Supporting information

Reproducibility of Crude Oil Spectra Obtained with Ultrahigh Resolution Mass Spectrometry

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Table S1. List of oil samples used in this study

Name	Location of field
Arabian	SAUDI ARABIA
West Bukha	OMAN
Pyrenees	AUSTRALIA
Upper Zakum	United Arab Emirates (U.A.E)

Table S2. Variations in class distributions based on absolute abundance values observed from Arabian heavy oil. These values were used to plot the figures in the left column of Fig. 1.

	Average value (set 1, absolute abundance)	**RSD of set 1** (set 1, absolute abundance)	**Error (set 1)**	**Average value** (set 2, absolute abundance)	**RSD** (set 2, absolute a bundance)	**Error (set 2)**	**Average value** (set 3, absolute abund ance)	**RSD** (set 3, absolute a bundance)	**Error (set 3)**	**Average value** (set 1, 2, and 3 combined, absolute a bundance)	**RSD** (set 1, 2, and 3 combined, absolut e abundance)	**Error** (set 1, 2, and 3 combined)
HC	31584259765.8	4.0	2899481141	30827758757.5	1.7	1207328821	32979758257.5	6.0	4470845692	31797258927	4.92	1227145758
S_1	25970455598.8	4.0	2342157129	24704023756.8	1.8	1019137200	26110532093.8	6.0	3536277538	25595003816	4.69	942624069
S_2	4727755682.0	4.6	488700144	4187928128.3	2.2	209254890	4106413171.5	6.4	601350217	4340698994	7.88	268388739
O_1	1790389912.5	4.6	187875943	1708909836.0	2.3	90998354	1730144424.5	6.3	247409248	1743148058	4.75	64905902
N_1	1793941763.0	4.1	165929494	1641668781.3	2.3	85785434	1625711922.8	6.7	246987723	1687107489	6.31	83572244
O_1S_1	1763950330.5	4.7	189561399	1619277940.5	2.5	90552832	1601766036.0	6.8	247681666	1661664769	6.41	83563724
N_1S_1	1630080032.8	5.0	184439818	1458171033.3	3.6	120000424	1408539896.8	5.7	180866725	1498930321	7.93	93240796
N_1S_2	1086567666.0	4.8	118206115	976341890.8	2.9	65236259	928153178.3	5.2	109221007	997020911.7	8.02	62727599
N_1O_1	546939728.8	11.0	136235162	507805842.3	4.8	55555444	582248779.3	3.8	50482918	545664783.4	8.77	37534641
S_3	433190641.5	1.9	18256632	342210588.3	3.1	24114756	316611212.3	11.3	80972271	364004147.3	15.36	43864184

Table S3. Variations in class distributions based on relative abundance values observed from Arabian heavy oil. These values were used to plot the figures in the right column of Fig. 1.

	Average value (set 1, relative abundance)	**RSD of set 1** (set 1, relative abundance)	**Error (set 1)**	**Average value** (set 2, relative abundance)	**RSD** (set 2, relative abundance)	**Error (set 2)**	**Average value** (set 3, relative abundance)	**RSD** (set 3, relative abundance)	**Error (set 3)**	**Average value** (set 1, 2, and 3 combined, relative abundance)	**RSD** (set 1, 2, and 3 combined, relative abundance)	**Error** (set 1, 2, and 3 combined)
HC	0.55	0.05	0.0006	0.56	0.05	0.0006	0.56	0.22	0.0027	0.55	0.7	0.0032
S_1	0.45	0.06	0.0006	0.44	0.06	0.0006	0.44	0.27	0.0027	0.45	0.9	0.0032
S_2	0.08	0.82	0.0015	0.08	0.72	0.0012	0.07	0.86	0.0014	0.08	7.2	0.0043
O_1	0.03	2.7	0.0019	0.03	1.5	0.0010	0.03	1.5	0.0010	0.03	3.3	0.0008
N_1	0.03	0.4	0.0003	0.03	1.1	0.0007	0.03	1.3	0.0008	0.03	5.4	0.0012
O_1S_1	0.03	2.8	0.0019	0.03	1.1	0.0007	0.03	0.93	0.0006	0.03	5.5	0.0013
N_1S_1	0.03	4.2	0.0027	0.03	1.9	0.0011	0.02	3.6	0.0020	0.03	7.9	0.0016
N_1S_2	0.02	2.8	0.0012	0.02	1.7	0.0007	0.02	2.0	0.0007	0.02	8.1	0.0011
N_1O_1	0.01	12	0.0027	0.01	3.2	0.0007	0.01	5.4	0.0012	0.01	8.0	0.0006
S_3	0.01	4.0	0.0007	0.01	4.3	0.0006	0.01	6.2	0.0007	0.01	15	0.0008

Table S4. Variations in DBE distributions of HC class compounds observed from Arabian heavy oil. These values were used to plot Fig. 2a.

