Supplementary Information

Integrative Approach Based on Simplex-Centroid Design, ESI-MS and Chemometric Analysis for Comprehensive Characterization of Phenolic Compounds from *Endopleura uchi* Bark

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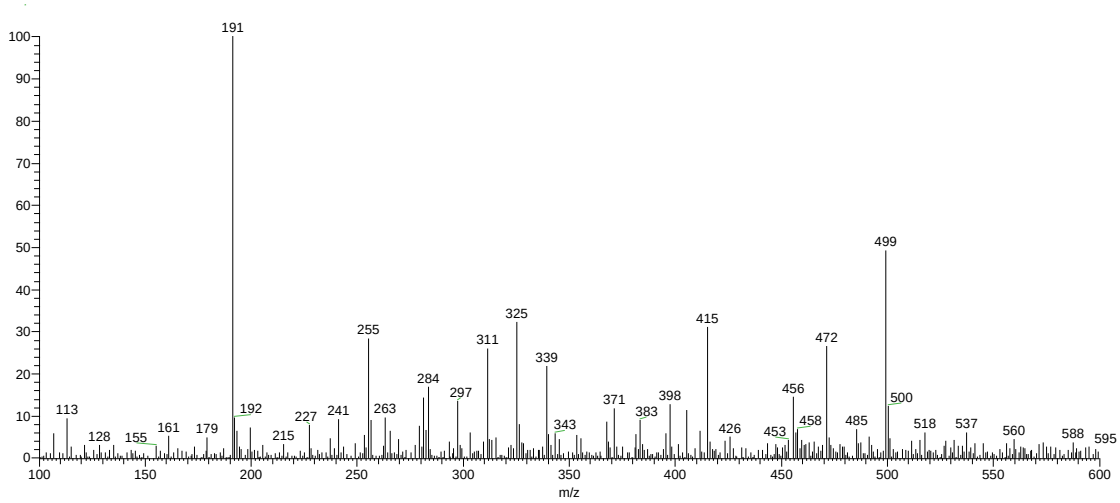

Figure S1. ESI-MS spectrum (negative mode) of the dc extract of *E. uchi* bark.

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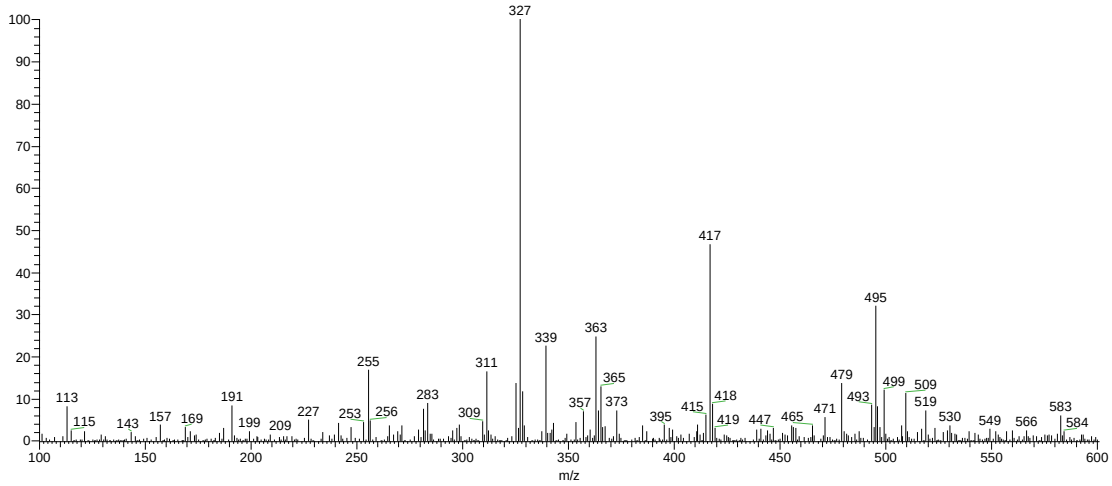

Figure S2. ESI-MS spectrum (negative mode) of the ea extract of *E. uchi* bark.

