

Supplemental Information

for

Spotting Isomer Mixtures in Forensic Illicit Drug Casework with GC–VUV using Automated Coelution Detection and Spectral Deconvolution

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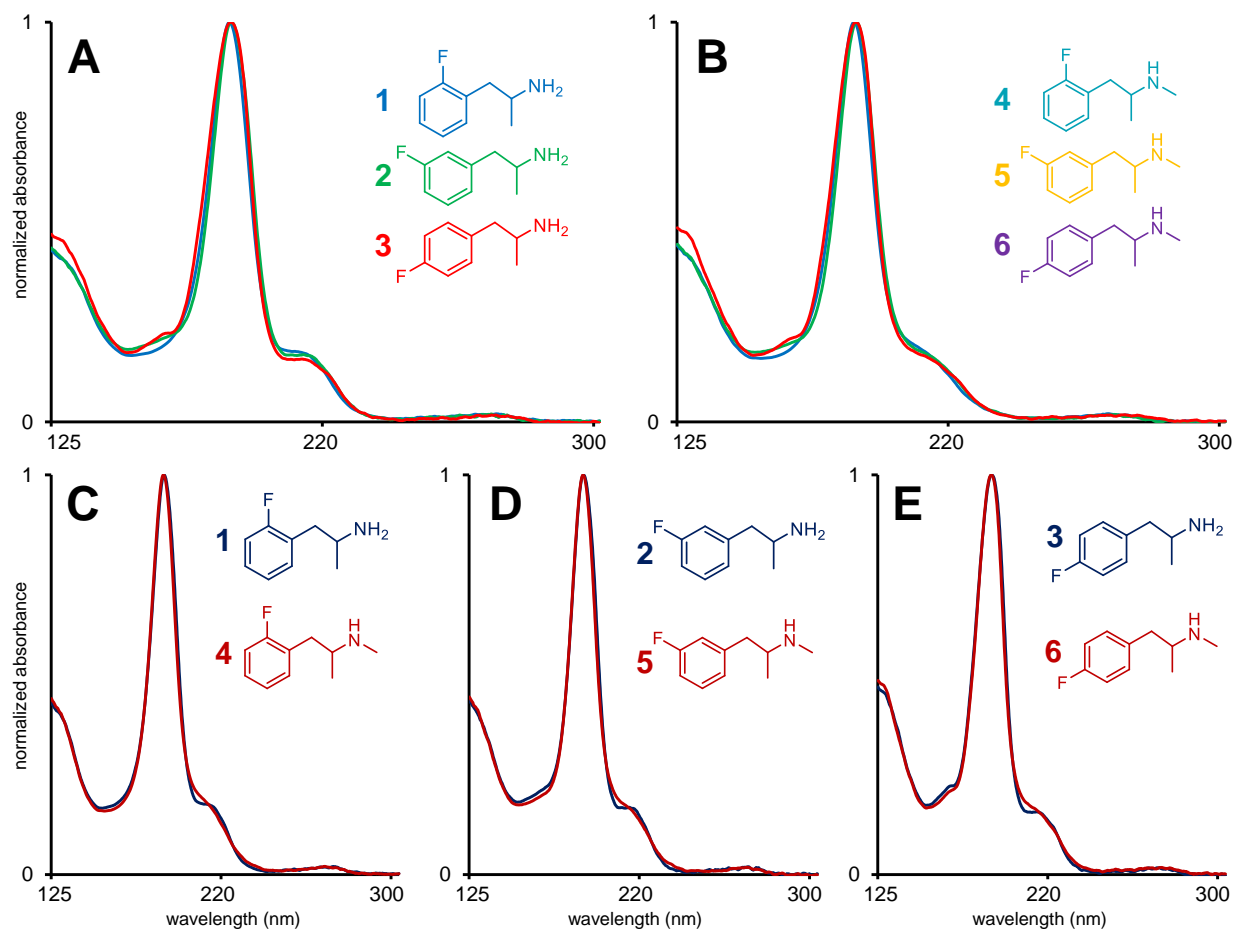


Fig. S1. VUV spectra from all fluoroamphetamine and fluoromethamphetamine isomers with overlays per isomeric group (A and B) and per ring positional class (C, D and E). 2-FA (1); 3-FA (2); 4-FA (3); 2-FMA (4); 3-FMA (5) and 4-FMA (6).