	Average value (set 1, relative abundance)	**RSD of set 1** (set 1, relative abundance)	**Error (set 1)**	**Average value** (set 2, relative abundance)	**RSD** (set 2, relative abundance)	**Error (set 2)**	**Average value** (set 3, relative abundance)	**RSD** (set 3, relative abundance)	**Error (set 3)**	**Average value** (set 1, 2, and 3 combined, relative abundance)	**RSD** (set 1, 2, and 3 combined, relative abundance)	**Error** (set 1, 2, and 3 combined)
2	1.4E-03	1.3	4.0E-05	7.5E-05	3.8	1.2E-04	6.4E-05	3.5	1.0E-04	1.4E-03	4.3	4.6E-05
2.5	4.1E-03	2.1	1.9E-04	2.7E-03	0.6	5.7E-05	2.5E-03	0.6	5.6E-05	4.2E-03	2.9	9.5E-05
3	3.3E-03	0.4	3.0E-05	1.1E-03	0.2	1.5E-05	1.1E-03	1.3	9.5E-05	3.2E-03	3.1	7.9E-05
3.5	8.8E-03	0.4	7.3E-05	3.5E-03	0.6	1.2E-04	3.3E-03	0.8	1.7E-04	8.9E-03	1.9	1.3E-04
4	3.9E-02	0.6	5.0E-04	1.8E-03	0.6	5.9E-04	1.7E-03	1.7	1.8E-03	4.3E-02	7.0	2.4E-03
4.5	1.3E-02	0.5	1.4E-04	3.7E-03	0.9	2.6E-04	3.5E-03	1.4	4.0E-04	1.3E-02	1.7	1.7E-04
5	3.5E-02	0.7	5.8E-04	5.3E-03	0.5	4.4E-04	5.4E-03	0.8	7.5E-04	3.8E-02	4.8	1.4E-03
5.5	1.4E-02	0.6	1.8E-04	4.3E-03	0.7	2.2E-04	4.1E-03	0.3	9.8E-05	1.4E-02	2.2	2.4E-04
6	3.2E-02	0.4	3.0E-04	4.2E-02	0.3	2.1E-04	4.6E-02	0.5	3.7E-04	3.4E-02	4.4	1.2E-03
6.5	1.2E-02	0.9	2.4E-04	3.4E-03	0.9	2.6E-04	3.3E-03	0.3	8.3E-05	1.3E-02	1.9	1.9E-04
7	3.1E-02	0.7	4.8E-04	2.6E-02	0.2	1.5E-04	2.6E-02	0.8	5.7E-04	3.2E-02	3.6	9.0E-04
7.5	1.1E-02	0.6	1.6E-04	2.7E-03	0.5	1.3E-04	2.6E-03	0.6	1.4E-04	1.1E-02	1.5	1.4E-04
8	3.0E-02	0.4	2.5E-04	1.9E-02	0.2	1.2E-04	1.9E-02	0.5	3.4E-04	3.1E-02	3.4	8.4E-04
8.5	8.3E-03	0.5	1.0E-04	2.7E-03	0.4	8.5E-05	2.6E-03	0.8	1.4E-04	8.3E-03	1.2	7.6E-05
9	3.1E-02	0.6	3.8E-04	3.6E-02	0.3	2.4E-04	3.8E-02	0.3	2.1E-04	3.2E-02	4.4	1.1E-03
9.5	5.7E-03	1.3	1.7E-04	2.8E-03	0.5	6.4E-05	2.6E-03	1.3	1.7E-04	5.7E-03	1.7	7.8E-05
10	2.7E-02	0.4	2.6E-04	3.0E-02	0.2	1.2E-04	3.2E-02	1.0	6.8E-04	2.8E-02	2.9	6.4E-04
10.5	3.1E-03	2.0	1.4E-04	2.2E-03	4.6	2.9E-04	2.0E-03	2.5	1.4E-04	2.8E-03	10.2	2.2E-04
11	2.3E-02	0.5	2.6E-04	2.7E-02	0.5	2.6E-04	2.8E-02	1.6	8.6E-04	2.4E-02	1.4	2.6E-04
11.5	2.5E-03	3.6	2.0E-04	1.9E-03	8.4	3.9E-04	1.7E-03	7.0	2.7E-04	2.1E-03	16.0	2.6E-04
12	2.1E-02	0.7	3.4E-04	2.5E-02	0.5	2.1E-04	2.5E-02	1.2	5.9E-04	2.1E-02	1.2	2.0E-04
12.5	2.0E-03	4.8	2.2E-04	1.5E-03	4.5	1.8E-04	1.3E-03	7.1	2.6E-04	1.8E-03	11.6	1.6E-04
13	1.8E-02	0.6	2.3E-04	2.1E-02	0.5	2.0E-04	2.1E-02	0.2	9.1E-05	1.8E-02	1.0	1.4E-04
13.5	1.1E-03	4.3	1.0E-04	1.2E-03	12.6	2.3E-04	1.1E-03	13.4	2.1E-04	8.4E-04	21.2	1.4E-04
14	1.4E-02	1.0	2.9E-04	1.8E-02	0.4	1.1E-04	1.8E-02	0.7	2.1E-04	1.4E-02	0.8	8.9E-05
14.5	1.2E-03	6.3	1.8E-04	1.0E-03	6.9	1.3E-04	9.6E-04	12.4	3.3E-04	1.1E-03	18.1	1.6E-04
15	1.1E-02	0.5	1.3E-04	1.5E-02	1.4	3.4E-04	1.5E-02	0.9	2.1E-04	1.1E-02	1.1	9.1E-05
15.5	9.3E-04	4.9	1.0E-04	3.9E-04	21.1	3.5E-04	2.8E-04	12.7	2.3E-04	8.1E-04	16.6	1.1E-04
16	8.6E-03	0.3	5.1E-05	1.2E-02	1.7	3.2E-04	1.2E-02	1.1	2.1E-04	8.4E-03	2.1	1.4E-04
16.5	5.2E-04	18.8	2.2E-04	2.7E-04	4.4	4.4E-05	1.8E-04	23.7	2.3E-04	4.7E-04	18.5	6.8E-05
17	6.7E-03	1.6	2.4E-04	1.0E-02	2.4	3.5E-04	9.8E-03	3.6	5.1E-04	6.5E-03	3.8	1.9E-04
17.5	5.1E-04	6.9	7.9E-05	2.2E-04	5.4	9.1E-05	1.7E-04	11.9	1.9E-04	6.5E-04	18.1	9.2E-05
18	5.3E-03	1.0	1.2E-04	8.3E-03	1.1	1.2E-04	7.8E-03	0.4	4.4E-05	4.8E-03	8.0	3.0E-04
18.5	4.5E-04	19.9	2.0E-04	9.6E-05	26.9	2.6E-04	6.6E-05	30.8	3.5E-04	4.6E-04	24.9	9.0E-05
19	4.0E-03	1.5	1.4E-04	6.5E-03	4.8	3.7E-04	6.0E-03	1.1	7.8E-05	3.6E-03	9.9	2.8E-04
19.5	3.5E-04	21.4	1.7E-04	1.5E-04	6.2	9.6E-05	1.6E-04	13.4	1.7E-04	5.3E-04	29.6	1.2E-04
20	3.1E-03	1.6	1.1E-04	5.0E-03	1.7	1.0E-04	4.5E-03	1.4	8.0E-05	2.8E-03	11.0	2.4E-04
20.5	2.1E-04	23.8	1.1E-04	1.5E-04	38.6	1.5E-04	1.1E-04	10.8	3.5E-05	1.8E-04	30.5	4.2E-05
21	2.4E-03	2.4	1.3E-04	4.2E-03	3.7	1.6E-04	3.6E-03	2.2	8.9E-05	2.0E-03	13.4	2.1E-04
21.5	2.0E-04	42.2	1.9E-04	1.8E-04	19.4	1.3E-04	1.2E-04	28.0	2.3E-04	2.8E-04	35.3	7.9E-05
22	1.8E-03	6.2	2.5E-04	3.2E-03	2.5	8.1E-05	2.9E-03	1.5	4.2E-05	1.5E-03	14.4	1.7E-04
22.5	2.0E-04	10.3	4.6E-05	5.7E-05	64.9	1.9E-04	5.0E-05	26.0	1.1E-04	1.7E-04	35.4	4.7E-05
23	1.3E-03	5.0	1.5E-04	2.4E-03	4.9	1.2E-04	2.1E-03	4.2	8.4E-05	1.1E-03	19.1	1.6E-04
23.5	9.2E-05	16.6	3.5E-05	1.7E-04	9.1	1.6E-05	1.6E-04	70.4	1.5E-04	8.7E-05	41.1	2.8E-05
24	9.3E-04	8.4	1.8E-04	1.7E-03	9.8	1.5E-04	1.5E-03	5.9	7.5E-05	7.2E-04	23.5	1.3E-04
24.5	9.2E-05	45.6	9.5E-05	1.3E-04	21.7	5.7E-05	1.4E-04	8.8	4.1E-05	1.4E-04	41.8	4.5E-05
25	6.1E-04	6.3	8.7E-05	1.3E-03	14.2	1.5E-04	1.1E-03	6.2	4.6E-05	4.6E-04	27.2	9.9E-05
25.5	5.6E-05	46.3	5.8E-05	4.7E-05	81.1	1.4E-04	8.9E-05	54.9	1.5E-04	8.3E-05	66.9	4.4E-05
26	4.5E-04	9.3	9.5E-05	9.6E-04	25.3	1.3E-04	7.3E-04	14.0	4.6E-05	2.7E-04	51.8	1.1E-04

Table S5. Variations in DBE distributions of S_1 class compounds observed from Arabian heavy oil. These values were used to plot Fig. 2b.