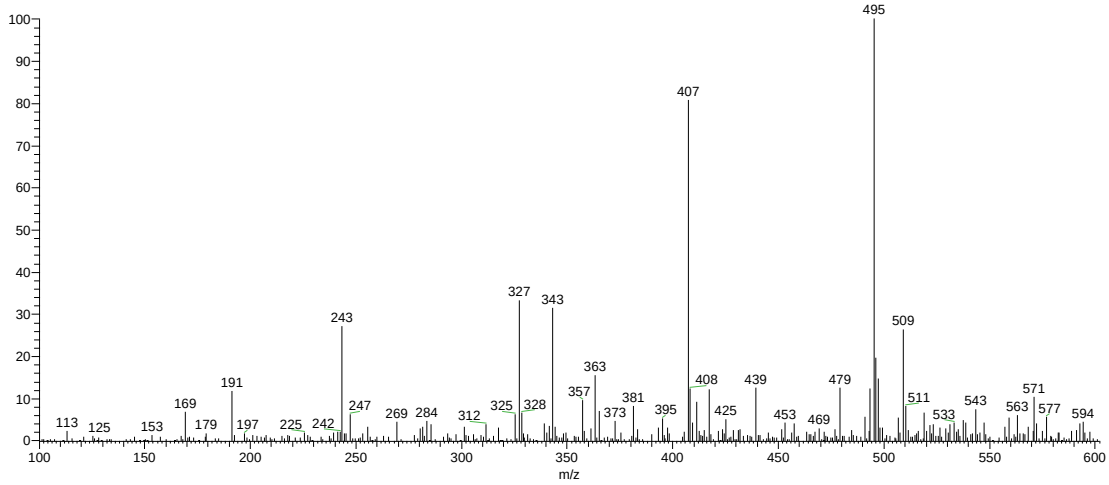

Figure S3. ESI-MS spectrum (negative mode) of the et extract of *E. uchi* bark.

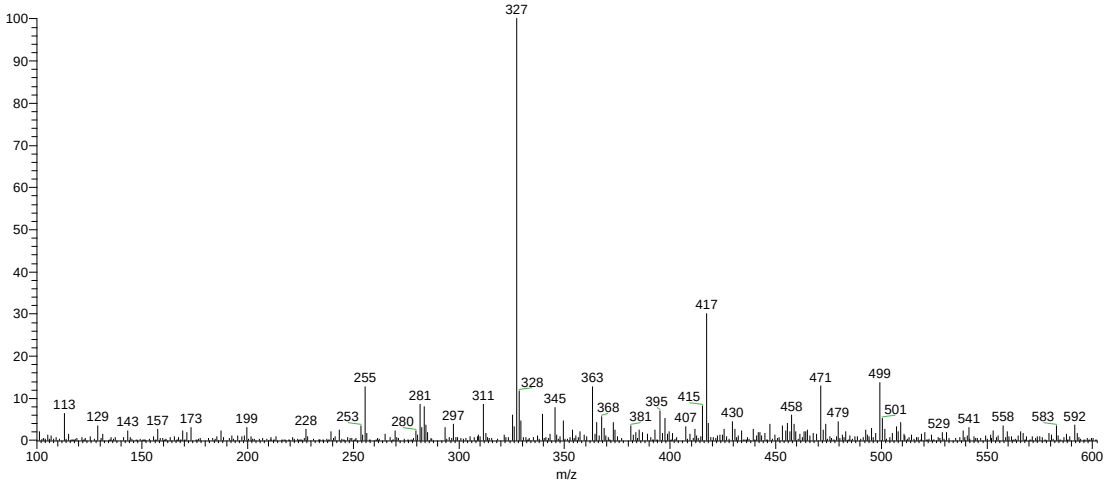

Figure S4. ESI-MS spectrum (negative mode) of the ea + dc extract of *E. uchi* bark.