Table S1A. Match scores from coeluted 3-MMC : 4-MMC mixtures – full library

mixture	GC method	library	1st match		next highest matches				remarks		
			score 1	match 1	score 2	match 2	score 1	match 1		score 2	match 2
3-MMC : 4-MMC 9:1	4 (150 C)	both present	0.9989	3-MMC	0.9989	4-MMC	0.9945	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	both present	0.9990	3-MMC	0.9990	4-MMC	0.9947	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	both present	0.9989	3-MMC	0.9987	4-MMC	0.9948	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	both present	0.9989	3-MMC	0.9986	4-MMC	0.9946	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	both present	0.9994	3-MMC	0.9986	4-MMC	0.9954	3-MEC	0.9940	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	both present	0.9994	3-MMC	0.9984	4-MMC	0.9951	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	both present	0.9992	3-MMC	0.9907	4-MEC	0.9953	3-MEC	0.9985	4-MMC	#1
3-MMC : 4-MMC 9:1	6 (250 C)	both present	0.9987	3-MMC	0.9973	4-MMC	0.9953	3-MEC	0.9910	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	both present	0.9993	3-MMC	0.9953	4-MMC	0.9961	3-MEC	0.9878	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	both present	0.9988	3-MMC	0.9988	4-MMC	0.9947	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	both present	0.9990	3-MMC	0.9989	4-MMC	0.9951	3-MEC	0.9947	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	both present	0.9991	3-MMC	0.9989	4-MMC	0.9953	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	both present	0.9991	3-MMC	0.9985	4-MMC	0.9950	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	both present	0.9991	3-MMC	0.9985	4-MMC	0.9952	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	both present	0.9991	3-MMC	0.9984	4-MMC	0.9951	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	both present	0.9992	3-MMC	0.9985	4-MMC	0.9952	3-MEC	0.9927	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	both present	0.9991	3-MMC	0.9983	4-MMC	0.9949	3-MEC	0.9919	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	both present	0.9990	3-MMC	0.9985	4-MMC	0.9955	3-MEC	0.9946	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	both present	0.9993	3-MMC	0.9989	4-MMC	0.9960	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	both present	0.9993	3-MMC	0.9989	4-MMC	0.9958	3-MEC	0.9945	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	both present	0.9993	3-MMC	0.9989	4-MMC	0.9960	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	both present	0.9991	3-MMC	0.9987	4-MMC	0.9958	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	both present	0.9991	3-MMC	0.9985	4-MMC	0.9946	3-MEC	0.9933	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	both present	0.9991	3-MMC	0.9986	4-MMC	0.9956	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	both present	0.9990	3-MMC	0.9981	4-MMC	0.9944	3-MEC	0.9924	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	both present	0.9991	3-MMC	0.9982	4-MMC	0.9949	3-MEC	0.9907	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	both present	0.9985	3-MMC	0.9982	4-MMC	0.9941	3-MEC	0.9924	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	both present	0.9991	3-MMC	0.9989	4-MMC	0.9949	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	both present	0.9993	3-MMC	0.9989	4-MMC	0.9956	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	both present	0.9990	3-MMC	0.9990	4-MMC	0.9951	3-MEC	0.9946	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	both present	0.9988	3-MMC	0.9989	4-MMC	0.9948	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	both present	0.9989	3-MMC	0.9988	4-MMC	0.9949	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	both present	0.9990	3-MMC	0.9989	4-MMC	0.9941	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	both present	0.9987	3-MMC	0.9980	4-MMC	0.9957	3-MEC	0.9929	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	both present	0.9992	3-MMC	0.9980	4-MMC	0.9952	3-MEC	0.9928	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	both present	0.9985	3-MMC	0.9980	4-MMC	0.9940	3-MEC	0.9928	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	both present	0.9992	3-MMC	0.9987	4-MMC	0.9955	3-MEC	0.9934	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	both present	0.9989	3-MMC	0.9988	4-MMC	0.9947	3-MEC	0.9940	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	both present	0.9992	3-MMC	0.9988	4-MMC	0.9955	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	both present	0.9992	3-MMC	0.9985	4-MMC	0.9949	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	both present	0.9992	3-MMC	0.9984	4-MMC	0.9949	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	both present	0.9992	3-MMC	0.9981	4-MMC	0.9954	3-MEC	0.9934	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	both present	0.9990	3-MMC	0.9981	4-MMC	0.9960	3-MEC	0.9928	4-MEC	#2
3-MMC : 4-MMC 1:9	6 (250 C)	both present	0.9988	3-MMC	0.9980	4-MMC	0.9955	3-MEC	0.9927	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	both present	0.9983	3-MMC	0.9980	4-MMC	0.9962	3-MEC	0.9931	4-MEC	

Remarks (erroneous results).

#1. the highest match was obtained from the incorrect combination of 3-MMC and 4-MEC.

#2. the highest match was obtained from a predicted coelution of three substances: 3-MMC, 4-MMC and 4-MEC.