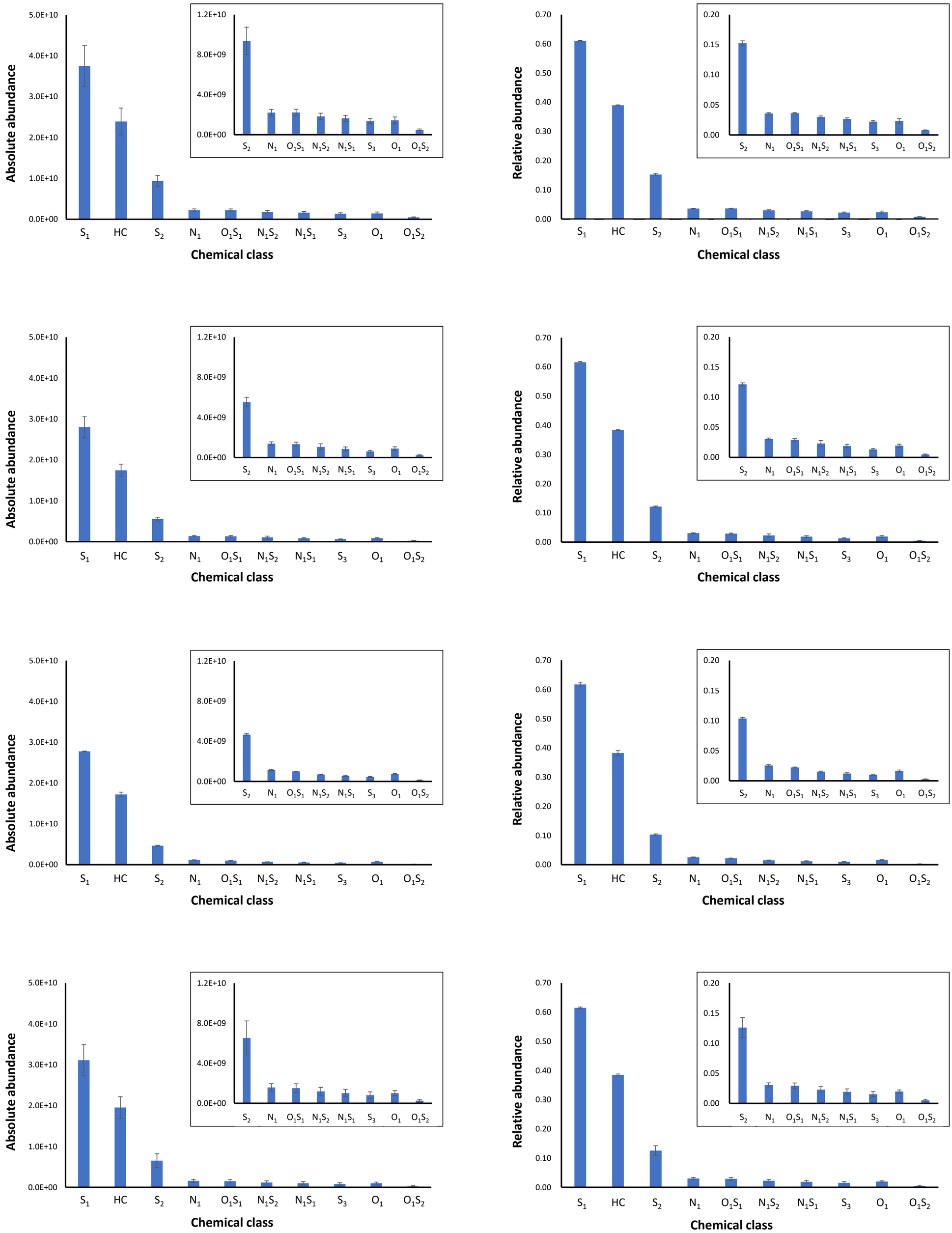
	Average value (set 1, relative abundance)	**RSD of set 1** (set 1, relative abundance)	**Error (set 1)**	**Average value** (set 2, relative abundance)	**% RSD** (set 2, relative abundance)	**Error (set 2)**	**Average value** (set 3, relative abundance)	**% RSD** (set 3, relative abundance)	**Error (set 3)**	**Average value** (set 1, 2, and 3 combined, relative abundance)	**% RSD** (set 1, 2, and 3 combined, relative abundance)	**Error** (set 1, 2, and 3 combined)
2	8.5E-05	18.8	3.6E-05	7.5E-05	29.4	5.0E-05	0.001	16.2	2.3E-05	7.5E-05	23.7	1.4E-05
2.5	2.8E-03	0.7	4.6E-05	2.7E-03	0.8	5.0E-05	0.004	0.8	4.2E-05	2.7E-03	5.6	1.2E-04
3	1.3E-03	2.7	8.3E-05	1.1E-03	3.3	8.1E-05	0.003	6.2	1.6E-04	1.2E-03	11.3	1.0E-04
3.5	3.7E-03	1.7	1.5E-04	3.5E-03	1.6	1.2E-04	0.009	1.3	1.0E-04	3.5E-03	4.4	1.2E-04
4	2.0E-03	4.4	2.0E-04	1.8E-03	1.9	7.8E-05	0.046	4.2	1.6E-04	1.8E-03	8.9	1.3E-04
4.5	3.7E-03	1.6	1.4E-04	3.7E-03	2.4	2.0E-04	0.013	2.1	1.7E-04	3.6E-03	3.8	1.1E-04
5	5.9E-03	1.1	1.5E-04	5.3E-03	1.3	1.6E-04	0.039	2.0	2.5E-04	5.5E-03	4.9	2.1E-04
5.5	4.6E-03	2.9	3.0E-04	4.3E-03	3.7	3.6E-04	0.014	0.9	8.6E-05	4.3E-03	4.7	1.6E-04
6	3.9E-02	0.2	2.0E-04	4.2E-02	0.6	5.4E-04	0.036	1.6	1.7E-03	4.2E-02	6.5	2.2E-03
6.5	3.7E-03	1.3	1.1E-04	3.4E-03	0.9	6.9E-05	0.013	3.2	2.4E-04	3.5E-03	4.8	1.3E-04
7	2.5E-02	0.7	4.0E-04	2.6E-02	0.9	5.4E-04	0.033	1.5	8.9E-04	2.6E-02	1.8	3.7E-04
7.5	2.7E-03	2.3	1.4E-04	2.7E-03	1.2	7.6E-05	0.012	2.6	1.5E-04	2.7E-03	3.5	7.3E-05
8	1.9E-02	0.4	1.5E-04	1.9E-02	0.4	1.8E-04	0.033	0.1	3.0E-05	1.9E-02	1.0	1.5E-04
8.5	2.9E-03	3.5	2.3E-04	2.7E-03	2.8	1.7E-04	0.008	2.8	1.7E-04	2.7E-03	5.5	1.2E-04
9	3.4E-02	0.4	3.0E-04	3.6E-02	0.1	1.1E-04	0.034	0.6	5.1E-04	3.6E-02	4.1	1.2E-03
9.5	3.0E-03	2.2	1.5E-04	2.8E-03	2.3	1.4E-04	0.006	2.1	1.3E-04	2.8E-03	5.9	1.3E-04
10	2.9E-02	0.3	2.1E-04	3.0E-02	0.3	2.0E-04	0.029	0.3	1.8E-04	3.0E-02	3.2	7.6E-04
10.5	2.3E-03	2.1	1.1E-04	2.2E-03	1.1	5.1E-05	0.002	1.5	6.8E-05	2.2E-03	5.4	9.1E-05
11	2.6E-02	0.7	3.9E-04	2.7E-02	0.2	1.2E-04	0.024	0.4	2.8E-04	2.7E-02	2.4	5.1E-04
11.5	2.0E-03	2.9	1.3E-04	1.9E-03	2.7	1.1E-04	0.002	3.6	1.4E-04	1.9E-03	5.8	8.5E-05
12	2.4E-02	0.6	3.4E-04	2.5E-02	0.3	1.6E-04	0.021	0.3	1.6E-04	2.5E-02	1.8	3.4E-04
12.5	1.6E-03	4.2	1.5E-04	1.5E-03	4.1	1.4E-04	0.002	4.7	1.4E-04	1.5E-03	8.4	9.5E-05
13	2.1E-02	0.5	2.5E-04	2.1E-02	0.7	3.2E-04	0.018	1.8	8.7E-04	2.1E-02	1.2	1.9E-04
13.5	1.3E-03	1.7	5.0E-05	1.2E-03	5.4	1.4E-04	0.001	2.5	6.1E-05	1.2E-03	7.9	7.4E-05
14	1.9E-02	0.4	1.8E-04	1.8E-02	0.7	3.0E-04	0.014	1.9	8.1E-04	1.9E-02	2.0	2.9E-04
14.5	1.1E-03	3.9	1.0E-04	1.0E-03	1.5	3.4E-05	0.001	0.8	1.6E-05	1.0E-03	6.9	5.6E-05
15	1.6E-02	0.7	2.6E-04	1.5E-02	0.2	6.2E-05	0.011	0.8	2.7E-04	1.5E-02	1.5	1.9E-04
15.5	4.7E-04	19.0	2.0E-04	3.9E-04	26.2	2.3E-04	0.001	13.5	8.6E-05	3.8E-04	28.7	8.5E-05
16	1.3E-02	0.4	1.2E-04	1.2E-02	0.4	1.1E-04	0.008	0.9	2.5E-04	1.2E-02	2.4	2.3E-04
16.5	3.3E-04	6.1	4.6E-05	2.7E-04	5.2	3.2E-05	0.0004	24.0	1.0E-04	2.6E-04	26.1	5.4E-05
17	1.1E-02	0.6	1.4E-04	1.0E-02	0.7	1.6E-04	0.006	0.9	2.1E-04	1.0E-02	3.5	2.8E-04
17.5	1.9E-04	12.2	5.4E-05	2.2E-04	26.5	1.3E-04	0.001	10.5	4.1E-05	1.9E-04	20.2	3.1E-05
18	8.6E-03	0.6	1.1E-04	8.3E-03	0.3	6.5E-05	0.004	0.3	5.4E-05	8.2E-03	3.9	2.5E-04
18.5	5.4E-05	41.5	5.1E-05	9.6E-05	52.9	1.2E-04	0.0005	43.4	6.5E-05	7.2E-05	51.8	2.9E-05
19	6.7E-03	0.7	1.1E-04	6.5E-03	0.9	1.3E-04	0.003	0.5	7.4E-05	6.4E-03	4.8	2.4E-04
19.5	1.3E-04	35.1	1.0E-04	1.5E-04	62.7	2.2E-04	0.001	45.3	1.7E-04	1.5E-04	46.6	5.4E-05
20	5.4E-03	0.9	1.1E-04	5.0E-03	0.9	9.8E-05	0.002	1.9	1.9E-04	5.0E-03	7.7	3.0E-04
20.5	1.1E-04	22.8	5.5E-05	1.5E-04	22.8	7.7E-05	0.0001	31.5	7.9E-05	1.2E-04	28.4	2.7E-05
21	4.4E-03	1.8	1.8E-04	4.2E-03	1.2	1.2E-04	0.002	1.6	1.4E-04	4.1E-03	8.0	2.5E-04
21.5	1.1E-04	36.6	9.3E-05	1.8E-04	14.6	6.0E-05	0.0004	52.2	1.5E-04	1.4E-04	38.1	4.2E-05
22	3.3E-03	3.5	2.7E-04	3.2E-03	2.0	1.5E-04	0.001	1.3	8.4E-05	3.1E-03	6.9	1.7E-04
22.5	7.3E-05	45.4	7.5E-05	5.7E-05	18.6	2.4E-05	0.0002	33.8	3.9E-05	6.0E-05	37.4	1.8E-05
23	2.5E-03	2.3	1.3E-04	2.4E-03	2.0	1.1E-04	0.001	5.5	2.6E-04	2.3E-03	8.5	1.5E-04
23.5	1.5E-04	21.8	7.2E-05	1.7E-04	21.4	8.4E-05	0.0001	34.2	1.3E-04	1.6E-04	25.2	3.2E-05
24	1.9E-03	2.3	9.7E-05	1.7E-03	6.4	2.5E-04	0.001	5.6	1.9E-04	1.7E-03	10.5	1.4E-04
24.5	7.6E-05	43.1	7.5E-05	1.3E-04	41.9	1.2E-04	0.0002	23.7	7.6E-05	1.2E-04	41.1	3.7E-05
25	1.4E-03	1.0	3.2E-05	1.3E-03	1.8	5.2E-05	0.0003	5.6	1.4E-04	1.3E-03	10.6	1.1E-04
25.5	7.9E-05	38.7	6.9E-05	4.7E-05	22.3	2.4E-05	0.0001	40.9	8.3E-05	7.2E-05	43.7	2.5E-05
26	9.8E-04	2.0	4.4E-05	9.6E-04	6.4	1.4E-04	0.0001	2.7	4.5E-05	8.9E-04	14.0	9.8E-05

Table S6. Variations in carbon number distributions of S_1 class compounds with DBE=9 observed from Arabian heavy oil. These values were used to plot Fig. 4.

