

Supporting Information

Renewable Aromatic Hydrocarbons from Waste Cooking Oil over Hierarchical Imidazole Supported Zeolites

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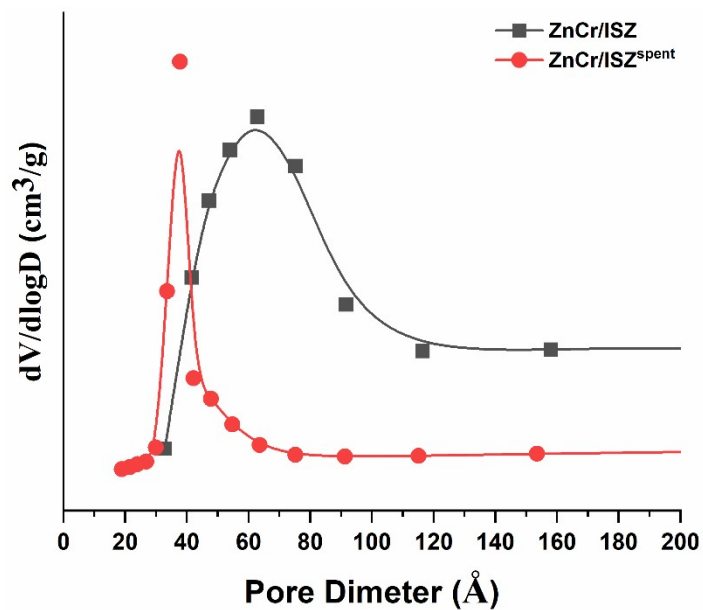


Figure S1. Pore diameter of fresh and spent ZnCr/ISZ catalyst.

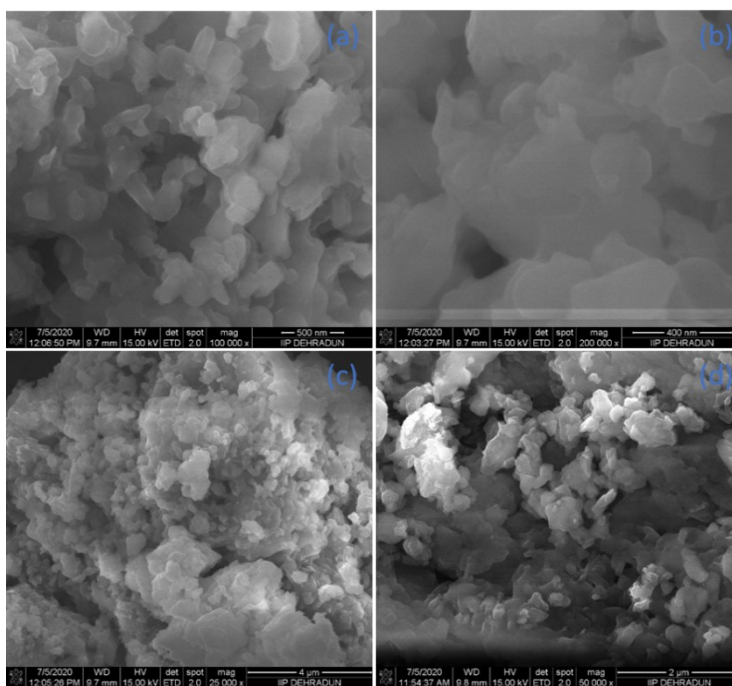
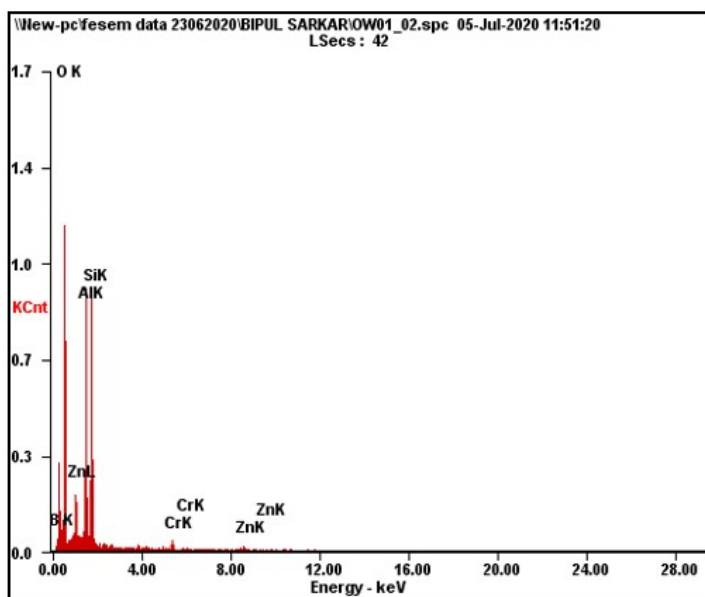
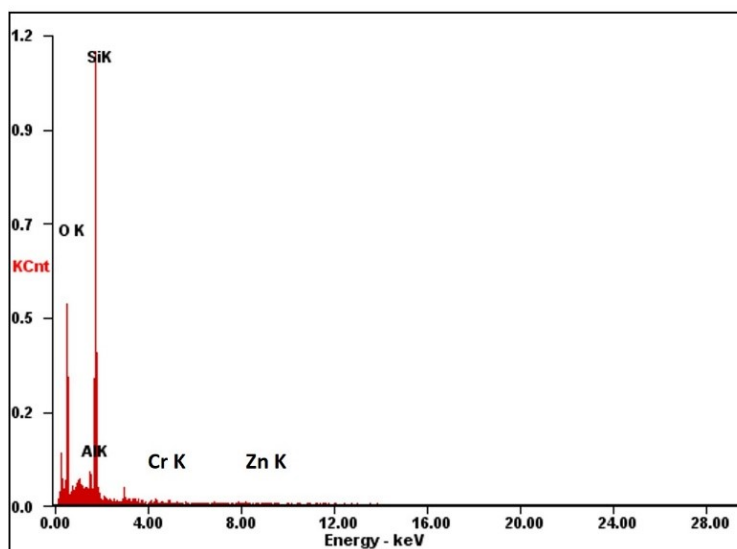


