

Oxidation of hydroxymethylpyrazines and hydroxylated phenyl compounds in a gas chromatography inlet

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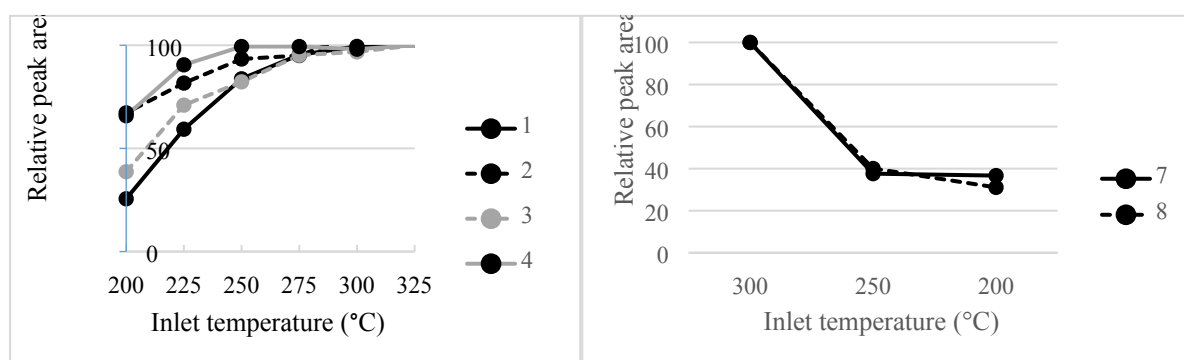
Supplementary data

S1. Percentage of aldehyde formed at different inlet temperatures

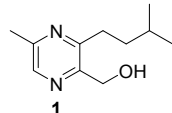
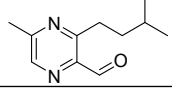
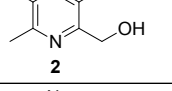
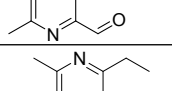
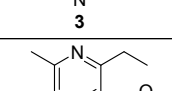
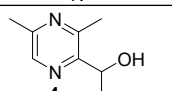
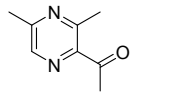
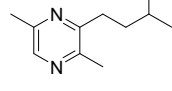
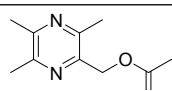
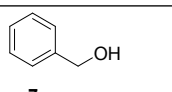
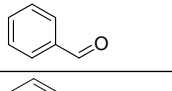
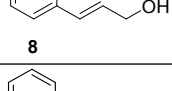
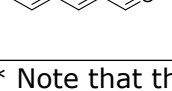
Compound	Inlet temperature (°C)					
	200	225	250	275	300	325
1	13	22	34	50	66	74
2	2	6	14	26	39	51
3	8	11	22	36	47	53
4	0	2	4	9	15	18
7	3		7		24	
8	1		9		34	

S2. Total peak area of TIC of hydroxymethylpyrazines **1-4**, benzyl alcohol **7**, and cinnamyl alcohol **8** and respective aldehyde at different injector temperatures.

Measured as the relative peak area compared to when injected at 325 °C (**1-4**) and 300 °C (**7-8**).



S3. Retention indices and mass fragmentations of alcohols **1-8 and formed aldehydes**

Compound	RT	Ten most abundant mass fragments
 1	13.68	138(100), 109(16), 137(14), 139(9), 133(8), 163(8), 151(7), 108(7), 123(4), 161(4)
 2	12.28	136(100), 108(76), 107(22), 163(19), 149(16), 121(16), 41(15), 66(11), 42(9), 137(9)
 3	10.80	123(100), 152(79), 151(35), 52(30), 53(30), 134(25), 121(24), 69(20), 54(18), 80(13)
 4	9.39	150(100), 42(78), 121(78), 122(76), 80(44), 53(40), 68(32), 54(21), 52(19), 107(17)
 5	12.62	180(100), 161(77), 165(55), 162(42), 151(39), 147(38), 67(30), 52(21), 66(20), 56(19)
 6	11.40	135(100), 178(70), 149(63), 150(36), 39(28), 53(24), 159(22), 56(21), 41(19), 122(17)
 7	9.73	137(100), 107(56), 109(27), 108(15), 66(13), 133(12), 152(11), 135(10), 138(8), 54(6)
 8	9.02	150(100), 107(90), 108(66), 42(46), 43(42), 66(39), 122(27), 67(16), 135(11), 151(9)
 9	10.92	122(100), 135(16), 121(13), 123(10), 163(10), 42(8), 41(6), 53(5), 80(4), 107(3)
 10	15.35	152(100), 151(89), 53(23), 135(22), 136(11), 134(10), 57(10), 153(10), 194(9), 121(8)
 11	8.80	79(100), 108(86), 77(64), 107(61), 51(25), 91(16), 50(14), 78(13), 80(9), 89(8)
 12	7.70	106(100), 105(95), 77(94), 51(43), 50(26), 78(18), 74(11), 52(10), 107(8), 76(6)
 13	12.96	92(100), 91(85), 134(74), 78(61), 105(56), 115(55), 77(51), 79(29), 103(29), 51(28)
 14	12.53	131(100), 132(62), 103(55), 77(40), 78(32), 51(28), 104(26), 50(13), 102(12), 74(8)

* Note that there was an error in previously reported data for this compound^{32, 41}