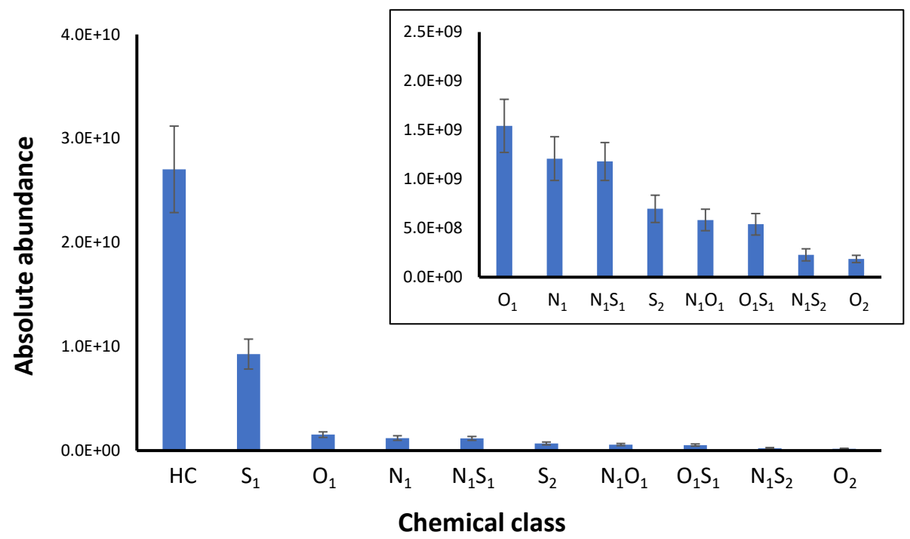
	Average value (set 1, relative abundance)	**RSD of set 1** (set 1, relative abundance)	**Error (set 1)**	**Average value** (set 2, relative abundance)	**RSD** (set 2, relative abundance)	**Error (set 2)**	**Average value** (set 3, relative abundance)	**RSD** (set 3, relative abundance)	**Error (set 3)**	**Average value** (set 1, 2, and 3 combined, relative abundance)	**RSD** (set 1, 2, and 3 combined, relative abundance)	**Error** (set 1, 2, and 3 combined)
16	2.0E-04	4.7	2.2E-05	2.0E-04	3.5	1.5E-05	2.0E-04	6.6	2.9E-05	2.0E-04	4.8	7.8E-06
17	1.9E-04	1.6	6.8E-06	1.6E-04	4.0	1.5E-05	1.6E-04	5.0	1.8E-05	1.7E-04	8.9	1.3E-05
18	1.9E-04	4.4	1.9E-05	1.7E-04	2.1	8.2E-06	1.8E-04	7.4	3.0E-05	1.8E-04	6.5	9.5E-06
19	2.8E-04	2.3	1.4E-05	2.7E-04	2.6	1.6E-05	3.1E-04	3.5	2.4E-05	2.9E-04	5.9	1.4E-05
20	4.4E-04	3.3	3.2E-05	4.5E-04	4.3	4.4E-05	4.9E-04	2.9	3.2E-05	4.6E-04	5.9	2.2E-05
21	6.3E-04	2.4	3.4E-05	6.2E-04	1.8	2.5E-05	7.4E-04	2.2	3.7E-05	6.6E-04	9.1	4.9E-05
22	7.5E-04	1.2	2.0E-05	7.8E-04	0.5	8.4E-06	8.7E-04	2.2	4.3E-05	8.0E-04	6.9	4.5E-05
23	8.1E-04	0.6	1.2E-05	9.2E-04	2.3	4.7E-05	1.0E-03	3.4	7.8E-05	9.2E-04	9.9	7.5E-05
24	9.4E-04	1.3	2.8E-05	1.0E-03	1.3	2.9E-05	1.1E-03	1.9	4.8E-05	1.0E-03	6.6	5.5E-05
25	9.6E-04	0.7	1.6E-05	1.0E-03	1.6	3.6E-05	1.1E-03	0.8	1.9E-05	1.0E-03	6.3	5.4E-05
26	1.1E-03	0.5	1.3E-05	1.2E-03	1.3	3.5E-05	1.4E-03	2.2	7.1E-05	1.2E-03	9.9	1.0E-04
27	1.1E-03	0.6	1.5E-05	1.2E-03	0.3	7.8E-06	1.3E-03	1.8	5.3E-05	1.2E-03	7.8	7.7E-05
28	1.1E-03	1.2	3.1E-05	1.2E-03	0.8	2.2E-05	1.4E-03	3.1	9.8E-05	1.2E-03	8.5	8.6E-05
29	1.2E-03	1.0	2.8E-05	1.3E-03	1.0	2.9E-05	1.4E-03	1.2	4.0E-05	1.3E-03	7.6	8.2E-05
30	1.3E-03	1.4	3.9E-05	1.3E-03	2.1	6.0E-05	1.5E-03	1.1	3.8E-05	1.3E-03	9.3	1.0E-04
31	1.2E-03	0.9	2.4E-05	1.3E-03	2.1	5.9E-05	1.4E-03	1.1	3.5E-05	1.3E-03	7.8	8.3E-05
32	1.1E-03	1.4	3.4E-05	1.2E-03	1.0	2.8E-05	1.3E-03	2.5	7.5E-05	1.2E-03	7.3	7.2E-05
33	1.2E-03	1.6	4.1E-05	1.3E-03	1.1	3.0E-05	1.3E-03	1.3	3.9E-05	1.2E-03	5.7	5.8E-05
34	1.3E-03	0.3	7.6E-06	1.4E-03	0.3	1.1E-05	1.5E-03	1.5	5.0E-05	1.4E-03	6.4	7.1E-05
35	1.3E-03	0.8	2.4E-05	1.4E-03	1.0	3.2E-05	1.6E-03	1.5	5.5E-05	1.5E-03	10.7	1.3E-04
36	1.2E-03	1.5	4.3E-05	1.4E-03	0.8	2.5E-05	1.6E-03	1.5	5.6E-05	1.4E-03	11.6	1.3E-04
37	1.2E-03	0.8	2.1E-05	1.3E-03	1.4	4.2E-05	1.5E-03	1.0	3.5E-05	1.4E-03	10.4	1.2E-04
38	1.2E-03	1.0	2.7E-05	1.3E-03	1.6	4.8E-05	1.5E-03	3.2	1.1E-04	1.3E-03	8.9	9.6E-05
39	1.2E-03	1.0	2.6E-05	1.3E-03	1.6	4.5E-05	1.4E-03	1.1	3.6E-05	1.3E-03	7.2	7.6E-05
40	1.2E-03	2.3	6.0E-05	1.2E-03	1.4	3.7E-05	1.3E-03	1.4	4.1E-05	1.2E-03	6.0	6.0E-05
41	1.1E-03	1.3	3.2E-05	1.1E-03	0.8	2.0E-05	1.2E-03	1.3	3.5E-05	1.1E-03	4.5	4.2E-05
42	1.0E-03	1.3	3.1E-05	1.1E-03	0.5	1.3E-05	1.1E-03	2.6	6.5E-05	1.1E-03	3.4	3.0E-05
43	9.5E-04	2.0	4.3E-05	9.8E-04	1.4	3.2E-05	9.6E-04	1.9	4.1E-05	9.6E-04	2.1	1.7E-05
44	8.5E-04	1.4	2.8E-05	8.7E-04	1.8	3.5E-05	8.5E-04	1.7	3.3E-05	8.6E-04	1.9	1.3E-05
45	7.4E-04	1.6	2.7E-05	7.7E-04	1.7	3.0E-05	7.2E-04	2.2	3.6E-05	7.4E-04	3.6	2.2E-05
46	6.5E-04	1.4	2.1E-05	7.0E-04	1.2	1.9E-05	6.5E-04	2.4	3.5E-05	6.7E-04	4.0	2.2E-05
47	5.6E-04	1.6	2.0E-05	6.0E-04	2.8	3.8E-05	5.5E-04	1.0	1.2E-05	5.7E-04	4.4	2.0E-05
48	5.2E-04	1.8	2.2E-05	5.4E-04	2.5	3.1E-05	5.0E-04	1.1	1.2E-05	5.2E-04	4.0	1.7E-05
49	4.4E-04	0.8	8.5E-06	4.4E-04	1.3	1.4E-05	4.0E-04	1.6	1.4E-05	4.3E-04	4.8	1.7E-05
50	4.0E-04	0.9	8.5E-06	4.1E-04	0.8	7.7E-06	3.7E-04	2.0	1.7E-05	4.0E-04	5.2	1.7E-05
51	3.5E-04	2.9	2.3E-05	3.6E-04	1.8	1.4E-05	3.3E-04	2.4	1.8E-05	3.5E-04	4.1	1.2E-05
52	3.2E-04	1.9	1.4E-05	3.1E-04	1.1	8.0E-06	2.7E-04	2.0	1.2E-05	3.0E-04	7.5	1.8E-05
53	2.9E-04	5.9	3.9E-05	3.1E-04	1.8	1.3E-05	2.6E-04	1.0	5.8E-06	2.8E-04	8.3	1.9E-05
54	2.4E-04	2.5	1.4E-05	2.4E-04	3.3	1.8E-05	2.0E-04	1.6	7.4E-06	2.3E-04	9.6	1.8E-05
55	2.2E-04	1.6	8.2E-06	2.3E-04	1.5	8.0E-06	1.8E-04	2.7	1.1E-05	2.1E-04	10.9	1.9E-05
56	2.1E-04	4.6	2.2E-05	2.2E-04	1.9	9.4E-06	1.8E-04	3.2	1.3E-05	2.0E-04	9.6	1.6E-05
57	1.9E-04	1.8	7.6E-06	2.0E-04	5.3	2.3E-05	1.6E-04	6.0	2.1E-05	1.8E-04	10.8	1.6E-05
58	1.7E-04	6.5	2.6E-05	1.9E-04	2.9	1.3E-05	1.5E-04	3.7	1.3E-05	1.7E-04	10.4	1.5E-05
59	1.6E-04	4.8	1.8E-05	1.7E-04	6.0	2.4E-05	1.3E-04	9.9	2.9E-05	1.6E-04	14.0	1.8E-05
60	1.5E-04	6.4	2.1E-05	1.3E-04	6.4	1.8E-05	7.8E-05	7.2	1.3E-05	1.2E-04	26.1	2.5E-05
61	1.3E-04	4.0	1.2E-05	1.0E-04	5.2	1.2E-05	5.8E-05	15.0	2.0E-05	9.8E-05	34.1	2.7E-05
62	1.2E-04	4.1	1.1E-05	7.6E-05	9.6	1.7E-05	4.5E-05	12.7	1.3E-05	8.0E-05	39.8	2.6E-05
63	1.0E-04	3.2	7.7E-06	6.5E-05	2.6	3.9E-06	3.3E-05	13.0	9.6E-06	6.5E-05	54.6	2.9E-05
64	8.6E-05	3.4	6.6E-06	4.3E-05	9.7	9.6E-06	2.7E-05	16.3	1.0E-05	5.2E-05	50.6	2.2E-05
65	7.0E-05	3.6	5.7E-06	3.2E-05	6.0	4.4E-06	2.3E-05	14.1	7.2E-06	4.2E-05	51.8	1.8E-05