Table S1B. Match scored from coeluted 3-MMC : 4-MMC mixtures – partial libraries

mixture	GC method	library	highest match scores						remarks
			score 1	match 1	score 2	match 2	score 3	match 3	
3-MMC : 4-MMC 9:1	4 (150 C)	3-MMC removed	0.9989	4-MMC	0.9947	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	3-MMC removed	0.9988	4-MMC	0.9947	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	3-MMC removed	0.9988	4-MMC	0.9946	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	3-MMC removed	0.9986	4-MMC	0.9948	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	3-MMC removed	0.9981	4-MMC	0.9953	3-MEC	0.9920	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	3-MMC removed	0.9981	4-MMC	0.9950	3-MEC	0.9930	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	3-MMC removed	0.9985	4-MMC	0.9968	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	3-MMC removed	0.9975	4-MMC	0.9963	3-MEC	0.9921	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	3-MMC removed	0.9953	4-MMC	0.9958	3-MEC	0.9855	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	3-MMC removed	0.9989	4-MMC	0.9947	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	3-MMC removed	0.9989	4-MMC	0.9954	3-MEC	0.9945	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	3-MMC removed	0.9989	4-MMC	0.9953	3-MEC	0.9945	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	3-MMC removed	0.9986	4-MMC	0.9950	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	3-MMC removed	0.9987	4-MMC	0.9953	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	3-MMC removed	0.9987	4-MMC	0.9949	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	3-MMC removed	0.9985	4-MMC	0.9954	3-MEC	0.9935	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	3-MMC removed	0.9985	4-MMC	0.9950	3-MEC	0.9931	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	3-MMC removed	0.9985	4-MMC	0.9953	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	3-MMC removed	0.9990	4-MMC	0.9960	3-MEC	0.9947	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	3-MMC removed	0.9989	4-MMC	0.9958	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	3-MMC removed	0.9989	4-MMC	0.9959	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	3-MMC removed	0.9987	4-MMC	0.9957	3-MEC	0.9946	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	3-MMC removed	0.9987	4-MMC	0.9949	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	3-MMC removed	0.9987	4-MMC	0.9956	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	3-MMC removed	0.9983	4-MMC	0.9961	3-MEC	0.9949	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	3-MMC removed	0.9981	4-MMC	0.9968	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	3-MMC removed	0.9983	4-MMC	0.9954	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	3-MMC removed	0.9988	4-MMC	0.9951	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	3-MMC removed	0.9986	4-MMC	0.9955	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	3-MMC removed	0.9984	4-MMC	0.9955	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	3-MMC removed	0.9988	4-MMC	0.9948	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	3-MMC removed	0.9987	4-MMC	0.9949	3-MEC	0.9933	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	3-MMC removed	0.9989	4-MMC	0.9943	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	3-MMC removed	0.9982	4-MMC	0.9964	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	3-MMC removed	0.9982	4-MMC	0.9961	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	3-MMC removed	0.9985	4-MMC	0.9965	3-MEC	0.9958	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	3-MMC removed	0.9986	4-MMC	0.9953	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	3-MMC removed	0.9985	4-MMC	0.9947	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	3-MMC removed	0.9984	4-MMC	0.9955	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	3-MMC removed	0.9988	4-MMC	0.9948	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	3-MMC removed	0.9984	4-MMC	0.9950	3-MEC	0.9937	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	3-MMC removed	0.9980	4-MMC	0.9949	3-MEC	0.9929	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	3-MMC removed	0.9982	4-MMC	0.9965	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	3-MMC removed	0.9981	4-MMC	0.9967	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	3-MMC removed	0.9984	4-MMC	0.9956	3-MEC	0.9953	4-MEC	

Table S1B. (continue)

mixture	GC method	library	highest match scores				remarks		
			score 1	match 1	score 2	match 2		score 3	match 3
3-MMC : 4-MMC 9:1	4 (150 C)	4-MMC removed	0.9989	3-MMC	0.9947	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	4-MMC removed	0.9989	3-MMC	0.9947	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	4-MMC removed	0.9989	3-MMC	0.9946	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	4-MMC removed	0.9989	3-MMC	0.9947	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	4-MMC removed	0.9993	3-MMC	0.9953	3-MEC	0.9922	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	4-MMC removed	0.9993	3-MMC	0.9952	3-MEC	0.9930	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	4-MMC removed	0.9992	3-MMC	0.9951	3-MEC	0.9912	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	4-MMC removed	0.9993	3-MMC	0.9959	3-MEC	0.9899	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	4-MMC removed	0.9993	3-MMC	0.9958	3-MEC	0.9855	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	4-MMC removed	0.9989	3-MMC	0.9947	3-MEC	0.9946	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	4-MMC removed	0.9991	3-MMC	0.9953	3-MEC	0.9946	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	4-MMC removed	0.9991	3-MMC	0.9953	3-MEC	0.9945	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	4-MMC removed	0.9989	3-MMC	0.9948	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	4-MMC removed	0.9990	3-MMC	0.9952	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	4-MMC removed	0.9990	3-MMC	0.9949	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	4-MMC removed	0.9992	3-MMC	0.9952	3-MEC	0.9927	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	4-MMC removed	0.9991	3-MMC	0.9947	3-MEC	0.9925	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	4-MMC removed	0.9992	3-MMC	0.9950	3-MEC	0.9923	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	4-MMC removed	0.9993	3-MMC	0.9960	3-MEC	0.9947	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	4-MMC removed	0.9993	3-MMC	0.9958	3-MEC	0.9949	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	4-MMC removed	0.9993	3-MMC	0.9959	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	4-MMC removed	0.9991	3-MMC	0.9957	3-MEC	0.9947	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	4-MMC removed	0.9991	3-MMC	0.9945	3-MEC	0.9935	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	4-MMC removed	0.9992	3-MMC	0.9956	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	4-MMC removed	0.9991	3-MMC	0.9944	3-MEC	0.9928	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	4-MMC removed	0.9992	3-MMC	0.9955	3-MEC	0.9913	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	4-MMC removed	0.9991	3-MMC	0.9940	3-MEC	0.9911	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	4-MMC removed	0.9991	3-MMC	0.9949	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	4-MMC removed	0.9992	3-MMC	0.9955	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	4-MMC removed	0.9990	3-MMC	0.9951	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	4-MMC removed	0.9988	3-MMC	0.9948	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	4-MMC removed	0.9989	3-MMC	0.9949	3-MEC	0.9931	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	4-MMC removed	0.9988	3-MMC	0.9937	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	4-MMC removed	0.9992	3-MMC			0.9928	4-MEC	#1
3-MMC : 4-MMC 1:3	6 (250 C)	4-MMC removed	0.9992	3-MMC			0.9926	4-MEC	#1
3-MMC : 4-MMC 1:3	6 (250 C)	4-MMC removed	0.9986	3-MMC			0.9940	4-MEC	#1
3-MMC : 4-MMC 1:9	4 (150 C)	4-MMC removed	0.9988	3-MMC	0.9953	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	4-MMC removed	0.9989	3-MMC	0.9947	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	4-MMC removed	0.9992	3-MMC	0.9955	3-MEC	0.9935	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	4-MMC removed	0.9991	3-MMC	0.9951	3-MEC	0.9935	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	4-MMC removed	0.9992	3-MMC	0.9949	3-MEC	0.9933	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	4-MMC removed	0.9992	3-MMC	0.9957	3-MEC	0.9925	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	4-MMC removed	0.9984	3-MMC			0.9925	4-MEC	#1
3-MMC : 4-MMC 1:9	6 (250 C)	4-MMC removed	0.9987	3-MMC			0.9923	4-MEC	#1
3-MMC : 4-MMC 1:9	6 (250 C)	4-MMC removed	0.9988	3-MMC			0.9928	4-MEC	#1

