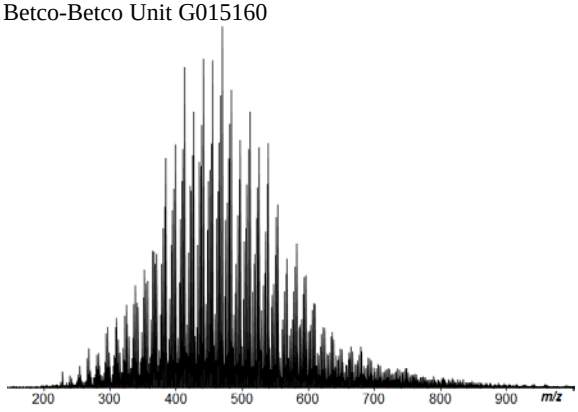
Supplementary data

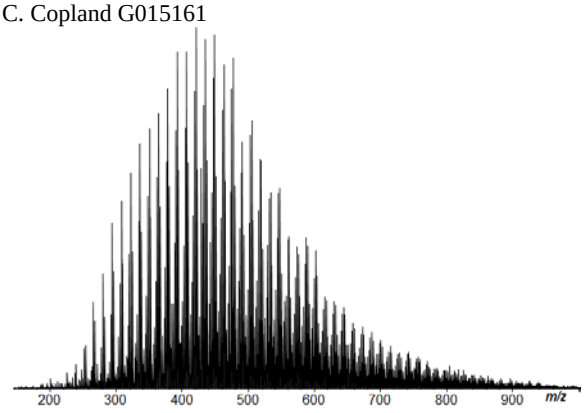
(1) (+)-ESI-FT-ICR-MS data

(a) (+)-ESI Broad band mass spectra

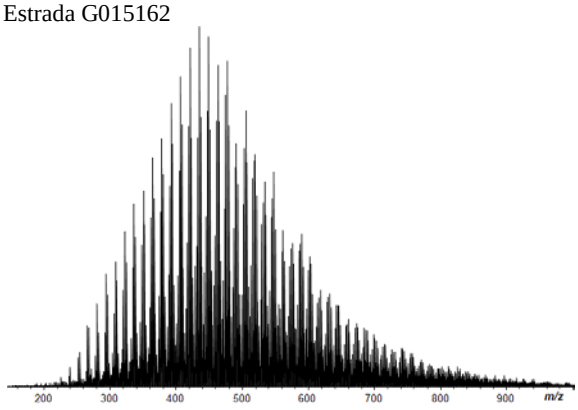
Betco-Betco Unit G015160



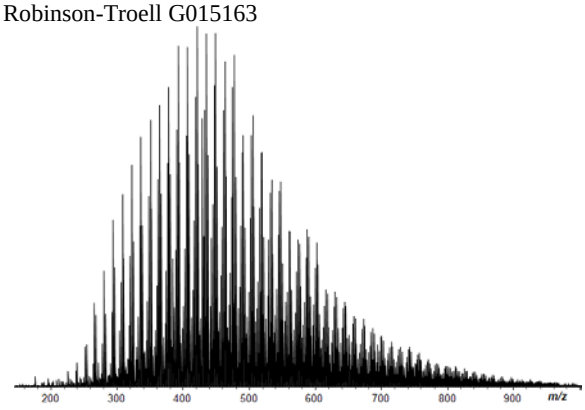
C. Copland G015161



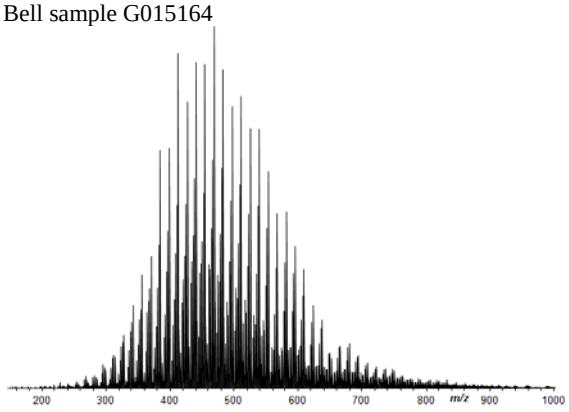
Estrada G015162



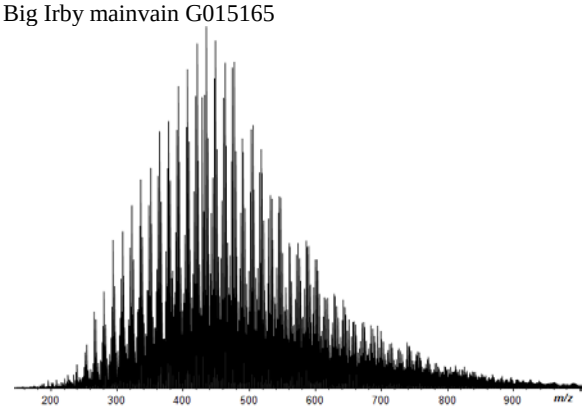
Robinson-Troell G015163



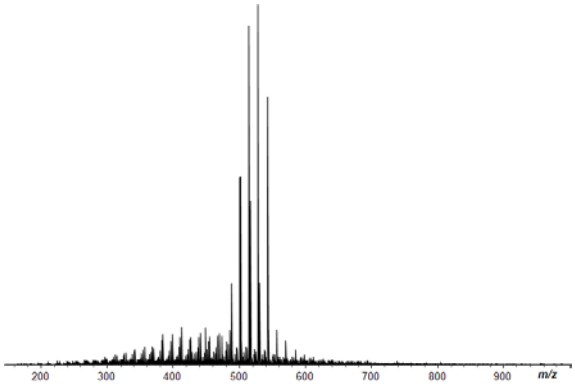
Bell sample G015164



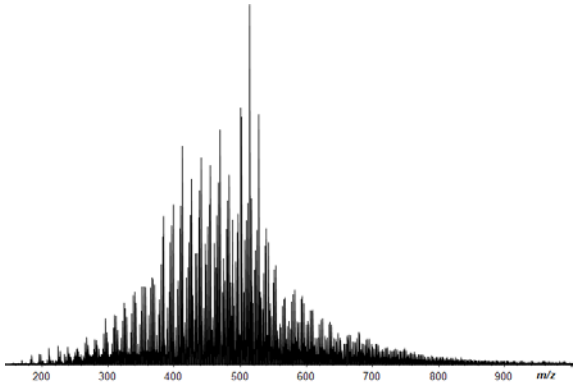
Big Irby mainvain G015165



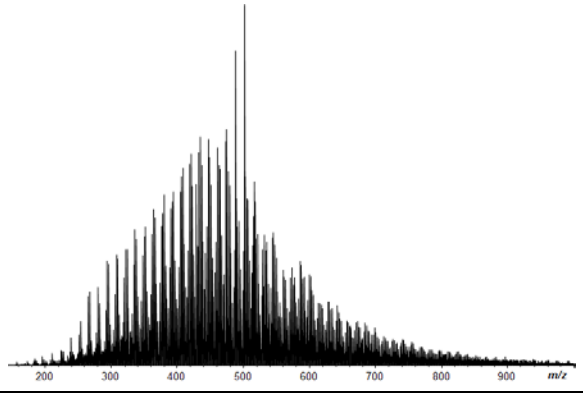
Well A G015548



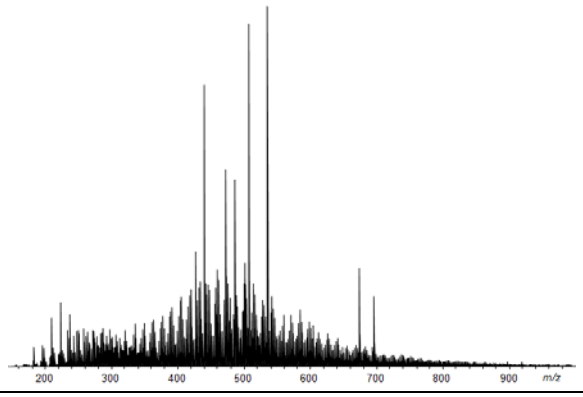
Well B G015550



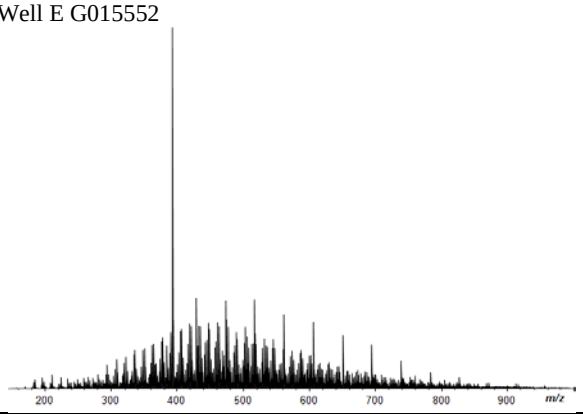
Well C G015151



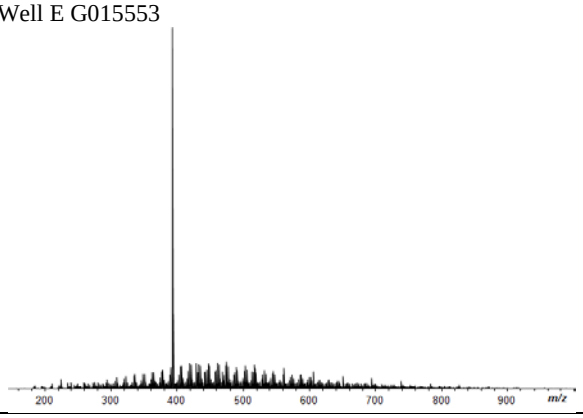
Well D G015394



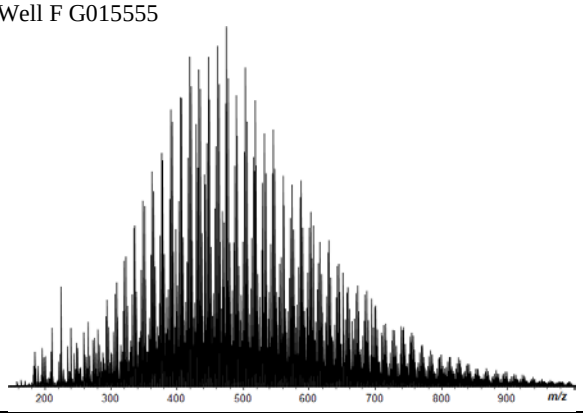
Well E G015552



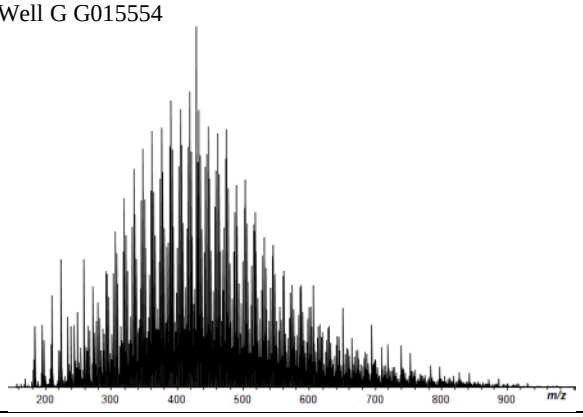
Well E G015553



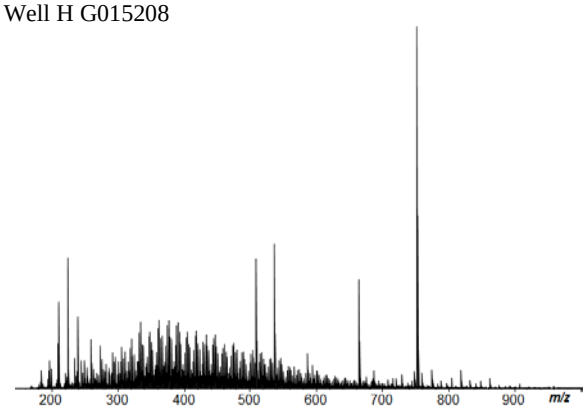