Figure S2: SEM images of (a,b)fresh and (c,d) spent ZnCr/ISZ catalyst



Element	Wt %	At %
Si K	40.36	35.89
AlK	07.69	04.06
ZnK	07.71	03.90
CrK	00.87	00.24
OK	01.05	00.23

Figure S3: EDX spectrum of ZnCr/ISZ catalyst



Element	Wt %	At %
Si K	40.36	34.17
AlK	07.69	04.08
ZnK	06.5	03.7
CrK	00.75	00.23
OK	01.00	00.21

Figure S4. EDX spectrum of spent ZnCr/ISZ catalyst

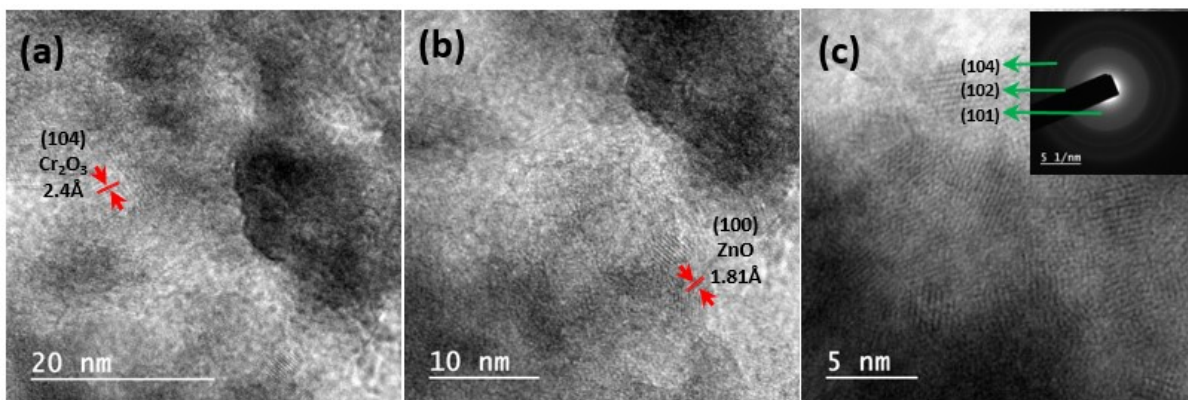


Figure S5: TEM image reduced ZnCr/ISZ catalyst

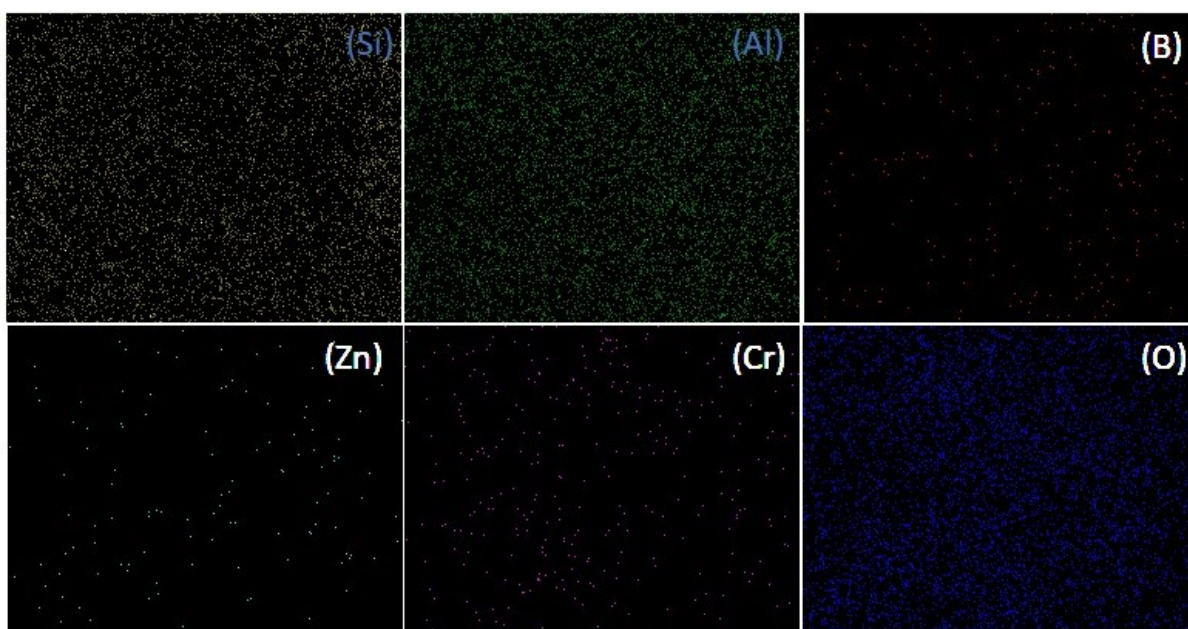


Figure S6: TEM image reduced ZnCr/ISZ catalyst

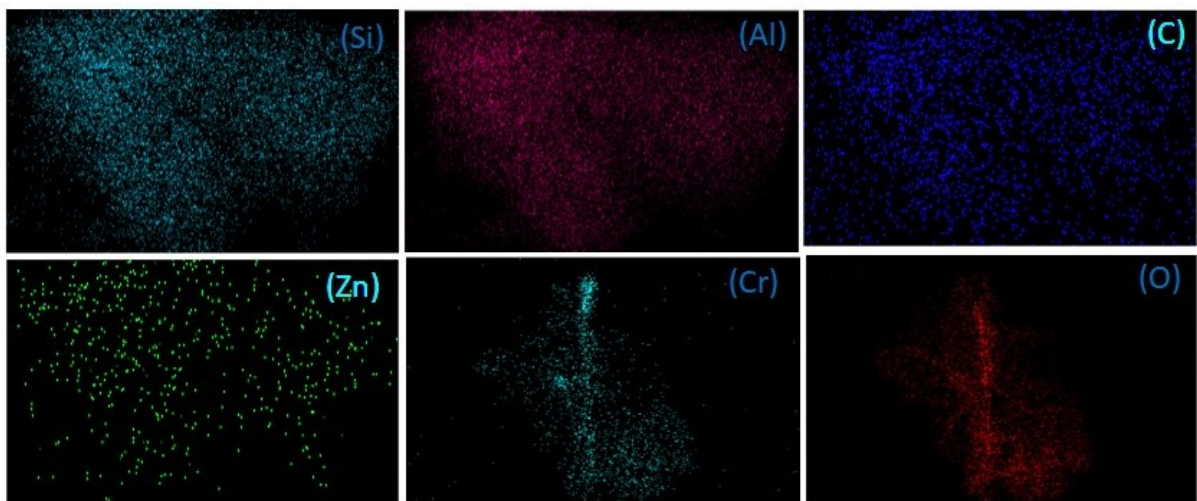


Figure S7. Elemental mapping of spent ZnCr/ISZ catalyst

