Table S1. SMILES* format for the targeted compound isolated from *Trigonella foenumgraecum*.

*: simplified molecular input line entry system.

Compound name	Formula	Smile ID	CID
Phenol, Phenol, 2-methoxy-3-(2-propenyl)	C10H12O2	COC1=C(C=CC=C1O)CC=C	596373
palmitic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	985
linolenic acid	C18H30O2	CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O	5280934
9,12-Octadecadienoic acid	C18H32O2	CCCCCC=CCC=CCCCCCCCC(=O)O	3931
butyl linoleate	C22H40O2	CCCCC/C=C\C/C=C\CCCCCCCC(=O)OCCCC	6436910
trimethylsilyl(9Z,12Z)-octadeca-9,12-dienoate	C21H40O2Si	CCCCCC=CCC=CCCCCCCCC(=O)O[Si](C)(C)C	5352430
3H,6H-Thieno [3,4-c]isoxazole	C8H13NOS	CC(C)C1C2=NOCC2CS1	598714
E,Z-1,3,12-Nonadecatriene	C19H34	CCCCCC/C=C\CCCCCCC/C=C/C=C	5365680
gamma.-Tocopherol	C28H48O2	CC1=C(C=C2CC[C@@](OC2=C1C)(C)CCC[C@H](C)CCC[C@H](C)CCCC(C)C)O	92729