

**Table S1: All the compounds with their abbreviations and retention times (RT), SIM ions**

S.No.	Compound full name	Abbreviation	RT(k-factor=2.93)	SIM Ions
1	2-Fluorobenzoic acid	2-FBA	15.82	95,123
2	3- Fluorobenzoic acid	3-FBA	14.74	95,123
3	4- Fluorobenzoic acid	4-FBA	14.74	95,123
4	2,3- di Fluorobenzoic acid	2,3- DFBA	15.66	113, 141
5	2,4- di Fluorobenzoic acid	2,4- DFBA	14.57	113, 141
6	2,5- di Fluorobenzoic acid	2,5- DFBA	15.03	113, 141
7	2,6- di Fluorobenzoic acid	2,6- DFBA	15.00	113, 141
8	3,4- di Fluorobenzoic acid	3,4- DFBA	14.46	113, 141
9	3,5- di Fluorobenzoic acid	3,5-DFBA	13.31	113, 141
10	2,3,4- tri Fluorobenzoic acid	2,3,4- TFBA	14.81	131, 159
11	2,3,5- tri Fluorobenzoic acid	2,3,5- TFBA	13.97	131, 159
12	2,3,6- tri Fluorobenzoic acid	2,3,6- TFBA	14.56	131, 159
13	2,4,5- tri Fluorobenzoic acid	2,4,5- TFBA	14.02	131, 159
14	2,4,6- tri Fluorobenzoic acid	2,4,6- TFBA	13.13	131, 159
15	3,4,5- tri Fluorobenzoic acid	3,4,5-TFBA	13.38	131, 159
16	2,3,4,5- tetra Fluorobenzoic acid	2,3,4,5- TetraFBA	13.39	149, 177
17	2,3,5,6- tetra Fluorobenzoic acid	2,3,5,6-TetraFBA	13.23	149, 177

18	2,3,4,5,6-penta Fluorobenzoic acid	2,3,4,5,6-PFBA	12.17	167,195
19	2,6-Bis (Trifluoromethyl) benzoic acid	2,6-Bis FBA	14.53	213, 241
20	3,5-Bis (Trifluoromethyl) benzoic acid	3,5-Bis FBA	13.01	213, 241
21	2-(Trifluoromethyl) benzoic acid	2-TFM	15.44	145,173
22	4-(Trifluoromethyl) benzoic acid	4-TFM	14.75	145,173
23	3-(Trifluoromethyl) benzoic acid	3-TFM	15.02	145,173

**Table S2 - Regression equation for different substituted FBAs**

Type of FBA	Regression equation	Value of R <sup>2</sup> (%)
Mono FBA	Response = -20853896 - 1661757 SV + 197169 W - 1891474 t + 409936 Temp + 13602417 VH + 1178061 SV <sup>2</sup> + 89018 t <sup>2</sup> - 680 Temp <sup>2</sup> + 4875387 VH <sup>2</sup> + 6740 SV*W + 522765 SV*t - 38001 SV*Temp - 5621688 SV*VH + 1959 W*t + 648.5 W*Temp - 78945 W*VH - 5668 t*Temp + 218202 t*VH - 292347 Temp*VH + 26684 SV*Temp*VH - 2218 t*Temp*VH + 1143.4 Temp <sup>2</sup> *VH - 22608 Temp*VH <sup>2</sup>	99.99
Di-FBA	Response = -3938150 - 313814 SV + 37234 W - 357195 t + 77414 Temp + 2568746 VH + 222471 SV <sup>2</sup> + 16811 t <sup>2</sup> - 128.3 Temp <sup>2</sup> + 920691 VH <sup>2</sup> + 1273 SV*W + 98721 SV*t - 7176 SV*Temp - 1061626 SV*VH + 370 W*t + 122.5 W*Temp - 14908 W*VH - 1070 t*Temp + 41206 t*VH - 55208 Temp*VH + 5039 SV*Temp*VH - 419.0 t*Temp*VH + 215.9 Temp <sup>2</sup> *VH - 4269 Temp*VH <sup>2</sup>	99.99
Tri-FBA	Response = -8044897 - 215691 SV + 68477 W - 628723 t + 157441 Temp + 4910092 VH + 449641 SV <sup>2</sup> + 34991 t <sup>2</sup> - 230.6 Temp <sup>2</sup> + 1986187 VH <sup>2</sup> + 4952 SV*W + 194018 SV*t - 18397 SV*Temp - 2288602 SV*VH - 483 W*t + 168.5 W*Temp - 26302 W*VH - 3148 t*Temp + 57923 t*VH - 110182 Temp*VH + 11414 SV*Temp*VH - 533.6 t*Temp*VH + 434.75 Temp <sup>2</sup> *VH - 9634 Temp*VH <sup>2</sup>	100.00
Tetra- FBA	Response = -4546301 - 362275 SV + 42984 W - 412355 t + 89369 Temp + 2965426 VH + 256826 SV <sup>2</sup> + 19407 t <sup>2</sup> - 148.1 Temp <sup>2</sup> + 1062870 VH <sup>2</sup> + 1469 SV*W + 113966 SV*t - 8284 SV*Temp - 1225569 SV*VH + 427 W*t + 141.4 W*Temp - 17211 W*VH - 1236 t*Temp + 47570 t*VH - 63734 Temp*VH + 5817 SV*Temp*VH - 483.6 t*Temp*VH + 249.3 Temp <sup>2</sup> *VH - 4929 Temp*VH <sup>2</sup>	99.99