Table S1B. (continue)

mixture	GC method	library	highest match scores						remarks
			score 1	match 1	score 2	match 2	score 3	match 3	
3-MMC : 4-MMC 9:1	4 (150 C)	both removed			0.9946	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	both removed			0.9947	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 9:1	4 (150 C)	both removed			0.9946	3-MEC	0.9940	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	both removed			0.9938	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	both removed			0.9953	3-MEC	0.9922	4-MEC	
3-MMC : 4-MMC 9:1	5 (200 C)	both removed			0.9938	3-MEC	0.9931	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	both removed			0.9951	3-MEC	0.9912	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	both removed			0.9958	3-MEC	0.9908	4-MEC	
3-MMC : 4-MMC 9:1	6 (250 C)	both removed			0.9961	3-MEC	0.9881	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	both removed			0.9947	3-MEC	0.9948	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	both removed			0.9951	3-MEC	0.9947	4-MEC	
3-MMC : 4-MMC 3:1	4 (150 C)	both removed			0.9954	3-MEC	0.9947	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	both removed			0.9948	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	both removed			0.9948	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 3:1	5 (200 C)	both removed			0.9947	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	both removed			0.9952	3-MEC	0.9927	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	both removed			0.9947	3-MEC	0.9925	4-MEC	
3-MMC : 4-MMC 3:1	6 (250 C)	both removed			0.9954	3-MEC	0.9952	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	both removed			0.9957	3-MEC	0.9941	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	both removed			0.9955	3-MEC	0.9944	4-MEC	
3-MMC : 4-MMC 1:1	4 (150 C)	both removed			0.9956	3-MEC	0.9949	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	both removed			0.9953	3-MEC	0.9946	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	both removed			0.9946	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:1	5 (200 C)	both removed			0.9952	3-MEC	0.9938	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	both removed			0.9963	3-MEC	0.9950	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	both removed			0.9967	3-MEC	0.9940	4-MEC	
3-MMC : 4-MMC 1:1	6 (250 C)	both removed			0.9944	3-MEC	0.9924	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	both removed			0.9947	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	both removed			0.9951	3-MEC	0.9942	4-MEC	
3-MMC : 4-MMC 1:3	4 (150 C)	both removed			0.9953	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	both removed			0.9949	3-MEC	0.9931	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	both removed			0.9937	3-MEC	0.9943	4-MEC	
3-MMC : 4-MMC 1:3	5 (200 C)	both removed			0.9950	3-MEC	0.9927	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	both removed			0.9957	3-MEC	0.9926	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	both removed			0.9971	3-MEC	0.9940	4-MEC	
3-MMC : 4-MMC 1:3	6 (250 C)	both removed			0.9962	3-MEC	0.9928	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	both removed			0.9953	3-MEC	0.9939	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	both removed			0.9947	3-MEC	0.9936	4-MEC	
3-MMC : 4-MMC 1:9	4 (150 C)	both removed			0.9955	3-MEC	0.9935	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	both removed			0.9950	3-MEC	0.9927	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	both removed			0.9949	3-MEC	0.9932	4-MEC	
3-MMC : 4-MMC 1:9	5 (200 C)	both removed			0.9956	3-MEC	0.9928	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	both removed			0.9962	3-MEC	0.9928	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	both removed			0.9965	3-MEC	0.9923	4-MEC	
3-MMC : 4-MMC 1:9	6 (250 C)	both removed			0.9958	3-MEC	0.9927	4-MEC	

Remarks (erroneous results).

#1. no other scores with a match above 0.9 were obtained.