Well F G015555



Well G G015554



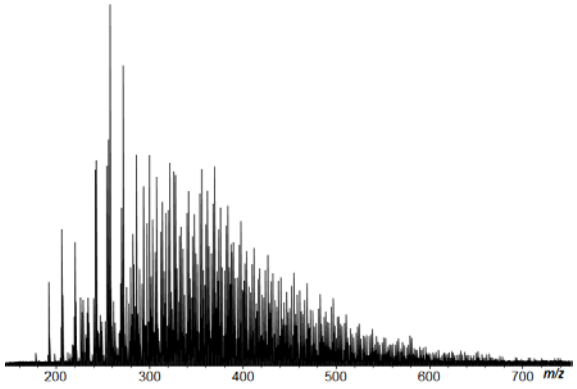
Well H G015208



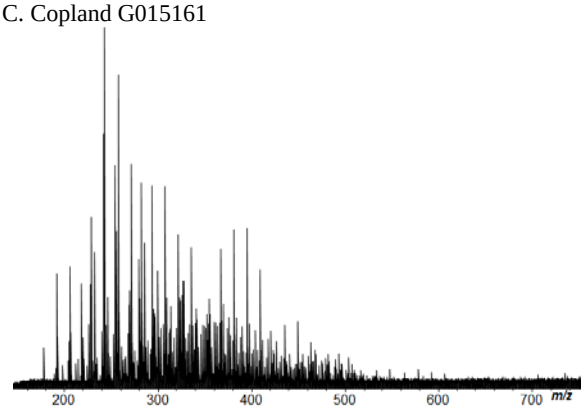
(2) (-)-ESI-FT-ICR-MS data

(a) (-)-ESI-Broad band mass spectra

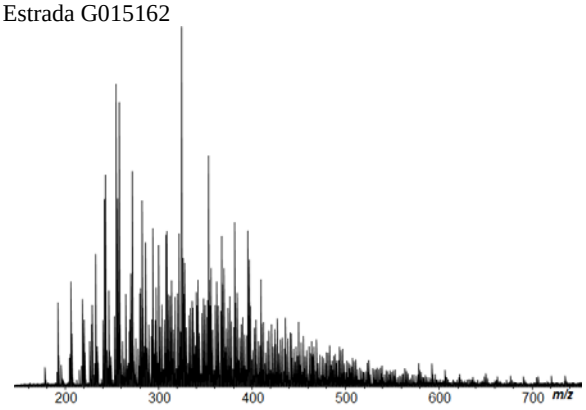
Betco-Betco Unit G015160



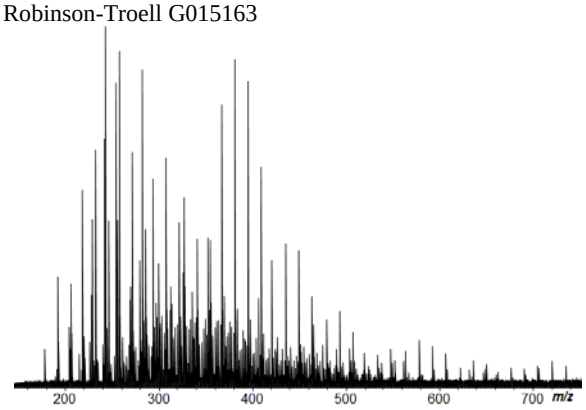
C. Copland G015161



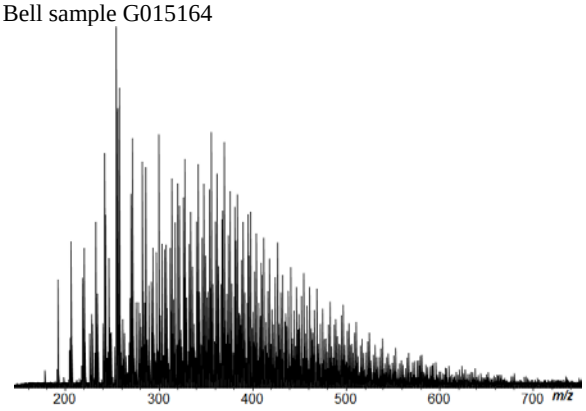
Estrada G015162



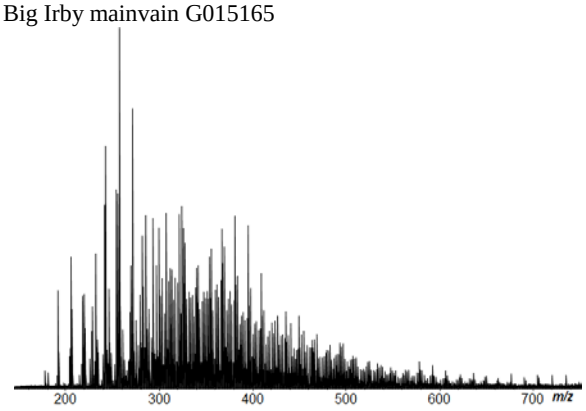
Robinson-Troell G015163



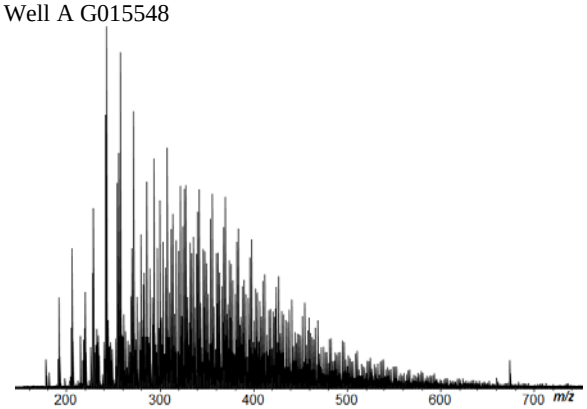
Bell sample G015164



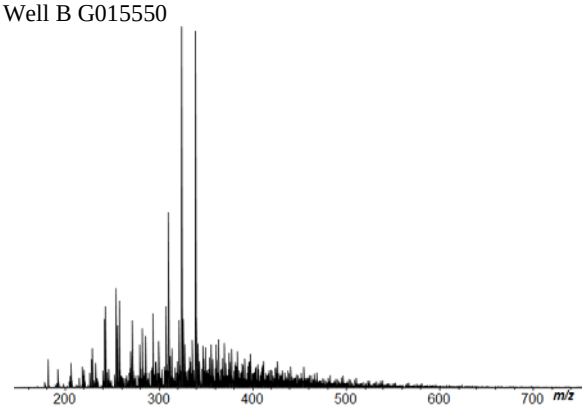
Big Irby mainvain G015165



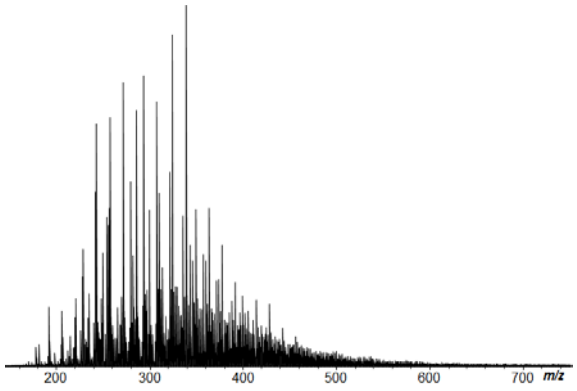
Well A G015548



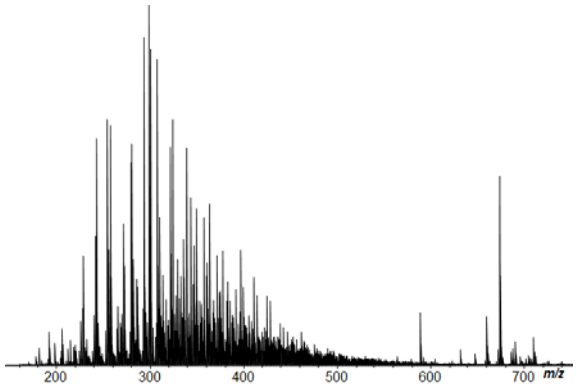
Well B G015550



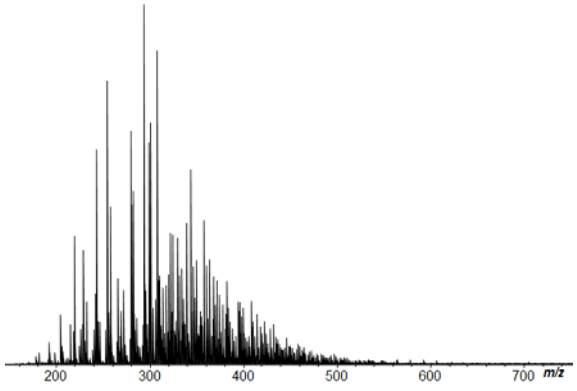
Well C G015151



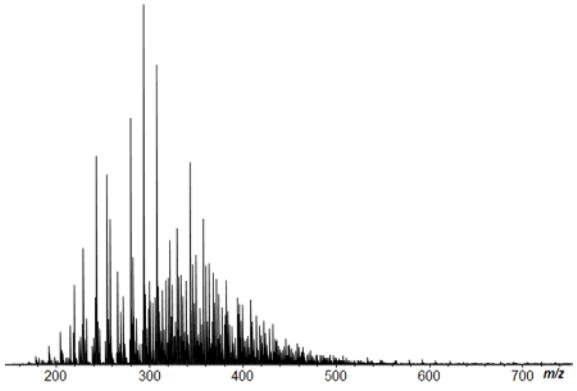
Well D G015394



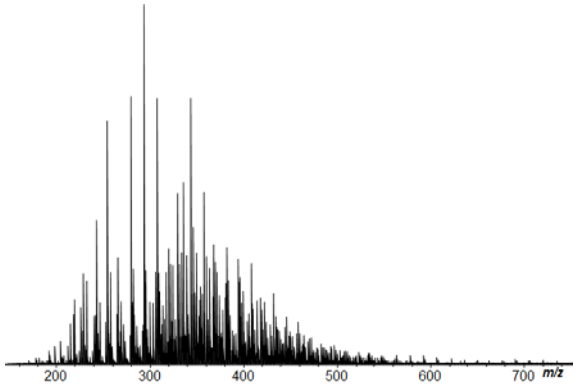
Well E G015552



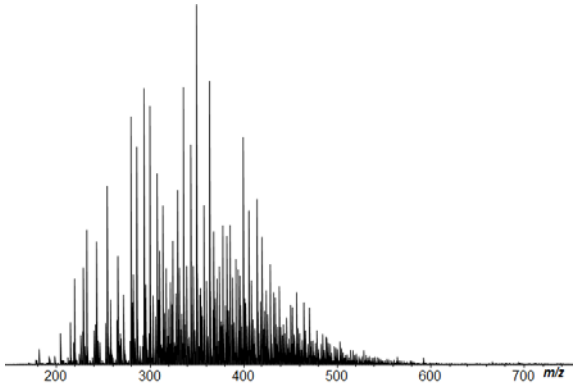