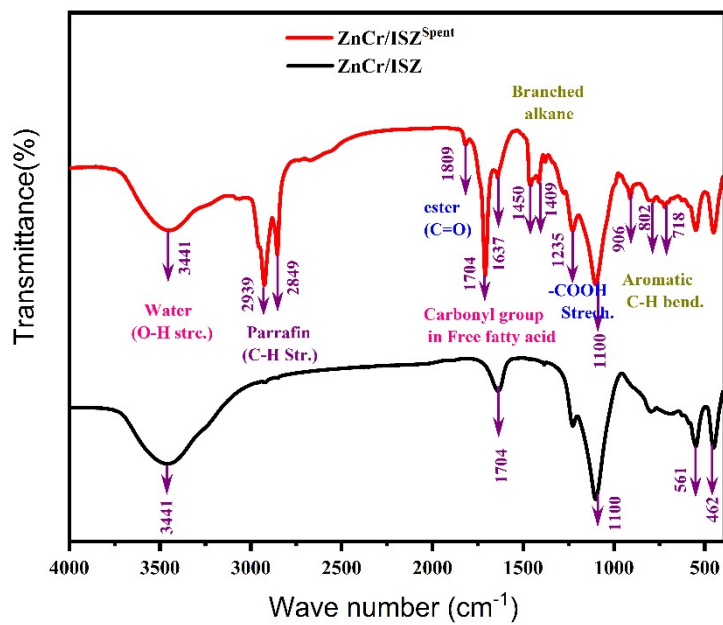


Figure S8. FTIR spectra of fresh and spent ZnCr/ISZ catalyst

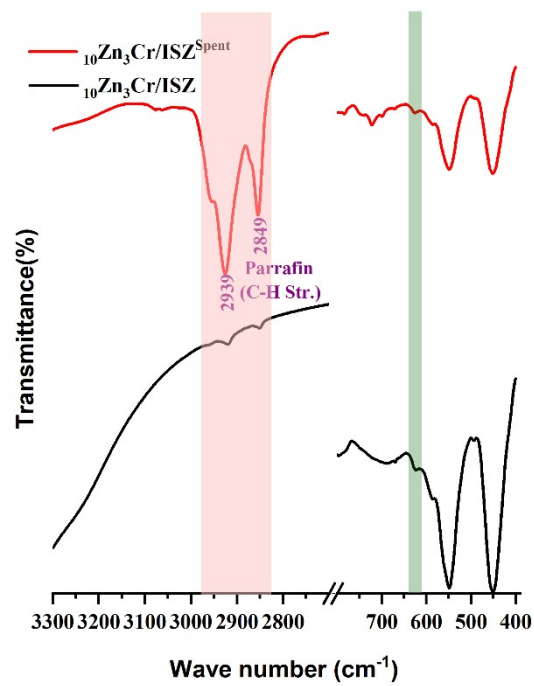


Figure S9. FT-IR of fresh and spent ZnCr/ISZ catalyst

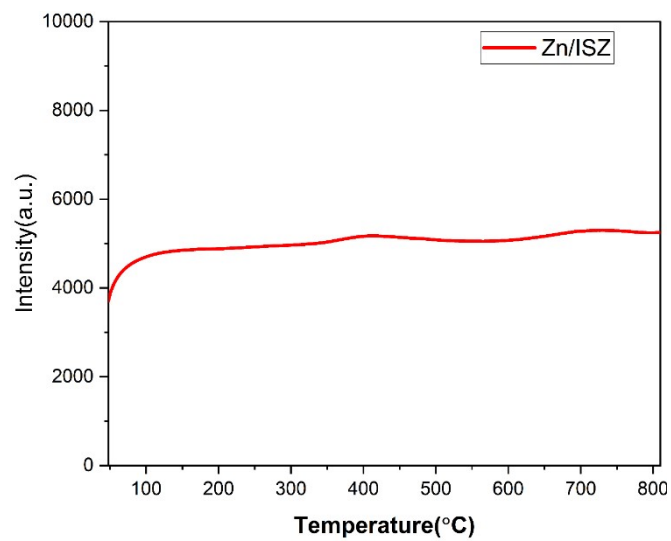


Figure S10. TPR profile of Zn/ISZ catalyst.