Table S1C. Match scores from coeluted 3-FA : 4-FA mixtures – full library

mixture	GC method	library	1st match		next highest match		remarks		
			score 1	match 1	score 2	match 2		score 1	match 1
3-FA : 4-FA 9:1	1 (30 C)	both present	0.9998	3-FA	0.9996	4-FA	0.9974	2-FA	
3-FA : 4-FA 9:1	1 (30 C)	both present	0.9997	3-FA	0.9996	4-FA	0.9974	2-FA	
3-FA : 4-FA 9:1	1 (30 C)	both present	0.9997	3-FA	0.9997	4-FA	0.9975	2-FA	
3-FA : 4-FA 9:1	3 (100 C)	both present	0.9997	3-FA	0.9992	4-FA	0.9976	2-FA	
3-FA : 4-FA 9:1	3 (100 C)	both present	0.9997	3-FA	0.9990	4-FA	0.9977	2-FA	
3-FA : 4-FA 9:1	3 (100 C)	both present	0.9997	3-FA	0.9994	4-FA	0.9978	2-FA	
3-FA : 4-FA 9:1	4 (150 C)	both present	0.9997	3-FA	N.A.	none	0.9988	4-FA	#1
3-FA : 4-FA 9:1	4 (150 C)	both present	0.9998	3-FA	N.A.	none	0.9986	4-FA	#1
3-FA : 4-FA 9:1	4 (150 C)	both present	0.9998	3-FA	N.A.	none	0.9988	4-FA	#1
3-FA : 4-FA 9:1	5 (200 C)	both present	0.9988	3-FA	0.9932	2-FA	0.9899	4-FA	#2
3-FA : 4-FA 9:1	5 (200 C)	both present	0.9988	3-FA	0.9933	2-FA	0.9903	4-FA	#2
3-FA : 4-FA 9:1	5 (200 C)	both present	0.9982	3-FA	0.9944	2-FA	0.9910	4-FA	#2
3-FA : 4-FA 3:1	1 (30 C)	both present	0.9998	3-FA	0.9998	4-FA	0.9973	4-FMA	
3-FA : 4-FA 3:1	1 (30 C)	both present	0.9998	3-FA	0.9997	4-FA	0.9972	4-FMA	
3-FA : 4-FA 3:1	1 (30 C)	both present	0.9998	3-FA	0.9997	4-FA	0.9973	4-FMA	
3-FA : 4-FA 3:1	3 (100 C)	both present	0.9997	3-FA	0.9996	4-FA	0.9977	2-FA	
3-FA : 4-FA 3:1	3 (100 C)	both present	0.9998	3-FA	0.9996	4-FA	0.9976	2-FA	
3-FA : 4-FA 3:1	3 (100 C)	both present	0.9997	3-FA	0.9995	4-FA	0.9976	2-FA	
3-FA : 4-FA 3:1	4 (150 C)	both present	0.9996	3-FA	0.9992	4-FA	0.9974	2-FA	
3-FA : 4-FA 3:1	4 (150 C)	both present	0.9998	3-FA	0.9995	4-FA	0.9977	2-FA	
3-FA : 4-FA 3:1	4 (150 C)	both present	0.9997	3-FA	0.9994	4-FA	0.9977	2-FA	
3-FA : 4-FA 3:1	5 (200 C)	both present	0.9951	2-FA	0.8526	o-xylene	0.9973	3-FA	#3
3-FA : 4-FA 3:1	5 (200 C)	both present	0.9975	3-FA	N.A.	none	0.9966	3-FMA	#1
3-FA : 4-FA 3:1	5 (200 C)	both present	0.9986	3-FA	0.9934	2-FA	0.9908	4-FA	#2
3-FA : 4-FA 1:1	1 (30 C)	both present	0.9997	3-FA	0.9998	4-FA	0.9973	4-FMA	
3-FA : 4-FA 1:1	1 (30 C)	both present	0.9996	3-FA	0.9998	4-FA	0.9973	4-FMA	
3-FA : 4-FA 1:1	1 (30 C)	both present	0.9996	3-FA	0.9998	4-FA	0.9974	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	both present	0.9995	3-FA	0.9997	4-FA	0.9974	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	both present	0.9997	3-FA	0.9998	4-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	both present	0.9992	3-FA	0.9995	4-FA	0.9972	3-FMA	
3-FA : 4-FA 1:1	4 (150 C)	both present	0.9994	3-FA	0.9997	4-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	both present	0.9994	3-FA	0.9997	4-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	both present	0.9994	3-FA	0.9997	4-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	5 (200 C)	both present	0.9981	3-FA	0.9918	4-FA	0.9929	3-FMA	
3-FA : 4-FA 1:1	5 (200 C)	both present	0.9918	3-FA	0.9980	4-FA	0.9928	3-FMA	
3-FA : 4-FA 1:1	5 (200 C)	both present	0.9981	3-FA	0.9917	4-FA	0.9928	3-FMA	
3-FA : 4-FA 1:3	1 (30 C)	both present	0.9996	3-FA	0.9998	4-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	both present	0.9997	3-FA	0.9997	4-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	both present	0.9997	3-FA	0.9998	4-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	both present	0.9997	3-FA	0.9998	4-FA	0.9974	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	both present	0.9994	3-FA	0.9997	4-FA	0.9975	2-FA	
3-FA : 4-FA 1:3	3 (100 C)	both present	0.9994	3-FA	0.9997	4-FA	0.9977	2-FA	
3-FA : 4-FA 1:3	4 (150 C)	both present	0.9992	3-FA	0.9997	4-FA	0.9976	2-FA	
3-FA : 4-FA 1:3	4 (150 C)	both present	0.9990	3-FA	0.9997	4-FA	0.9976	2-FA	
3-FA : 4-FA 1:3	4 (150 C)	both present	0.9993	3-FA	0.9997	4-FA	0.9976	2-FA	
3-FA : 4-FA 1:3	5 (200 C)	both present	0.9976	3-FA	N.A.	none	0.9966	3-FMA	#1
3-FA : 4-FA 1:3	5 (200 C)	both present	0.9975	3-FA	0.9953	2-FA	0.9902	4-FMA	#2
3-FA : 4-FA 1:3	5 (200 C)	both present	0.9991	3-FA	N.A.	none	0.9978	3-FMA	#2
3-FA : 4-FA 1:9	1 (30 C)	both present	0.9991	3-FA	0.9998	4-FA	0.9979	2-FA	
3-FA : 4-FA 1:9	1 (30 C)	both present	0.9990	3-FA	0.9998	4-FA	0.9976	2-FA	
3-FA : 4-FA 1:9	1 (30 C)	both present	0.9989	3-FA	0.9998	4-FA	0.9977	2-FA	
3-FA : 4-FA 1:9	3 (100 C)	both present	0.9991	3-FA	0.9998	4-FA	0.9970	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	both present	0.9986	3-FA	0.9998	4-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	both present	0.9997	4-FA	0.9968	2-FA	0.9986	3-FA	#2
3-FA : 4-FA 1:9	4 (150 C)	both present	0.9998	4-FA	N.A.	none	0.9973	4-FMA	#1
3-FA : 4-FA 1:9	4 (150 C)	both present	0.9997	4-FA	N.A.	none	0.9973	4-FMA	#1
3-FA : 4-FA 1:9	4 (150 C)	both present	0.9997	4-FA	N.A.	none	0.9974	2-FA	#1
3-FA : 4-FA 1:9	5 (200 C)	both present	0.9995	4-FA	0.9900	2-FMA	0.9955	2-FA	#2
3-FA : 4-FA 1:9	5 (200 C)	both present	0.9996	4-FA	0.9899	2-FMA	0.9956	2-FA	#2
3-FA : 4-FA 1:9	5 (200 C)	both present	0.9991	4-FA	0.9623	2-FMA	0.9950	2-FA	#2

Remarks (erroneous results).