Well E G015553



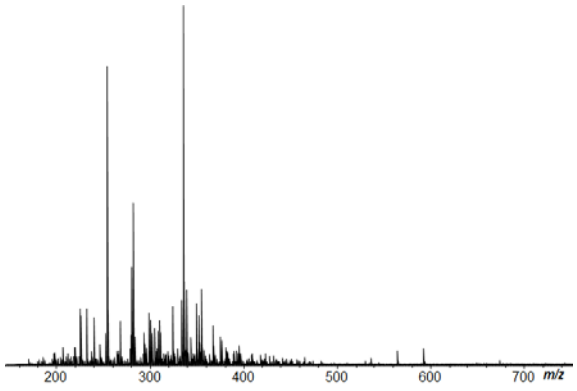
Well F G015555



Well G G015554



Well H G015208



(b) DBE distribution of N_2 compound classes

Sample name	ID G0-	DBE = 0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Betco-Betco Unit #1	15160	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00
C.Copland 1	15161	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Estrada et al 1	15162	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Robison-Troell 1	15163	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bell Sample 1	15164	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Big Irby Mainvein #1	15165	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well A	15548	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.44	0.34	1.25	1.04	0.95	1.10	0.67	1.73	0.99	0.40	0.75
Well B	15550	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.32	0.24	1.41	0.96	0.81	1.33	0.71	2.45	1.14	0.44	1.41