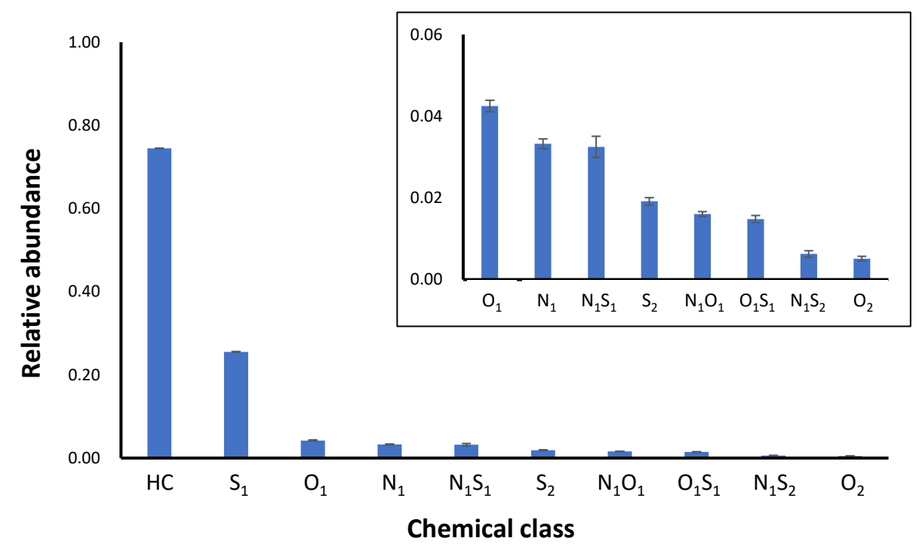
Figure S1. Class distributions of (a) Zakum, (b) Bukha, and (c) Pyrenees oils observed with (+)APPI FT-ICR-MS presented as summed absolute abundances (left column) and summed relative abundances (right column) for the 1st (first row), 2nd (second row), 3rd (third row), and combined datasets (fourth row).

