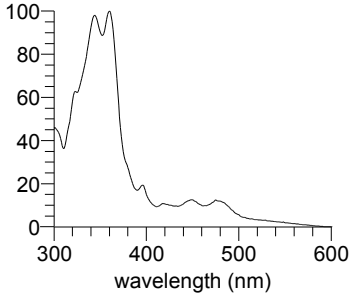
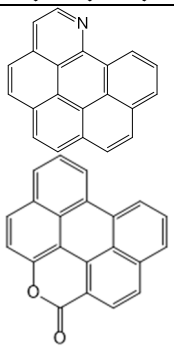
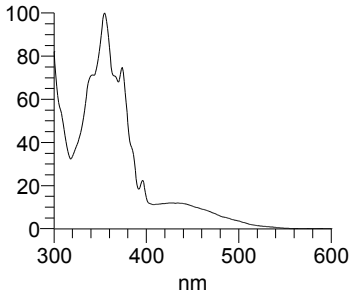
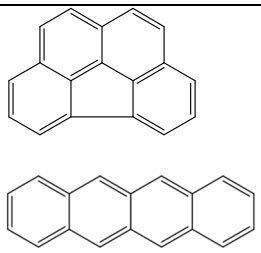
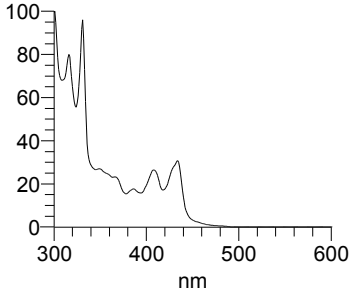
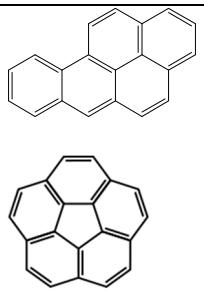
Figure S1. UV-Vis spectra of the BBOA sample extracted with three different solvents. The Absorption Ångström exponent (*AAE*) values were calculated by a linear regression fit of log(abs) vs log(λ) in the wavelength range of 300−600 nm. The *AAE* values for water, acetonitrile, and orgmix extracts are 5.3, 7.1 and 5.6, respectively.

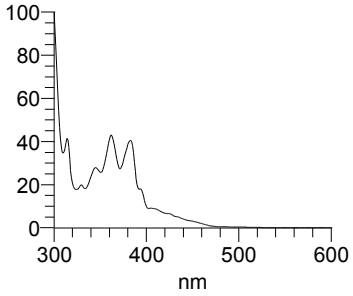
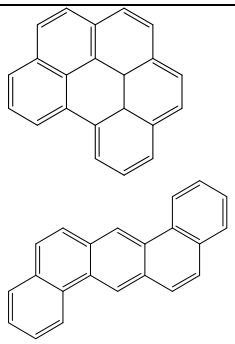
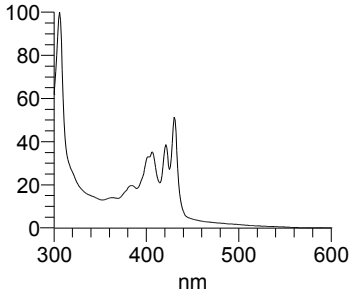
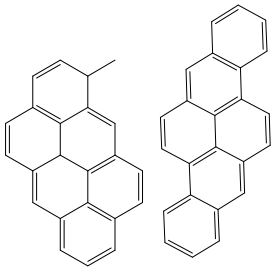
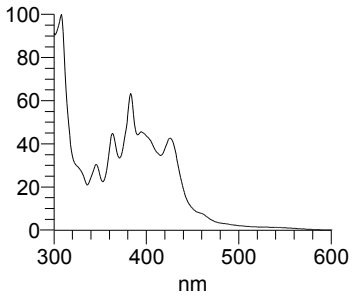
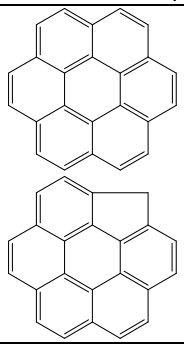
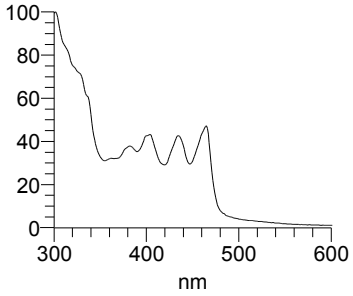
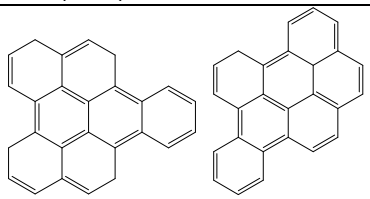
Table S1. For each BrC compound LC retention times (RT), PDA spectra, assigned elemental formulas, probable structures of the major BrC chromophores, measured m/z and detection mode are noted. For clarity, all detected compounds are reported as neutral species, unless stated otherwise.