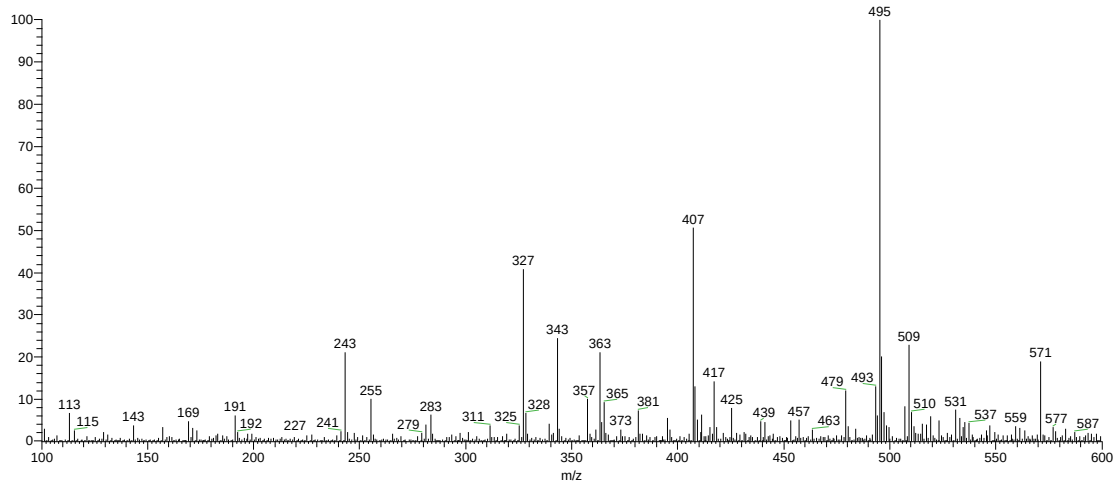

Figure S5. ESI-MS spectrum (negative mode) of the et + dc extract of *E. uchi* bark.

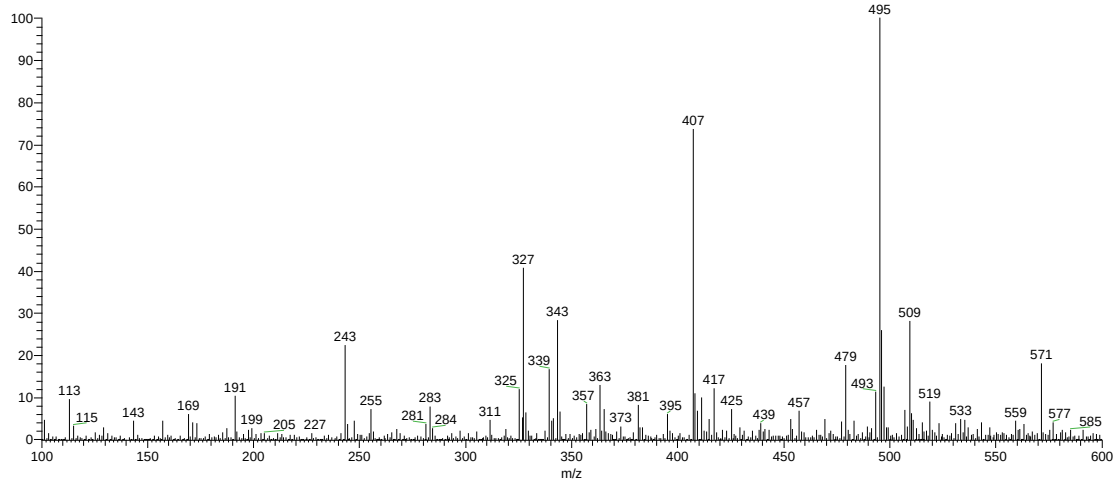

Figure S6. ESI-MS spectrum (negative mode) of the et + ea extract of *E. uchi* bark.