(a) Zakum

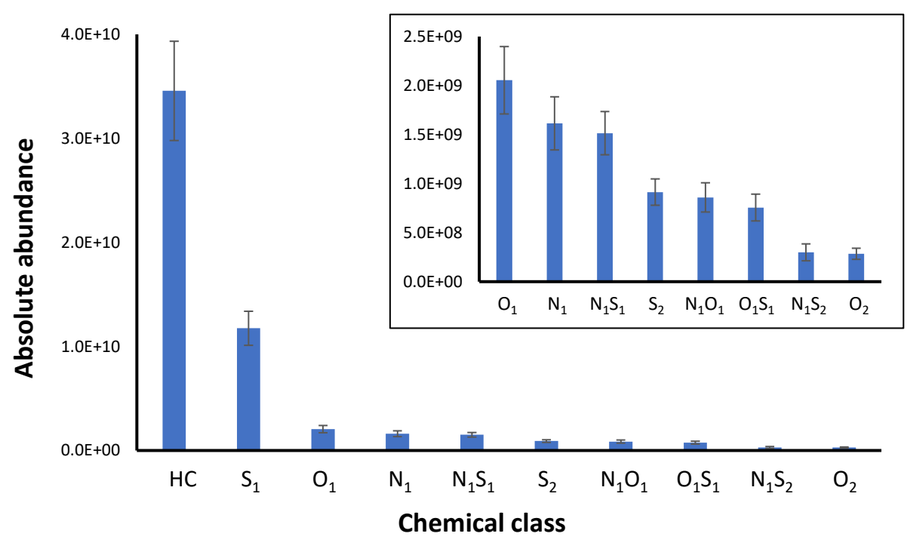


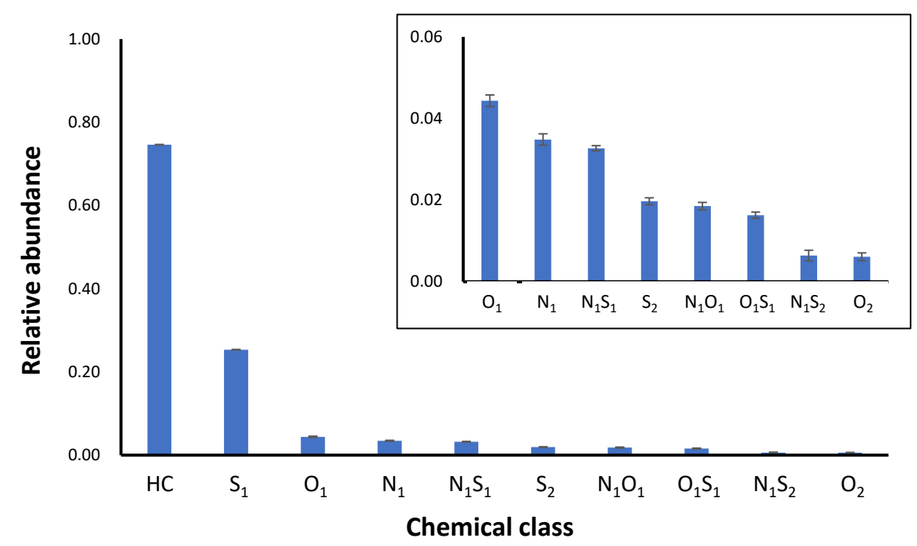
(b) Bukha



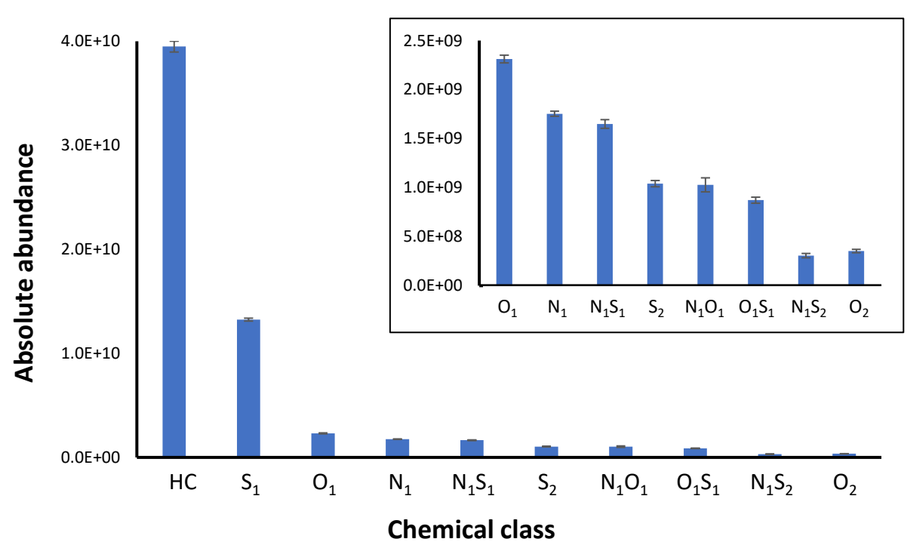


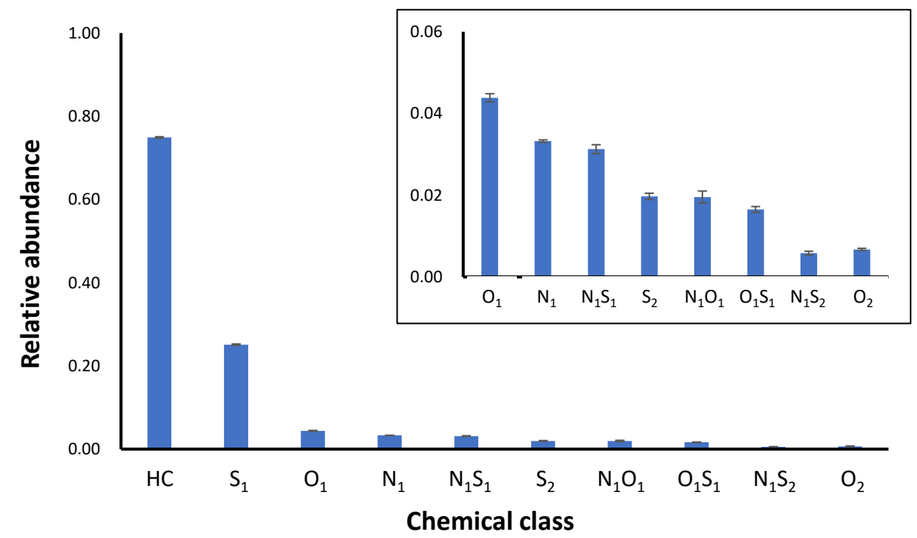
1st set



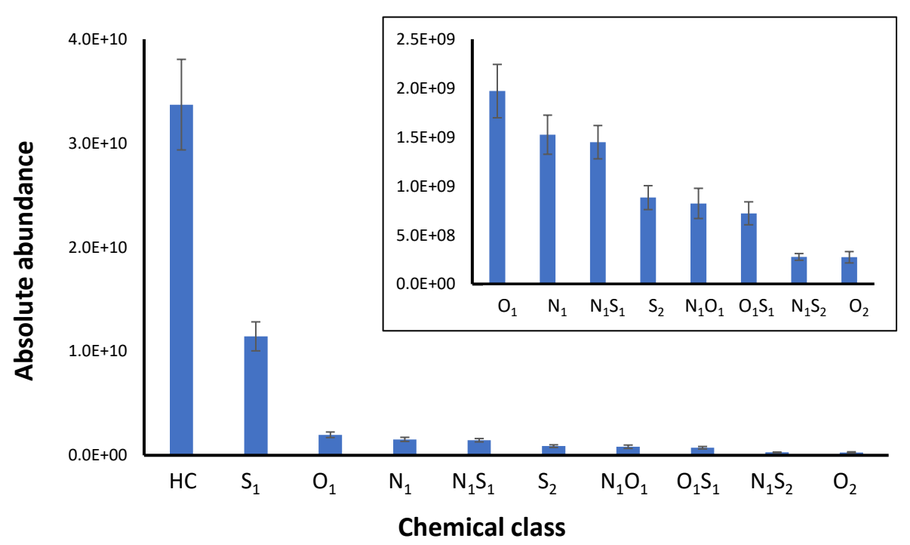


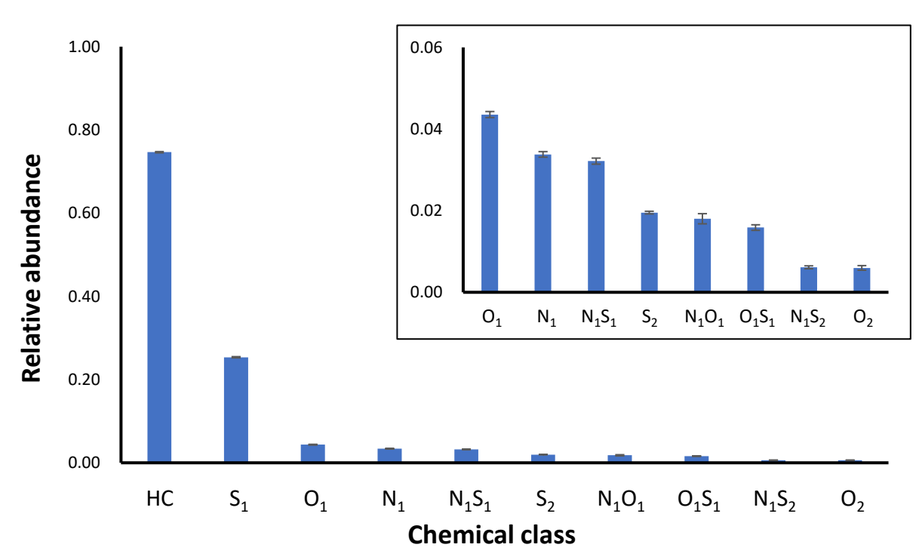
2nd set





3rd set





Three data sets combined

(c) Pyrenees

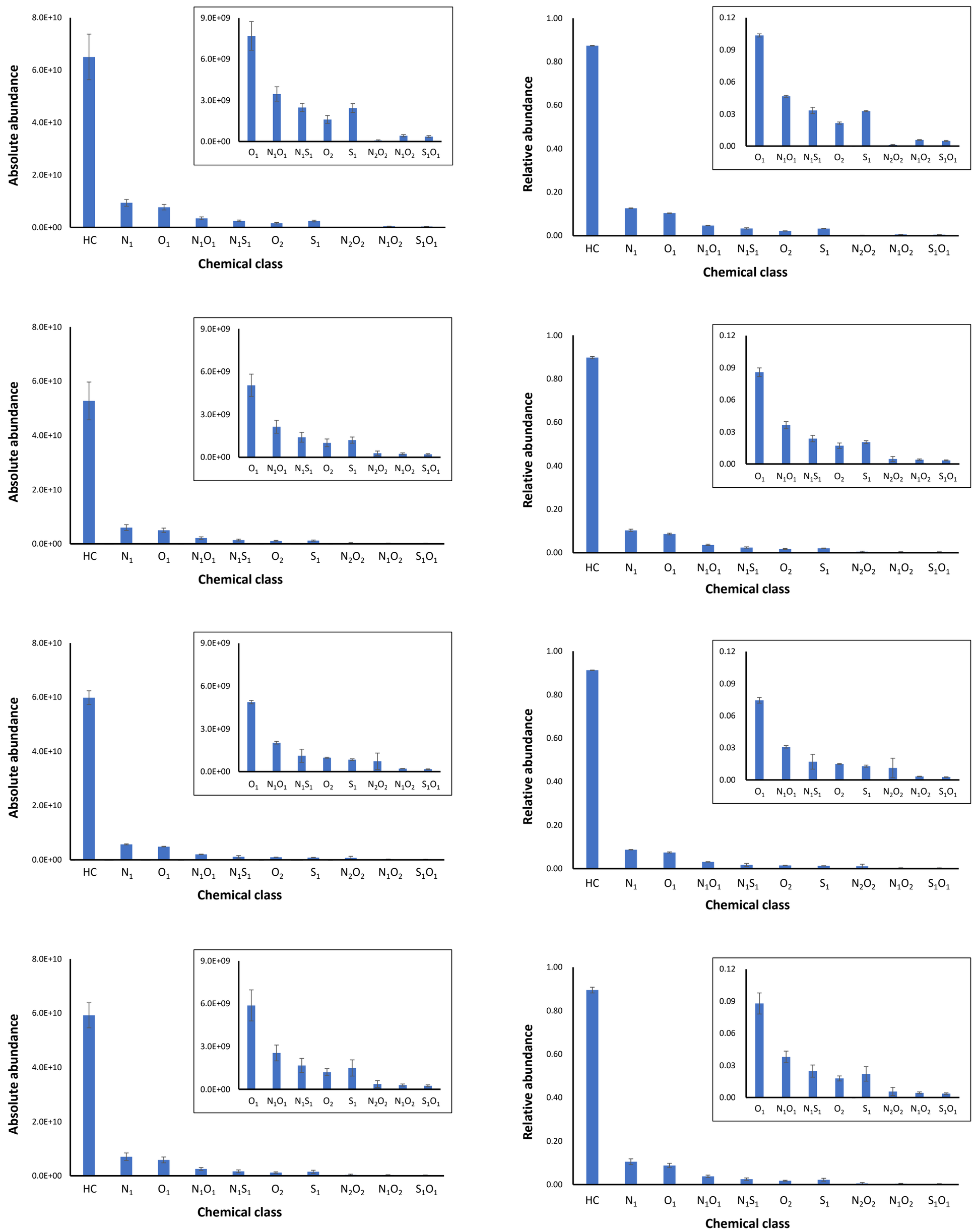
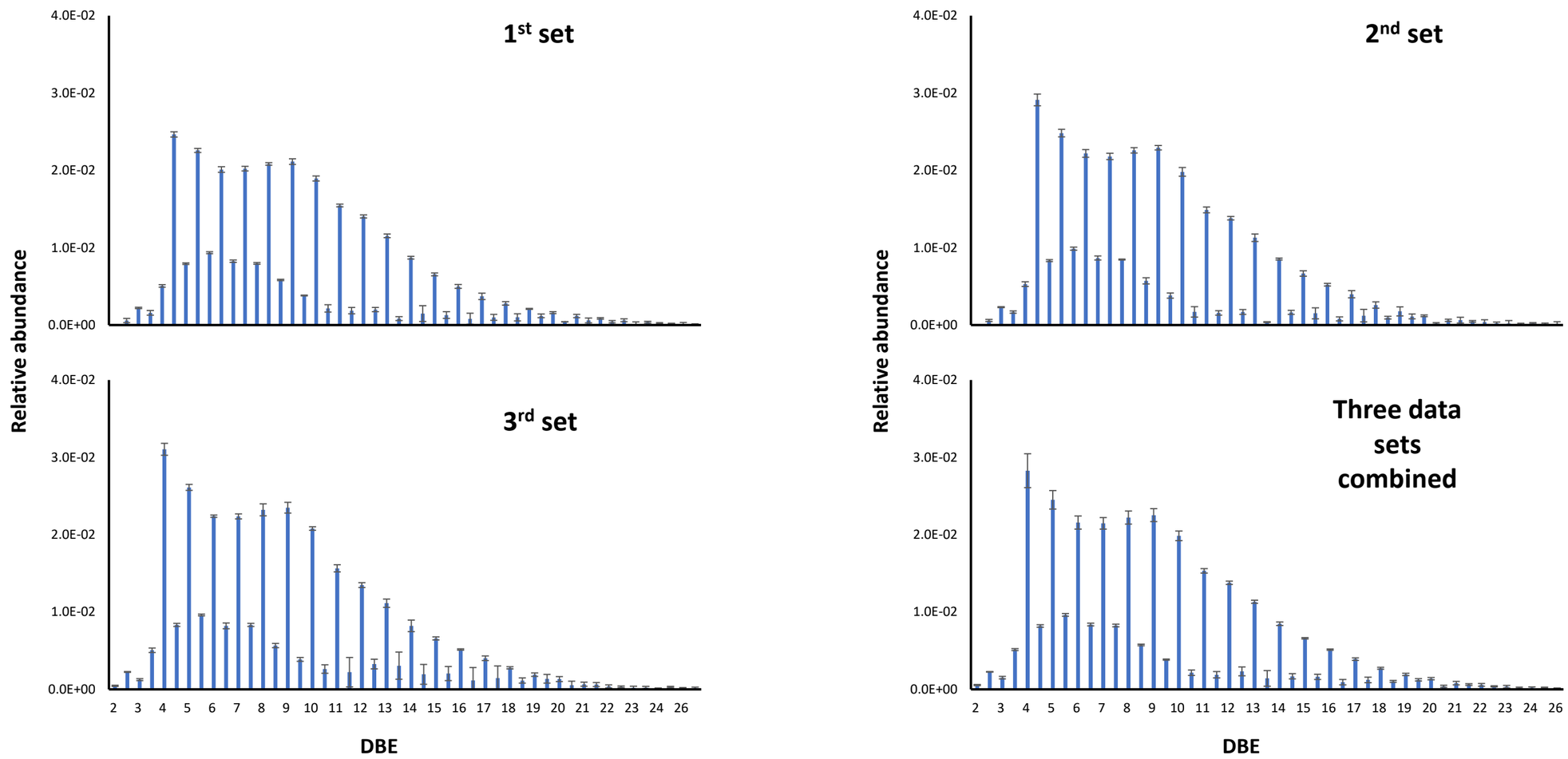