#1. the highest obtained match was a single component match (no coelution detected and no deconvolution performed).

#2. the highest obtained match was incorrect for the minor predicted constituent.

#3. the highest match was a coelution of 2 components, however both were incorrect.

Table S1D. Match scored from coeluted 3-FA : 4-FA mixtures – partial libraries

mixture	GC method	library	highest match scores				remarks	
			score 1	match 1	score 2	match 2		score 3
3-FA : 4-FA 9:1	1 (30 C)	3-FA removed	0.9996	4-FA	0.9974	2-FA	0.9971	3-FMA
3-FA : 4-FA 9:1	1 (30 C)	3-FA removed	0.9996	4-FA	0.9974	2-FA	0.9970	3-FMA
3-FA : 4-FA 9:1	1 (30 C)	3-FA removed	0.9997	4-FA	0.9975	2-FA	0.9970	3-FMA
3-FA : 4-FA 9:1	3 (100 C)	3-FA removed	0.9992	4-FA	0.9976	2-FA	0.9971	3-FMA
3-FA : 4-FA 9:1	3 (100 C)	3-FA removed	0.9990	4-FA	0.9977	2-FA	0.9971	3-FMA
3-FA : 4-FA 9:1	3 (100 C)	3-FA removed	0.9994	4-FA	0.9978	2-FA	0.9971	3-FMA
3-FA : 4-FA 9:1	4 (150 C)	3-FA removed	0.9988	4-FA	0.9977	2-FA	0.9970	4-FMA
3-FA : 4-FA 9:1	4 (150 C)	3-FA removed	0.9988	4-FA	0.9973	2-FA	0.9970	4-FMA
3-FA : 4-FA 9:1	4 (150 C)	3-FA removed	0.9988	4-FA	0.9975	2-FA	0.9971	4-FMA
3-FA : 4-FA 3:1	1 (30 C)	3-FA removed	0.9997	4-FA	0.9977	2-FA	0.9970	3-FMA
3-FA : 4-FA 3:1	1 (30 C)	3-FA removed	0.9997	4-FA	0.9977	2-FA	0.9977	3-FMA
3-FA : 4-FA 3:1	1 (30 C)	3-FA removed	0.9998	4-FA	0.9977	2-FA	0.9973	3-FMA
3-FA : 4-FA 3:1	3 (100 C)	3-FA removed	0.9996	4-FA	0.9977	2-FA	0.9976	3-FMA
3-FA : 4-FA 3:1	3 (100 C)	3-FA removed	0.9996	4-FA	0.9976	2-FA	0.9969	3-FMA
3-FA : 4-FA 3:1	3 (100 C)	3-FA removed	0.9995	4-FA	0.9976	2-FA	0.9970	3-FMA
3-FA : 4-FA 3:1	4 (150 C)	3-FA removed	0.9994	4-FA	0.9977	2-FA	0.9972	3-FMA
3-FA : 4-FA 3:1	4 (150 C)	3-FA removed	0.9995	4-FA	0.9977	2-FA	0.9968	3-FMA
3-FA : 4-FA 3:1	4 (150 C)	3-FA removed	0.9995	4-FA	0.9977	2-FA	0.9969	3-FMA
3-FA : 4-FA 1:1	1 (30 C)	3-FA removed	0.9998	4-FA	0.9978	2-FA	0.9972	3-FMA
3-FA : 4-FA 1:1	1 (30 C)	3-FA removed	0.9998	4-FA	0.9977	2-FA	0.9973	3-FMA
3-FA : 4-FA 1:1	1 (30 C)	3-FA removed	0.9998	4-FA	0.9978	2-FA	0.9973	3-FMA
3-FA : 4-FA 1:1	3 (100 C)	3-FA removed	0.9997	4-FA	0.9978	2-FA	0.9970	3-FMA
3-FA : 4-FA 1:1	3 (100 C)	3-FA removed	0.9998	4-FA	0.9976	2-FA	0.9970	3-FMA
3-FA : 4-FA 1:1	3 (100 C)	3-FA removed	0.9996	4-FA	0.9978	2-FA	0.9973	3-FMA
3-FA : 4-FA 1:1	4 (150 C)	3-FA removed	0.9997	4-FA	0.9977	2-FA	0.9966	3-FMA
3-FA : 4-FA 1:1	4 (150 C)	3-FA removed	0.9997	4-FA	0.9976	2-FA	0.9967	3-FMA
3-FA : 4-FA 1:1	4 (150 C)	3-FA removed	0.9997	4-FA	0.9977	2-FA	0.9966	3-FMA
3-FA : 4-FA 1:3	1 (30 C)	3-FA removed	0.9998	4-FA	0.9976	2-FA	0.9971	3-FMA
3-FA : 4-FA 1:3	1 (30 C)	3-FA removed	0.9997	4-FA	0.9977	2-FA	0.9971	3-FMA
3-FA : 4-FA 1:3	1 (30 C)	3-FA removed	0.9998	4-FA	0.9975	2-FA	0.9970	3-FMA
3-FA : 4-FA 1:3	3 (100 C)	3-FA removed	0.9998	4-FA	0.9977	2-FA	0.9971	3-FMA
3-FA : 4-FA 1:3	3 (100 C)	3-FA removed	0.9998	4-FA	0.9977	2-FA	0.9971	3-FMA
3-FA : 4-FA 1:3	3 (100 C)	3-FA removed	0.9997	4-FA	0.9977	2-FA	0.9969	3-FMA
3-FA : 4-FA 1:3	4 (150 C)	3-FA removed	0.9997	4-FA	0.9976	2-FA	0.9967	3-FMA
3-FA : 4-FA 1:3	4 (150 C)	3-FA removed	0.9997	4-FA	0.9976	2-FA	0.9968	3-FMA
3-FA : 4-FA 1:3	4 (150 C)	3-FA removed	0.9997	4-FA	0.9976	2-FA	0.9966	3-FMA
3-FA : 4-FA 1:9	1 (30 C)	3-FA removed	0.9997	4-FA	0.9974	2-FA	0.9959	3-FMA
3-FA : 4-FA 1:9	1 (30 C)	3-FA removed	0.9997	4-FA	0.9975	2-FA	0.9968	3-FMA
3-FA : 4-FA 1:9	1 (30 C)	3-FA removed	0.9997	4-FA	0.9975	2-FA	0.9971	4-FMA
3-FA : 4-FA 1:9	3 (100 C)	3-FA removed	0.9998	4-FA	0.9977	2-FA	0.9970	4-FMA
3-FA : 4-FA 1:9	3 (100 C)	3-FA removed	0.9998	4-FA	0.9978	2-FA	0.9971	4-FMA
3-FA : 4-FA 1:9	3 (100 C)	3-FA removed	0.9997	4-FA	0.9974	2-FA	0.9973	4-FMA
3-FA : 4-FA 1:9	4 (150 C)	3-FA removed	0.9997	4-FA	0.9966	2-FA	0.9973	4-FMA
3-FA : 4-FA 1:9	4 (150 C)	3-FA removed	0.9996	4-FA	0.9965	2-FA	0.9973	4-FMA
3-FA : 4-FA 1:9	4 (150 C)	3-FA removed	0.9997	4-FA	0.9962	2-FA	0.9973	4-FMA