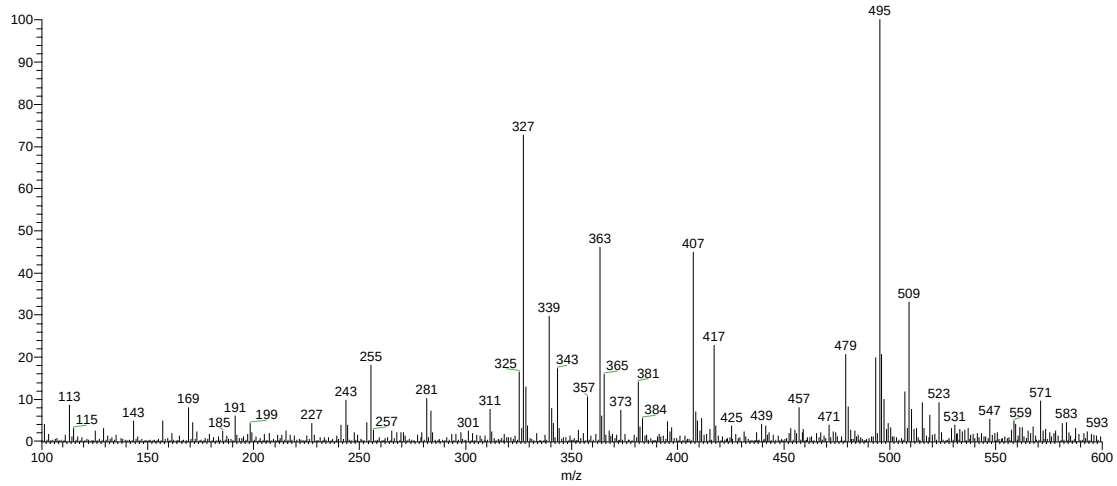

Figure S7. ESI-MS spectrum (negative mode) of the et + ea + dc extract of *E. uchi* bark.

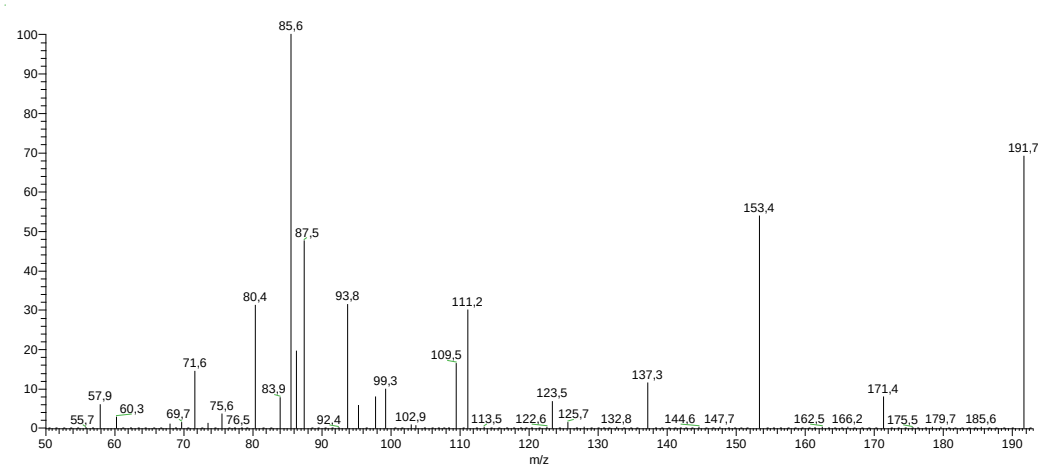

Figure S8. ESI-MS/MS spectra (negative mode) at 35 eV collision energy of the ion at *m/z* 191 present in the *E. uchi* bark.

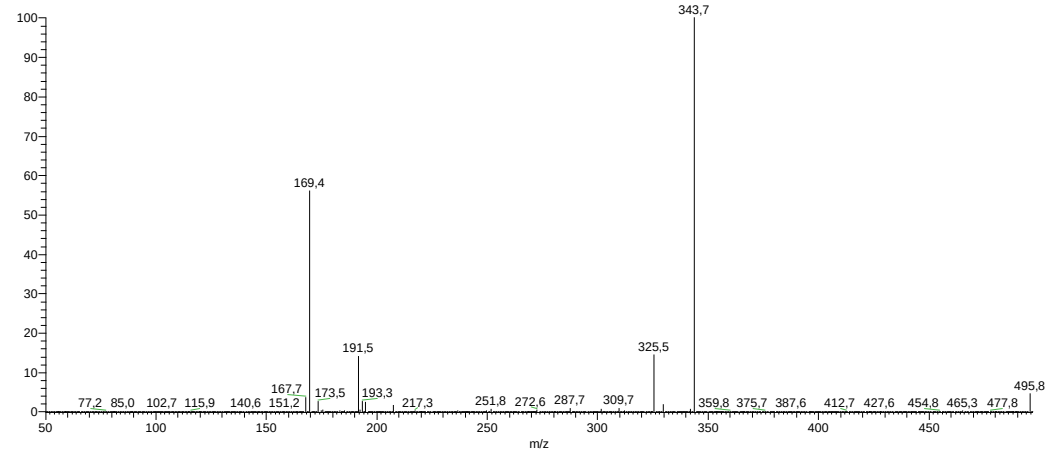

Figure S9. ESI-MS/MS spectra (negative mode) at 30 eV collision energy of the ion at *m/z* 495 present in the *E. uchi* bark.