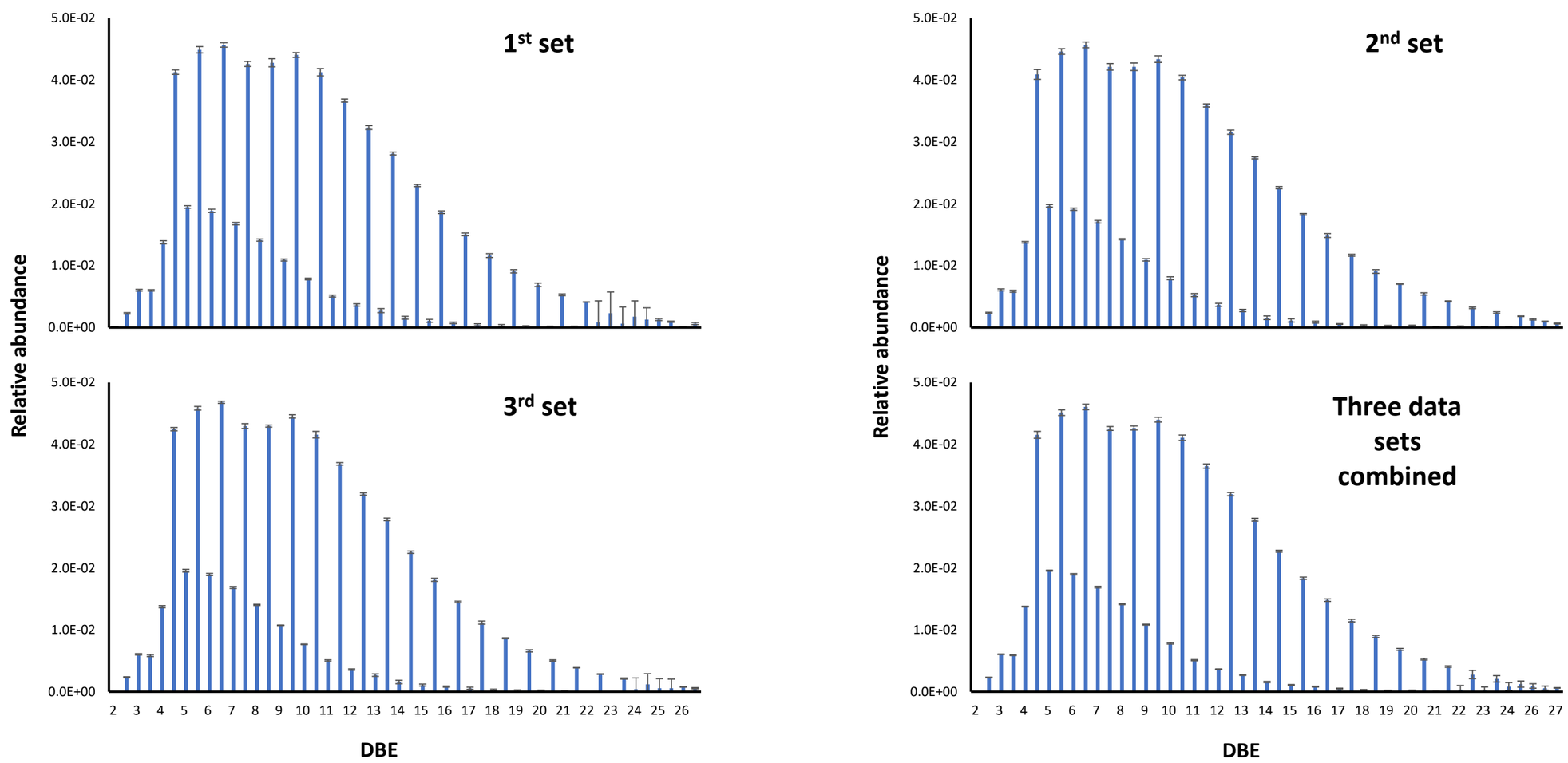

Absolute abundance
Relative abundance
Chemical class
HC
N_1
O_1
N_1O_1
N_1S_1
O_2
S_1
N_2O_2
N_1O_2
S_1O_1
1st set
2nd set
3rd set
Three data sets combined

Figure S2. DBE distributions of HC class in (a) Zakum, (b) Bukha, and (c) Pyrenees oils observed with (+)APPI FT-ICR-MS presented as summed relative abundances for the 1st , 2nd, 3rd, and combined datasets.