Table S1D. (continue)

mixture	GC method	library	highest match scores						remarks
			score 1	match 1	score 2	match 2	score 3	match 3	
3-FA : 4-FA 9:1	1 (30 C)	4-FA removed	0.9998	3-FA	0.9974	2-FA	0.9972	4-FMA	
3-FA : 4-FA 9:1	1 (30 C)	4-FA removed	0.9997	3-FA	0.9974	2-FA	0.9972	4-FMA	
3-FA : 4-FA 9:1	1 (30 C)	4-FA removed	0.9997	3-FA	0.9975	2-FA	0.9973	4-FMA	
3-FA : 4-FA 9:1	3 (100 C)	4-FA removed	0.9997	3-FA	0.9978	2-FA	0.9971	4-FMA	
3-FA : 4-FA 9:1	3 (100 C)	4-FA removed	0.9997	3-FA	0.9976	2-FA	0.9970	4-FMA	
3-FA : 4-FA 9:1	3 (100 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9970	4-FMA	
3-FA : 4-FA 9:1	4 (150 C)	4-FA removed	0.9998	3-FA	0.9977	2-FA	0.9959	3-FMA	
3-FA : 4-FA 9:1	4 (150 C)	4-FA removed	0.9997	3-FA	0.9973	2-FA	0.9962	4-FMA	
3-FA : 4-FA 9:1	4 (150 C)	4-FA removed	0.9998	3-FA	0.9975	2-FA	0.9969	3-FMA	
3-FA : 4-FA 3:1	1 (30 C)	4-FA removed	0.9997	3-FA	0.9974	2-FA	0.9973	4-FMA	
3-FA : 4-FA 3:1	1 (30 C)	4-FA removed	0.9997	3-FA	0.9975	2-FA	0.9972	4-FMA	
3-FA : 4-FA 3:1	1 (30 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9973	4-FMA	
3-FA : 4-FA 3:1	3 (100 C)	4-FA removed	0.9998	3-FA	0.9976	2-FA	0.9969	4-FMA	
3-FA : 4-FA 3:1	3 (100 C)	4-FA removed	0.9998	3-FA	0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 3:1	3 (100 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9970	4-FMA	
3-FA : 4-FA 3:1	4 (150 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9966	4-FMA	
3-FA : 4-FA 3:1	4 (150 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9970	4-FMA	
3-FA : 4-FA 3:1	4 (150 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9970	4-FMA	
3-FA : 4-FA 1:1	1 (30 C)	4-FA removed	0.9997	3-FA	0.9978	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:1	1 (30 C)	4-FA removed	0.9996	3-FA	0.9977	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:1	1 (30 C)	4-FA removed	0.9996	3-FA	0.9978	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	4-FA removed	0.9995	3-FA	0.9978	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	4-FA removed	0.9997	3-FA	0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	4-FA removed	0.9992	3-FA	0.9978	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	4-FA removed	0.9994	3-FA	0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	4-FA removed	0.9994	3-FA	0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	4-FA removed	0.9994	3-FA	0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	4-FA removed	0.9994	3-FA	0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	4-FA removed	0.9996	3-FA	0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	4-FA removed	0.9997	3-FA	0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	4-FA removed	0.9994	3-FA	0.9975	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	4-FA removed	0.9994	3-FA	0.9977	2-FA	0.9975	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	4-FA removed	0.9997	3-FA	0.9977	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:3	4 (150 C)	4-FA removed	0.9992	3-FA	0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	4 (150 C)	4-FA removed	0.9990	3-FA	0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	4 (150 C)	4-FA removed	0.9993	3-FA	0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	1 (30 C)	4-FA removed	0.9991	3-FA	0.9979	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	1 (30 C)	4-FA removed	0.9995	3-FA	0.9978	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:9	1 (30 C)	4-FA removed	0.9995	3-FA	0.9978	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	4-FA removed	0.9991	3-FA	0.9977	2-FA	0.9970	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	4-FA removed	0.9985	3-FA	0.9978	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	4-FA removed	0.9978	3-FA	0.9974	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:9	4 (150 C)	4-FA removed			0.9966	2-FA	0.9971	4-FMA	#1
3-FA : 4-FA 1:9	4 (150 C)	4-FA removed			0.9966	2-FA	0.9973	4-FMA	#1
3-FA : 4-FA 1:9	4 (150 C)	4-FA removed			0.9966	2-FA	0.9973	4-FMA	#1