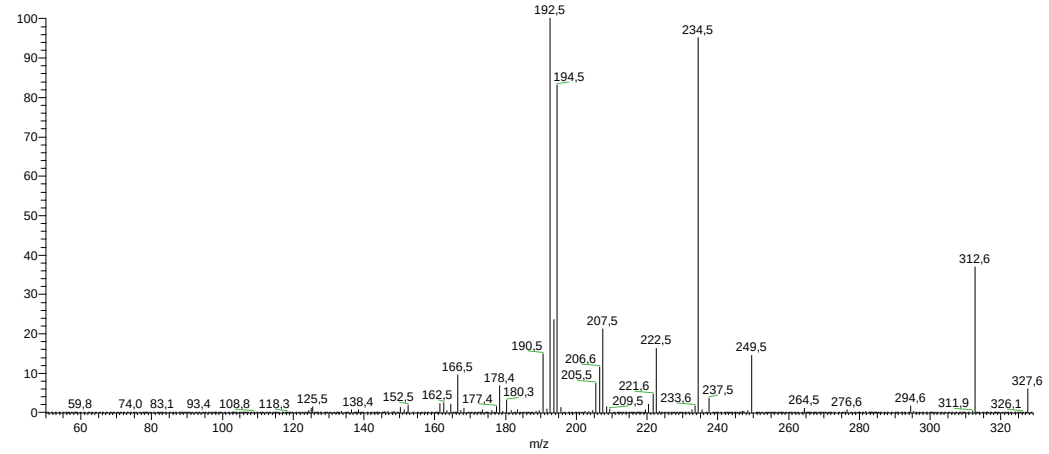

Figure S10. ESI-MS/MS spectra (negative mode) at 30 eV collision energy of the ion at *m/z* 327 present in the *E. uchi* bark.

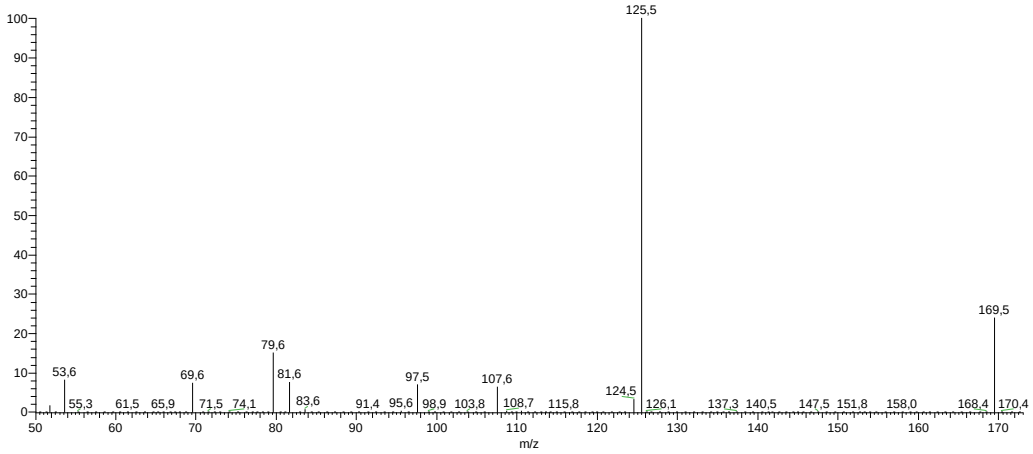

Figure S11. ESI-MS/MS spectra (negative mode) at 35 eV collision energy of the ion at *m/z* 169 present in the *E. uchi* bark.