Penta-FBA	Response = -2738096 - 104152 SV + 34912 W - 230648 t + 59425 Temp + 1497034 VH + 118116 SV <sup>2</sup> + 9244 t <sup>2</sup> - 165.1 Temp <sup>2</sup> + 722201 VH <sup>2</sup> - 234 SV*W + 58225 SV*t - 3226 SV*Temp - 733716 SV*VH - 115 W*t + 28.7 W*Temp - 9784 W*VH - 301 t*Temp + 36496 t*VH - 39474 Temp*VH + 3349 SV*Temp*VH - 349.1 t*Temp*VH + 173.0 Temp <sup>2</sup> *VH - 3530 Temp*VH <sup>2</sup>	99.94
TFM-BA	Response = -4557289 - 363151 SV + 43088 W - 413352 t + 89585 Temp + 2972593 VH + 257447 SV <sup>2</sup> + 19453 t <sup>2</sup> - 148.5 Temp <sup>2</sup> + 1065439 VH <sup>2</sup> + 1473 SV*W + 114242 SV*t - 8304 SV*Temp - 1228531 SV*VH + 428 W*t + 141.7 W*Temp - 17252 W*VH - 1239 t*Temp + 47685 t*VH - 63888 Temp*VH + 5831 SV*Temp*VH - 484.8 t*Temp*VH + 249.9 Temp <sup>2</sup> *VH - 4941 Temp*VH <sup>2</sup>	99.99
Bis-TFM-BA	Response = -2602706 - 207399 SV + 24608 W - 236069 t + 51163 Temp + 1697674 VH + 147030 SV <sup>2</sup> + 11110 t <sup>2</sup> - 84.8 Temp <sup>2</sup> + 608482 VH <sup>2</sup> + 841 SV*W + 65245 SV*t - 4743 SV*Temp - 701625 SV*VH + 244 W*t + 80.9 W*Temp - 9853 W*VH - 707 t*Temp + 27233 t*VH - 36487 Temp*VH + 3330 SV*Temp*VH - 276.9 t*Temp*VH + 142.70 Temp <sup>2</sup> *VH - 2822 Temp*VH <sup>2</sup>	99.99

Where SV = sample volume, W = weight of MOF, t = reaction time, VH = volume of hexane, T = temperature

**Table S3: Side products of the reaction with their confirmation probability in NIST library search.**

S.No.	Compound name	% Confirmation probability
1	1,1,3 trimethoxy propane	45.73
2	2,3,4, tri-FBA methyl phenyl ester	9.10
3	2,3,4 tri-FBA difluoro phenyl ester	6.25
4	2-fluorobenzohydrazide	20.87
5	Methyl styrene	14.67
6	Acetophenone	15.46
7	Benzene, (1-methoxy-1-methylethyl)	53.38
8	Benzoic acid 2-fluoro ethyl ester	34.41

**Table S4: GC-MS results of the five repeated cycles**

No of cycles	% RC -1	% RC -2
1	149.26	149.85
2	148.58	148.65
3	148.65	150.79
4	148.61	148.15
5	147.19	148.51