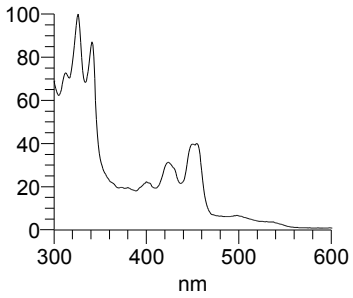
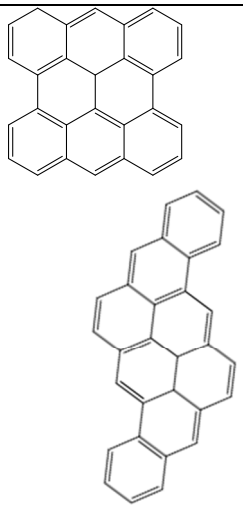
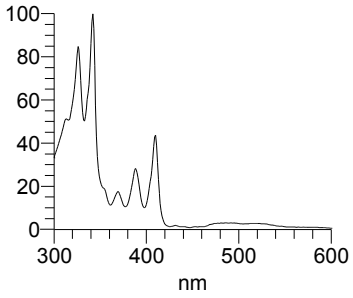
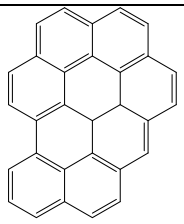
Peak #; RT range (min-min)	UV-Vis spectrum	Elemental formula	Tentative structures	Detection mode & measured *m/z*
1; (9.4-9.9)		$C_8 H_8 O_3$, $C_9 H_6 O_4$,		ESI-, 151.0403, 177.0196,
2; (10.3-10.8)		$C_6 H_5 N O_5$ $C_8 H_{10} O_5 S$		ESI-, 170.0097, 217.0178,
3; (14.0-14.5)		$C_{10} H_8 O_4$ $C_9 H_{10} O_3$ $C_{12} H_{12} O_4$		ESI-, 191.0352, 165.0559, 219.0664,
4; (15.9-16.4)		$C_6 H_5 N O_4$	 4-nitrocatechol based on the UV-vis spectrum and previous report of *Lin et al*.[44]	ESI-, 154.0147

5; (17.9-18.6)		C_{10} H_{10} O_3 C_{11} H_{12} O_4		ESI-, 177.0559, 207.0665,
6; (20.0-20.5)		C_8 H_7 N O_4 C_7 H_7 N O_4	 methyl-nitrocatechol (C_7 H_7 N O_4) based on the UV-vis spectrum and previous report of *Claeys et al*.[60]	ESI-, 180.0305, 168.0304,
7; (22.0-22.3)		C_8 H_9 N O_5	 4-nitrosyringol based on the UV-vis spectrum and previous report of *Lin et al*.[33]	ESI-, 198.0410,
8; (23.1-23.6)		C_7 H_7 N O_4	 4-nitroguaiacol based on the UV-vis spectrum and previous report of *Kitanovski et al*.[62]	ESI-, 168.0304,
9; (25.5-26.0)		C_8 H_9 N O_4 C_{10} H_{11} N O_5		ESI-, 182.0460, 224.0567,

10; (28.5-29.2)		C_{11} H_{13} N O_5 C_{18} H_{16} O_8		ESI- , 238.0724, 359.0779,
11; (32.4-32.9)		C_{10} H_7 N O_3 C_9 H_{11} N O_4	 2-Nitro-1-naphthol based on the UV-vis spectrum and previous report of *Xie et al*.[63]	ESI-, 188.0355, 196.0617,
12; (33.5-33.9)		C_{10} H_{13} N O_4 C_{13} H_{13} N O_4 C_{11} H_{13} N O_4		ESI-, 210.0775, 246.0777, 222.0776,
13; (38.8-39.5)		C_{17} H_{14} O_4 C_{15} H_{14} O_4		ESI+, 283.0979, 259.0981,
14; (41.5-41.9)		C_{17} H_{10} O C_{16} H_{10} O		ESI+, 231.0804, 219.0809,

15; (43.6-44.1)		C_{19} H_{10} O		ESI+, 271.0752,
16; (47.8-48.2)		C_{21} H_{12} O C_{17} H_{11} N		ESI+, 281.0959, 230.0964,
17; (51.3-51.9)		C_{21} H_{11} N C_{21} H_{10} O_2		ESI+, 278.0968, 295.0753,
18; (55.2-55.7)		C_{18} H_{10} C_{18} H_{12}		APPI+ , 226.0765, 228.0922,
19; (58.8-59.6)		C_{20} H_{12} C_{20} H_{14} C_{20} H_{10}		APPI+ , 252.0920, 254.1074, 250.0765,

20; (63.8-64.4)		C_{22} H_{12} C_{22} H_{14} C_{25} H_{12} O	 Benzo[ghi]perylene ($C_{22}H_{12}$) based on the UV-vis spectrum and previous report of *Friedel and Orchin*.[61] (spectrum #573)	APPI+ , 276.0918, 278.1096, 328.0867,
21; (65.3-65.8)		C_{24} H_{14} C_{23} H_{14} C_{27} H_{12} O	 Methylanthanthrene ($C_{23}H_{14}$) based on the UV-vis spectrum and previous report of *Friedel and Orchin*.[61] (spectrum #569)	APPI+ , 302.1073 290.1076, 352.0864,
22; (67.0-67.5)		C_{24} H_{12} C_{24} H_{14} C_{23} H_{12}		APPI+ , 300.0919, 302.1073, 288.0938,
23; (71.2-72.0)		C_{26} H_{14} C_{26} H_{12}		APPI+ , 326.1073, 324.0915,

24; (79.3-80.1)		C_{28} H_{14} C_{30} H_{16}		APPI+ , 350.1095, 376.1251,
25; (91.7-92.5)		C_{30} H_{14}		APPI+ , 374.1070,