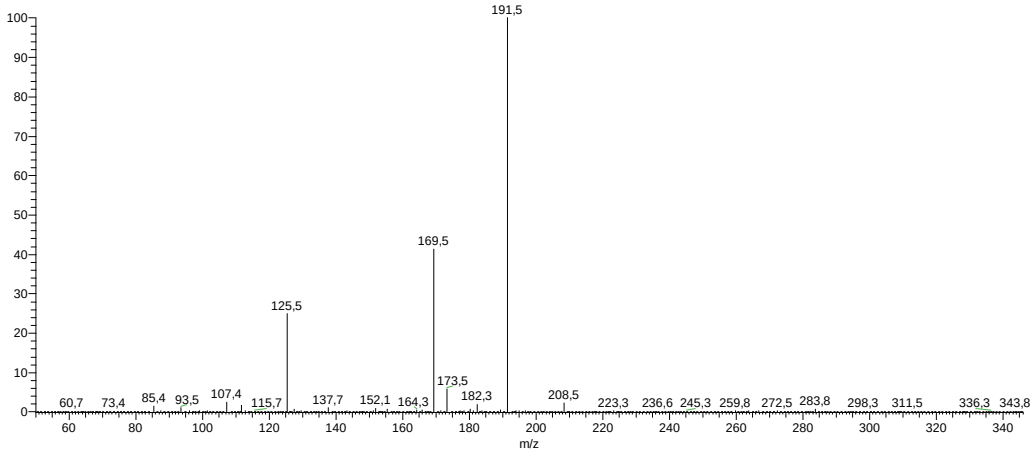

Figure S12. ESI-MS/MS spectra (negative mode) at 30 eV collision energy of the ion at *m/z* 343 present in the *E. uchi* bark.

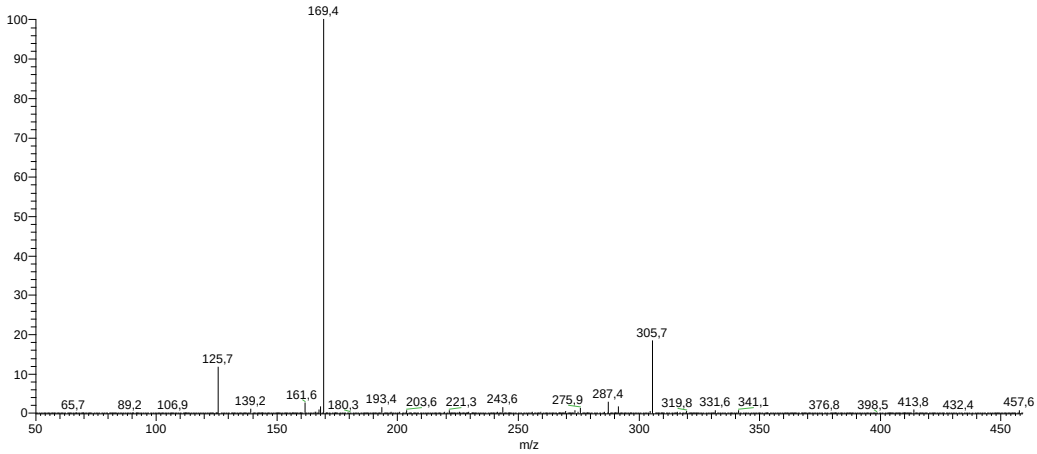

Figure S13. ESI-MS/MS spectra (negative mode) at 30 eV collision energy of the ion at *m/z* 457 present in the *E. uchi* bark.

Table S1. Data used in the PCA analysis based in the peak intensities obtained between 100 to 600 *m/z*, after elimination of those signals which had intensities below to 5% than the intensity of the base peak