Well C	15551	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.29	0.97	0.54	4.58	1.86	0.93	4.61	1.38	1.32	2.03	0.65	0.90
Well D	15394	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.17	0.09	2.06	1.06	0.80	2.05	0.95	2.22	1.19	0.56	1.95
Well E	15552	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.39	0.19	0.04	0.73	0.34	0.61	0.50	0.21	0.68
Well E	15553	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.11	0.14	0.66	0.28	0.75	0.51	0.23	0.85
Well F	15555	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.21	0.06	0.00	0.49	0.21	0.57	0.39	0.23	0.90
Well G	15554	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.30	0.10	0.07	0.54	0.22	0.67	0.37	0.22	1.09
Well H	15208	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	ID G0-	DBE = 21	22	23	24	25	26	27	28	29	30
Betco-Betco Unit #1	15160	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C.Copland 1	15161	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Estrada et al 1	15162	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Robison-Troell 1	15163	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bell Sample 1	15164	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Big Irby Mainvein #1	15165	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well A	15548	0.37	0.13	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well B	15550	0.56	0.28	0.28	0.07	0.00	0.00	0.00	0.00	0.00	0.00
Well C	15551	0.39	0.15	0.23	0.09	0.00	0.00	0.00	0.00	0.00	0.00
Well D	15394	0.72	0.47	0.67	0.30	0.19	0.10	0.04	0.00	0.00	0.00
Well E	15552	0.37	0.18	0.28	0.14	0.10	0.03	0.00	0.00	0.00	0.00
Well E	15553	0.43	0.27	0.34	0.21	0.12	0.00	0.00	0.00	0.00	0.00
Well F	15555	0.39	0.31	0.50	0.20	0.21	0.11	0.06	0.00	0.00	0.00
Well G	15554	0.36	0.37	0.54	0.21	0.23	0.14	0.07	0.03	0.00	0.00
Well H	15208	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

All abundances in [%TMIA]

(c) DBE distribution of N_1O_1 compound classes