Table S1D. (continue)

mixture	GC method	library	highest match scores				remarks		
			score 1	match 1	score 2	match 2		score 3	match 3
3-FA : 4-FA 9:1	1 (30 C)	both removed			0.9974	2-FA	0.9971	3-FMA	
3-FA : 4-FA 9:1	1 (30 C)	both removed			0.9973	2-FA	0.9971	3-FMA	
3-FA : 4-FA 9:1	1 (30 C)	both removed			0.9975	2-FA	0.9971	3-FMA	
3-FA : 4-FA 9:1	3 (100 C)	both removed			0.9975	2-FA	0.9972	3-FMA	
3-FA : 4-FA 9:1	3 (100 C)	both removed			0.9977	2-FA	0.9972	3-FMA	
3-FA : 4-FA 9:1	3 (100 C)	both removed			0.9978	2-FA	0.9972	3-FMA	
3-FA : 4-FA 9:1	4 (150 C)	both removed			0.9972	2-FA	0.9968	3-FMA	
3-FA : 4-FA 9:1	4 (150 C)	both removed			0.9972	2-FA	0.9969	3-FMA	
3-FA : 4-FA 9:1	4 (150 C)	both removed			0.9974	2-FA	0.9969	3-FMA	
3-FA : 4-FA 3:1	1 (30 C)	both removed			0.9977	2-FA	0.9973	4-FMA	
3-FA : 4-FA 3:1	1 (30 C)	both removed			0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 3:1	1 (30 C)	both removed			0.9976	2-FA	0.9973	4-FMA	
3-FA : 4-FA 3:1	3 (100 C)	both removed			0.9976	2-FA	0.9962	3-FMA	
3-FA : 4-FA 3:1	3 (100 C)	both removed			0.9975	2-FA	0.9972	4-FMA	
3-FA : 4-FA 3:1	3 (100 C)	both removed			0.9976	2-FA	0.9970	4-FMA	
3-FA : 4-FA 3:1	4 (150 C)	both removed			0.9974	2-FA	0.9972	3-FMA	
3-FA : 4-FA 3:1	4 (150 C)	both removed			0.9977	2-FA	0.9968	3-FMA	
3-FA : 4-FA 3:1	4 (150 C)	both removed			0.9977	2-FA	0.9969	3-FMA	
3-FA : 4-FA 1:1	1 (30 C)	both removed			0.9977	3-FMA	0.9980	4-FMA	#2
3-FA : 4-FA 1:1	1 (30 C)	both removed			0.9977	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:1	1 (30 C)	both removed			0.9978	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	both removed			0.9978	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	both removed			0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	3 (100 C)	both removed			0.9978	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	both removed			0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	both removed			0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:1	4 (150 C)	both removed			0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	both removed			0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	both removed			0.9977	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:3	1 (30 C)	both removed			0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	both removed			0.9977	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	both removed			0.9977	2-FA	0.9975	4-FMA	
3-FA : 4-FA 1:3	3 (100 C)	both removed			0.9977	2-FA	0.9974	4-FMA	
3-FA : 4-FA 1:3	4 (150 C)	both removed			0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	4 (150 C)	both removed			0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:3	4 (150 C)	both removed			0.9975	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	1 (30 C)	both removed			0.9979	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	1 (30 C)	both removed			0.9976	2-FA	0.9972	4-FMA	
3-FA : 4-FA 1:9	1 (30 C)	both removed			0.9976	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	both removed			0.9976	2-FA	0.9970	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	both removed			0.9978	2-FA	0.9971	4-FMA	
3-FA : 4-FA 1:9	3 (100 C)	both removed			0.9974	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:9	4 (150 C)	both removed			0.9966	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:9	4 (150 C)	both removed			0.9965	2-FA	0.9973	4-FMA	
3-FA : 4-FA 1:9	4 (150 C)	both removed			0.9962	2-FA	0.9973	4-FMA	

Remarks (erroneous results).

#1. the highest match was the 2-FA : 4-FMA combination; 3-FA was only detected in lower scoring matches.

#2. the highest match was the combination 3-FMA and 4-FMA; lower matches included 2-FA with a 0.9978 individual match score.