	dc	ea	et	ea+dc	et+dc	et+ea	et+ea+dc
107	5.75	0	0	0	0	0	0
113	9.32	8.22	0	6.36	6.59	9.63	8.5
161	5.24	0	0	0	0	0	0
169	0	0	6.72	0	0	6.08	7.99
191	100	8.33	11.67	0	5.93	10.43	5.99
192	9.65	0	0	0	0	0	0
193	6.47	0	0	0	0	0	0
199	7.14	0	0	0	0	0	0
227	7.75	0	0	0	0	0	0
241	9.19	0	0	0	0	0	0
243	0	0	27.18	0	21.08	22.43	9.67
247	0	0	6.17	0	0	0	0
253	5.52	0	0	0	0	0	0
255	28.31	16.78	0	12.7	9.96	7.22	18.12
256	9.03	0	0	0	0	0	0
263	9.55	0	0	0	0	0	0
265	6.41	0	0	0	0	0	0
279	7.63	0	0	0	0	0	0
281	14.25	0	0	8.62	0	0	10.2
282	0	7.6	0	0	0	0	0
283	6.61	8.91	0	0	6.22	7.77	0
284	16.78	0	0	8	0	0	7.28
297	13.52	0	0	0	0	0	0
303	6.02	0	0	0	0	0	0
311	25.98	16.47	0	8.53	0	0	7.68
325	32.16	13.72	6.28	5.92	0	11.86	16.47
326	7.94	0	0	0	0	0	0
327	0	100	33.26	100	40.77	40.76	72.68
328	0	11.67	6.61	11.77	6.63	6.37	12.94
339	21.82	22.62	0	6.31	0	16.61	29.63
340	5.59	0	0	0	0	0	7.77
343	5.73	0	31.51	0	24.4	28.34	17.25
344	0	0	0	0	0	6.55	0
345	0	0	0	7.74	0	0	0
353	5.46	0	0	0	0	0	0
357	0	6.91	9.56	0	9.94	8.35	10.5
363	0	24.8	15.49	12.63	20.95	12.93	45.99
364	0	7.11	0	0	0	0	5.97
365	0	12.92	7.07	0	9.21	7.15	15.8
368	8.59	0	0	5.53	0	0	0
371	11.8	0	0	0	0	0	0
373	0	7.18	0	0	0	0	7.3
381	5.58	0	8.25	0	7.16	8.09	14.08
383	9.04	0	0	0	0	0	0
384	0	0	0	0	0	0	5.33
395	0	0	5.31	6.95	5.34	5.93	0
396	5.77	0	0	0	0	0	0
398	12.78	0	0	5.28	0	0	0
405	11.42	0	0	0	0	0	0
407	0	0	80.82	0	50.61	73.7	44.87
408	0	0	12.39	0	12.89	10.96	6.96
409	0	0	0	0	5.01	6.83	0
411	0	0	9.14	0	6.19	9.98	5.45
412	6.42	0	0	0	0	0	0
415	31.03	6.25	0	8.22	0	0	0
417	0	46.74	12.17	30.13	14.11	12.17	22.72
418	0	8.74	0	0	0	0	0
425	0	0	0	0	7.82	7.18	0
426	5.02	0	0	0	0	0	0
439	0	0	12.54	0	0	0	0
456	14.41	0	0	0	0	0	0
457	6.02	0	0	0	5.04	6.85	8.04
458	6.8	0	0	5.92	0	0	0
471	0	5.56	0	13	0	0	0
472	26.54	0	0	0	0	0	0
479	0	13.7	12.57	0	11.93	17.6	20.66
480	0	0	0	0	0	0	8.2
485	6.9	0	0	0	0	0	0
491	5.08	0	5.64	0	0	0	0
493	0	8.57	12.31	0	13.01	11.34	19.87
494	0	0	0	0	5.97	0	0
495	0	32.08	100	0	100	100	100
496	0	8.23	19.69	0	19.98	25.88	20.53
497	0	0	14.6	0	6.83	12.48	10.06
499	49.2	12.05	0	13.65	0	0	0
500	12.39	0	0	0	0	0	0
501	0	0	0	5.17	0	0	0
507	0	0	5.34	0	8.25	6.95	11.69
508	0	0	0	0	0	0	0
509	0	11.32	26.24	0	22.76	28.12	33.07
510	0	0	0	0	6.85	6.28	7.68
511	0	0	8.1	0	0	0	0
515	0	0	0	0	0	0	9.1
518	5.93	0	0	0	0	0	0
519	0	7.26	6.64	0	5.87	8.99	6.3
523	0	0	0	0	0	0	9.23
531	0	0	0	0	7.45	0	0
533	0	0	0	0	5.49	0	0
537	6.08	0	0	0	0	0	0
543	0	0	7.46	0	0	0	0
547	0	0	0	0	0	0	5.28
559	0	0	5.43	0	0	0	0
563	0	0	6.01	0	0	0	0
571	0	0	10.36	0	18.77	18.09	9.5
577	0	0	5.52	0	0	0	0
583	0	5.93	0	0	0	0	0

dc: dichloromethane; ea: ethyl acetate; et: ethanol.