**A**

**B**

**C**

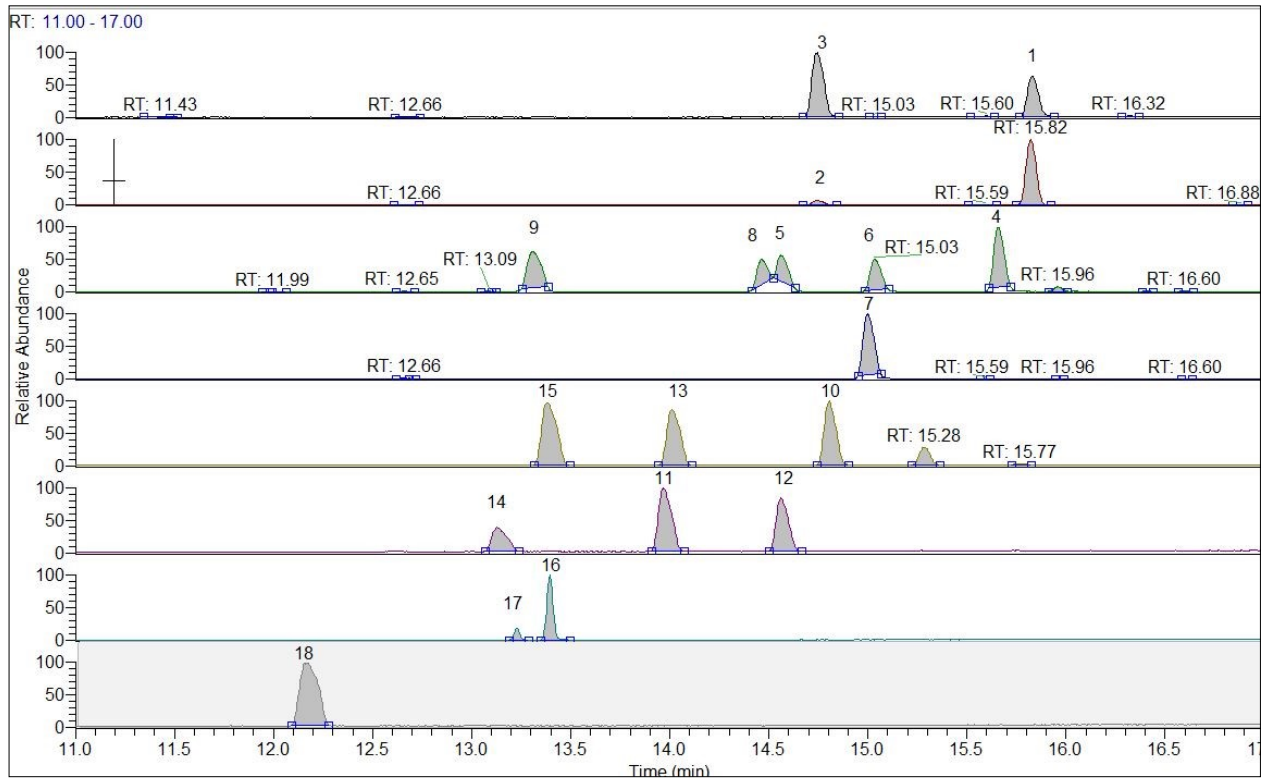
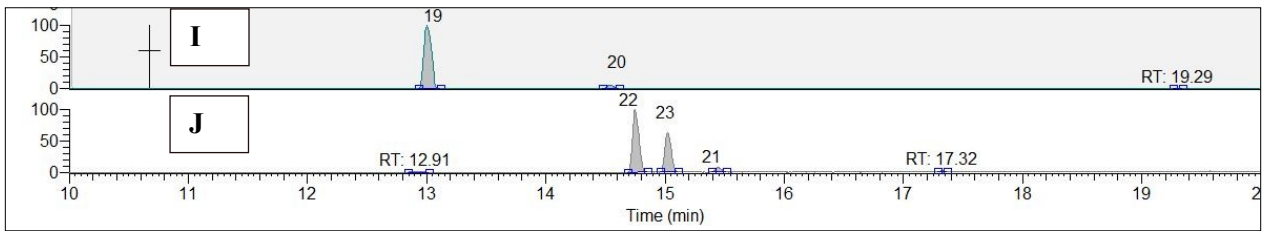
**D**

**E**

**F**

**G**

**H**



*Figure S1 - Chromatogram of (A) 2-FBA + 4-FBA, (B) 3-FBA, (C) Di-FBA mix without 2,6-DFBA, (D) 2,6 DFBA, (E) Mixture of 2,3,4 + 2,4,5 + 3,4,5 TFBA, (F) Mixture of 2,3,5 + 2,3,6 + 2,4,6 TFBA, (G) Mixture of Tetra-FBA, (H) Penta-FBA, (I) Mixture of Bis-FBAs, (J) Mixture of TFM-FBAs at their SIM ions (Peak numbering is done according to Table S1)*