Sample name	ID G0-	DBE = 0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Betco-Betco Unit #1	15160	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.75	1.18	0.58	0.54	1.00	0.27	0.04
C.Copland 1	15161	0.00	0.00	1.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.44	3.28	2.53	5.10	2.61	1.71	2.59	0.47	0.00
Estrada et al 1	15162	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	1.02	1.81	0.83	0.71	1.35	0.40	0.09
Robison-Troell 1	15163	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.56	1.53	3.48	0.92	0.56	2.00	0.13	0.00
Bell Sample 1	15164	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.98	1.77	0.62	0.64	1.10	0.20	0.00
Big Irby Mainvein #1	15165	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.79	1.75	0.84	0.75	1.39	0.43	0.00
Well A	15548	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.04	0.15	0.44	0.42	0.45	0.63	1.01	0.98	0.56	0.74	0.66	0.19	0.17
Well B	15550	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.61	0.69	0.77	1.16	1.65	1.77	1.04	1.13	1.22	0.52	0.39
Well C	15551	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.13	1.65	1.14	1.27	4.15	2.21	2.32	2.83	1.59	2.13	0.99	0.66
Well D	15394	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.31	0.56	1.02	1.14	1.65	1.16	1.11	1.78	0.69	0.66
Well E	15552	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.28	0.63	0.82	0.82	2.43	1.28	1.07	2.75	0.93	0.71
Well E	15553	0.00	0.00	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.10	0.24	0.64	0.87	0.88	2.60	1.42	1.21	3.20	1.12	0.90
Well F	15555	0.00	0.03	1.12	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.07	0.47	0.61	0.67	2.39	1.16	0.95	3.10	1.18	0.80
Well G	15554	0.00	0.00	0.34	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.03	0.17	0.22	0.28	1.60	0.55	0.53	1.99	0.54	0.54
Well H	15208	0.00	0.47	8.57	2.14	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.56	0.00	0.00