(a) Zakum_HC



(b) Bukha_HC



(c) Pyrenees_HC

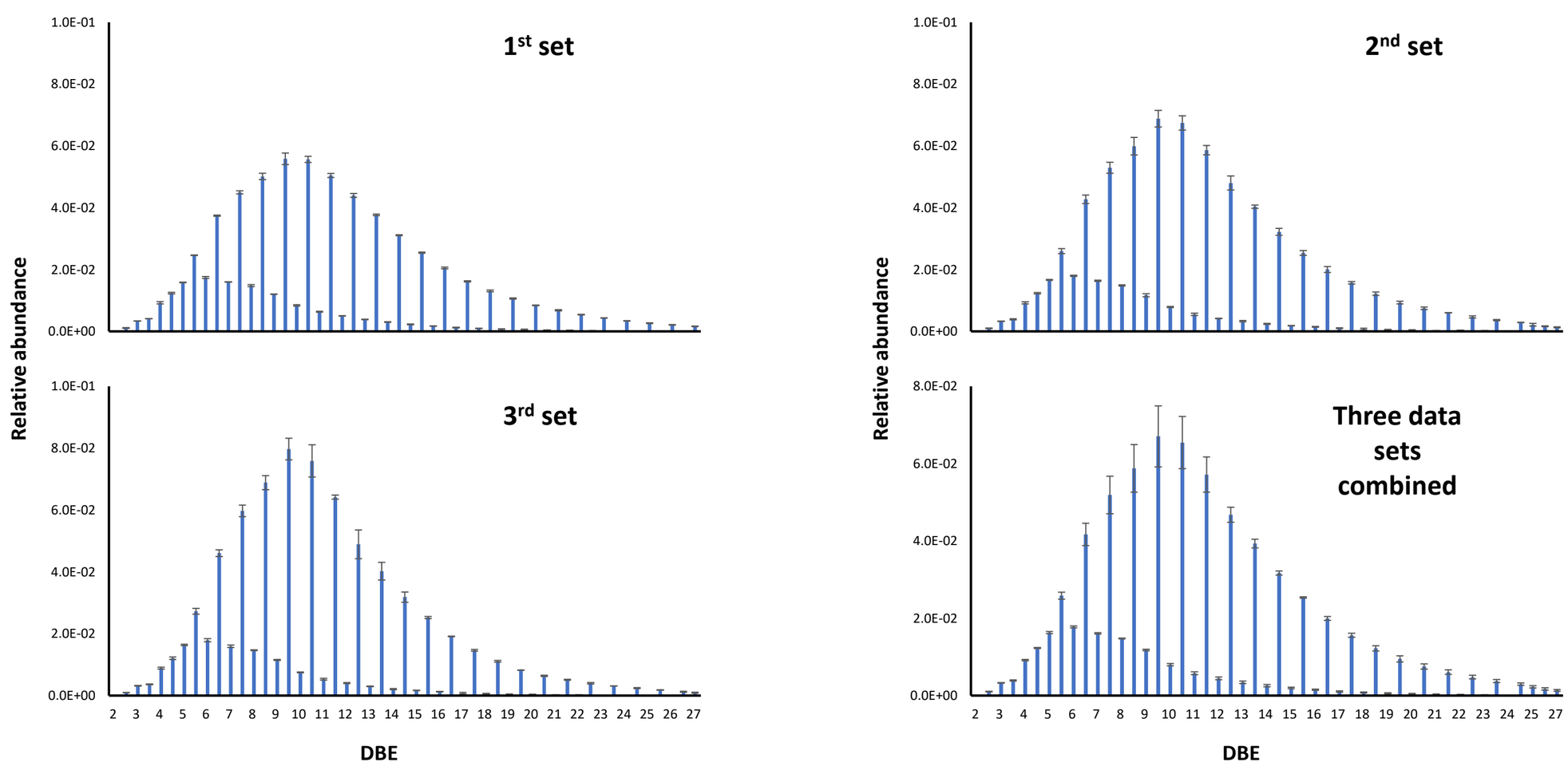
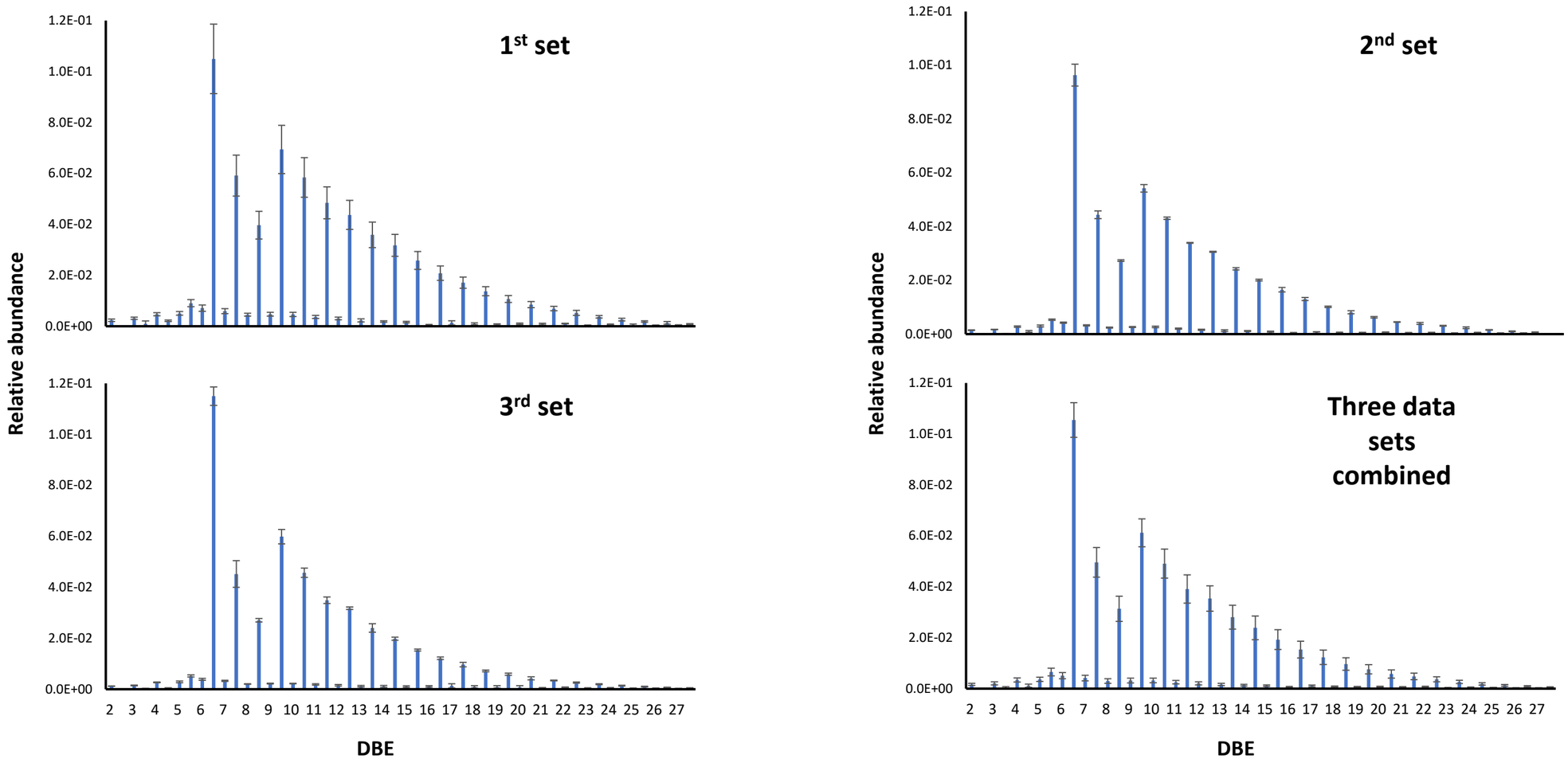
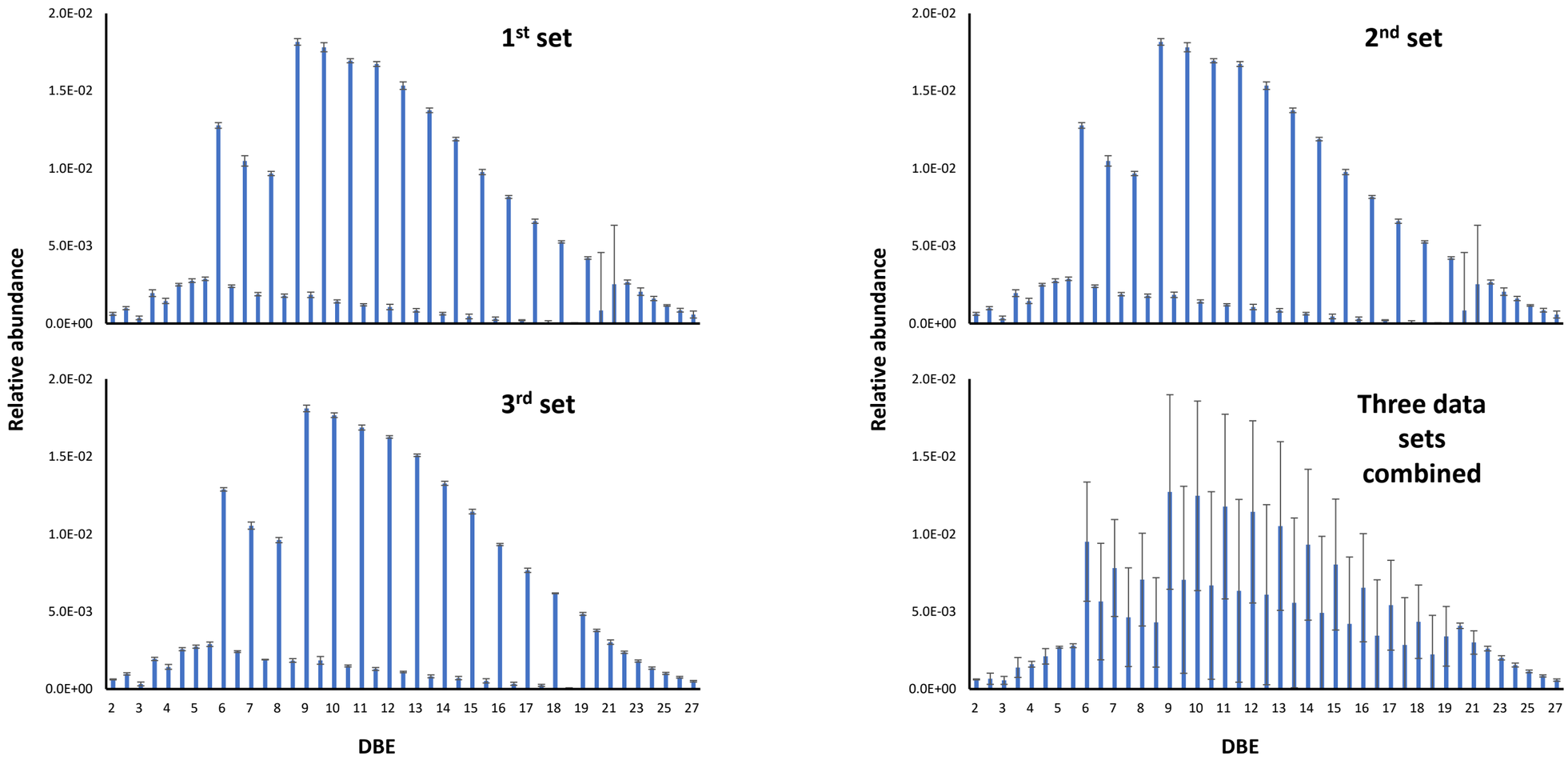


Figure S3. DBE distributions of S1 class in (a) Zakum, (b) Bukha, and (c) Pyrenees oils observed with (+)APPI FT-ICR-MS present-ed as summed relative abundances for the 1st , 2nd, 3rd, and com-bined datasets.

(a) Zakum_S_1



(b) Bukha_S_1



(c) Pyrenees_S_1