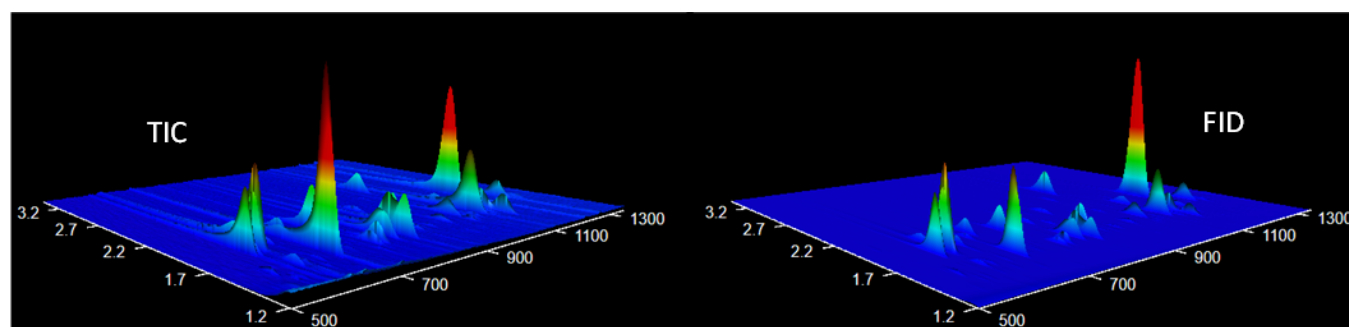


Instrument: Pegasus® BT 4D with Paradigm Shift

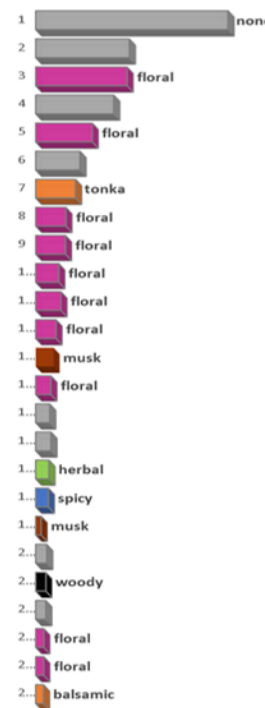
Reformulation of Perfume Sample with GCxGC-TOFMS/FID

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Key Words: Perfume, Reformulation, GCxGC, TOFMS, FID, Dual detection, RFF modulator



Name	R.T. (s)	Similarity	Retention Ind	Lib. RI	Area % S1
Diethyl Phthalate	1200, 2.050	886	1591.7	1594 ± 8(35)	15.45563
ex DPG	625, 1.850	888	1040.4	1042 ± 0(1)	7.51986
Linalool	697.5, 1.620	830	1102.2	1099 ± 2(966)	7.34045
ex DPG	600, 1.820	850	1019.1	1038 ± 0(1)	6.26595
α Isomethyl ionone	1100, 1.690	782	1482.1	1480 ± 5(17)	4.53998
ex DPG	620, 1.840	845	1036.2	1046 ± 0(1)	3.55505
Coumarin	1070, 2.460	879	1451.3	1440 ± 11(25)	3.19821
Citronellol	837.5, 1.630	849	1226.2	1228 ± 3(190)	2.42379
Benzyl acetate	770, 1.940	836	1165.2	1164 ± 2(65)	2.38983
Geraniol	865, 1.690	711	1252.4	1255 ± 3(343)	2.04998
Kharismal	1255, 1.820	832	1654.3	1656 ± 2(12)	2.01709
Hydroxy citronellal	905, 1.760	828	1290.5	1295 ± 7(16)	1.62833
Galaxolide	422.5, 1.810	799	1859.0	1851 ± 0(1)	1.43594
Phenylethyl Alcohol	715, 2.010	882	1117.4	1116 ± 5(269)	1.21486
Unknown	137.5, 1.700		1522.2		1.12173
ex DPG	657.5, 1.890	817	1068.1	1068 ± 0(1)	1.09226
Linalyl acetate	862.5, 1.580	819	1250.0	1257 ± 4(156)	1.06472
Methylisoeugenol	112.5, 1.960	836	1494.9	1492 ± 9(16)	1.01413
Ethylene brassylate	552.5, 1.940	848	2033.6		0.89351
Citronellal diethyl acetal	1140, 1.560	720	1525.0		0.88162
Acetylcedrene	1365, 1.770	801	1784.8	1764 ± 0(1)	0.81260
Unknown	1050, 1.740		1430.8		0.80796
Benzyl alcohol	620, 2.020	766	1036.2	1036 ± 4(186)	0.64401
Ethyl linalool	805, 1.610	802	1195.7		0.64164
Benzyl Benzoate	362.5, 2.120	800	1781.8	1763 ± 5(125)	0.62274



TIC and FID GCxGC chromatograms, that were detected simultaneously from one injection, are shown for a perfume sample. The table shows the major analyte components that were tentatively identified from MS and relatively quantified with Area% from FID.

A perfume sample was analyzed with GCxGC-TOFMS/FID to simultaneously identify and quantify the major components within the sample. GCxGC was crucial for handling the sample complexity, and dual detection allowed for analyte identifications with MS and quantitation based on FID Area % from a single injection. A GCxGC flow modulator allowing full transfer of analytes from the first dimension to the second dimension and a splitter capable of maintaining a constant split ratio between the MS and FID during the entire length of the run were critical for this work.