	ID G0-	DBE = 21	22	23	24	25	26	27	28	29	30
Betco-Betco Unit #1	15160	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C.Copland 1	15161	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Estrada et al 1	15162	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Robison-Troell 1	15163	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bell Sample 1	15164	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Big Irby Mainvein #1	15165	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well A	15548	0.15	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well B	15550	0.29	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well C	15551	0.71	0.29	0.21	0.10	0.00	0.00	0.00	0.00	0.00	0.00
Well D	15394	079	0.34	0.24	0.19	0.07	0.05	0.00	0.00	0.00	0.00
Well E	15552	1.18	0.50	0.38	0.26	0.13	0.05	0.00	0.00	0.00	0.00
Well E	15553	1.37	0.63	0.43	0.33	0.18	0.07	0.00	0.00	0.00	0.00
Well F	15555	1.51	0.68	0.46	0.36	0.21	0.18	0.05	0.00	0.00	0.00
Well G	15554	0.85	0.33	0.28	0.17	0.08	0.03	0.00	0.00	0.00	0.00
Well H	15208	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

All abundances in [%TMIA]

(d) DBE distribution of N_1S_1 compound classes

Sample name	ID G0-	DBE = 0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Betco-Betco Unit #1	15160	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.99	0.41	0.08	0.58	0.08	0.00	0.00
C.Copland 1	15161	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.47	0.00	0.00	1.21	0.00	0.00	0.00
Estrada et al 1	15162	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.46	0.49	0.00	0.90	0.25	0.00	0.05
Robison-Troell 1	15163	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.67	0.24	0.00	1.73	0.26	0.00	0.00
Bell Sample 1	15164	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.24	1.12	0.26	1.13	0.56	0.00	0.00
Big Irby Mainvein #1	15165	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.79	0.14	0.00	0.37	0.00	0.00	0.00
Well A	15548	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.63	0.76	0.53	2.34	1.57	1.04	1.78	0.95	0.75	0.54
Well B	15550	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.16	0.21	0.09	2.62	1.30	0.87	2.61	1.14	0.79	0.90
Well C	15551	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.96	0.54	0.64	2.61	0.70	0.77	1.22
Well D	15394	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.02	0.00	0.00	0.00	0.04	1.78	0.46	0.56	2.66	0.66	0.73	1.32
Well E	15552	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.86	0.20	0.37	2.46	0.73	0.59	1.28
Well E	15553	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	2.09	0.23	0.41	2.88	0.81	0.66	1.52
Well F	15555	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.04	1.29	0.03	0.19	2.40	0.80	0.64	1.54
Well G	15554	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.02	4.36	0.35	1.16	6.56	1.11	2.33	3.98
Well H	15208	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.21	0.00	0.00	0.46	0.11	0.00	0.25

	ID G0-	DBE = 21	22	23	24	25	26	27	28	29	30
Betco-Betco Unit #1	15160	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C.Copland 1	15161	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Estrada et al 1	15162	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Robison-Troell 1	15163	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bell Sample 1	15164	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Big Irby Mainvein #1	15165	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well A	15548	0.31	0.18	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Well B	15550	0.49	0.34	0.16	0.04	0.00	0.00	0.00	0.00	0.00	0.00
Well C	15551	0.52	0.44	0.30	0.14	0.10	0.01	0.00	0.00	0.00	0.00
Well D	15394	0.55	0.52	0.41	0.24	0.18	0.09	0.01	0.00	0.00	0.00
Well E	15552	0.52	0.52	0.42	0.20	0.20	0.08	0.02	0.00	0.00	0.00
Well E	15553	0.55	0.57	0.48	0.22	0.19	0.08	0.00	0.00	0.00	0.00
Well F	15555	0.70	0.83	0.68	0.35	0.40	0.24	0.11	0.12	0.00	0.00
Well G	15554	1.27	1.85	1.33	0.69	0.69	0.39	0.23	0.16	0.06	0.00
Well H	15208	0.00	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

All abundances in [%TMIA]