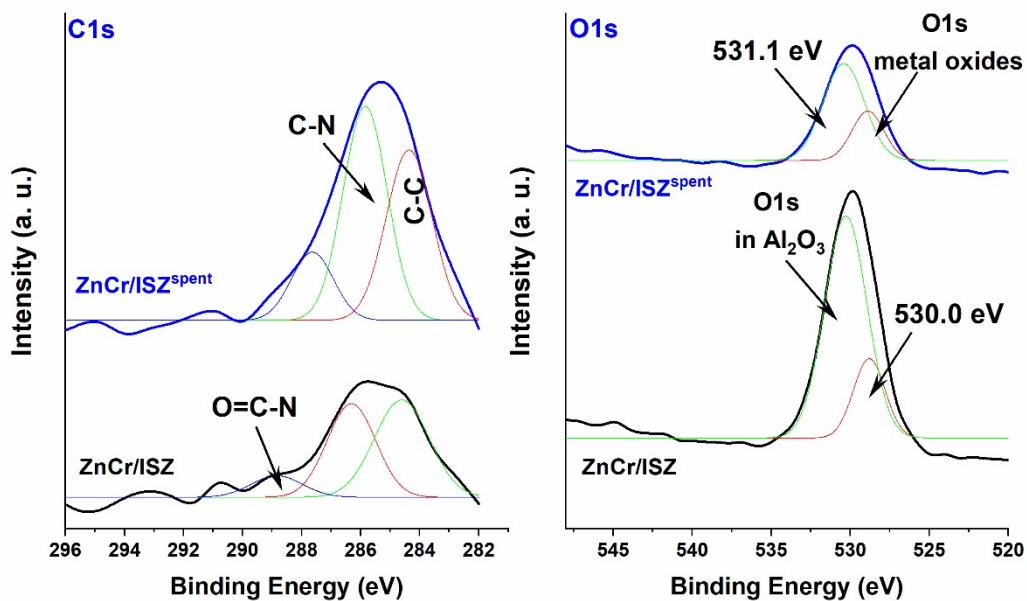


Figure S11. XP spectra of C1s and O1s of fresh and spent ZnCr/ISZ catalyst

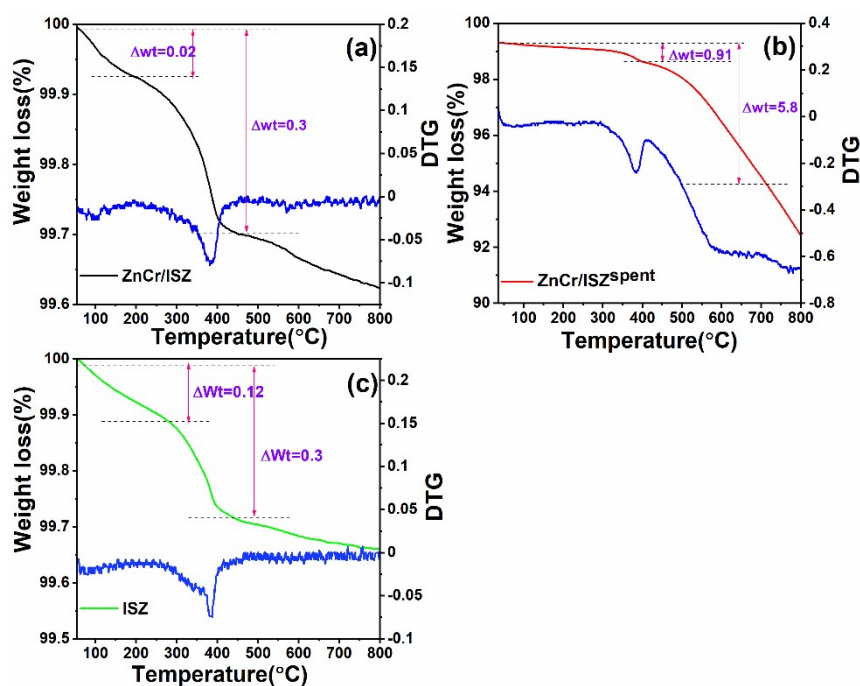


Figure S12. Thermogravimetric analysis (TGA) data of (a) fresh, (b) spent ZnCr/ISZ catalyst and (c) pure ISZ support. Note: spent catalyst was recovered after 4h time-on-stream.

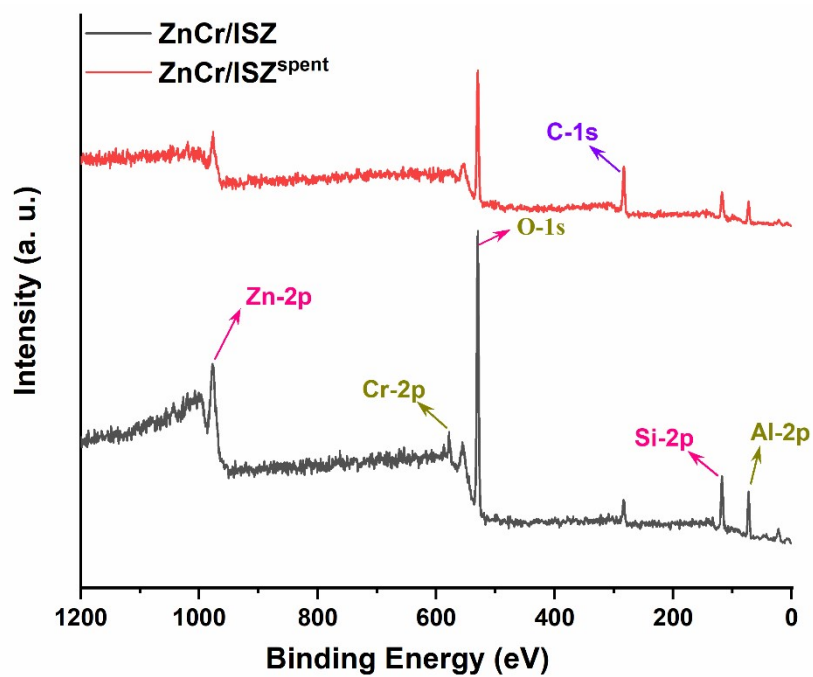


Figure S13. Survey scan of fresh and spent ZnCr/ISZ catalyst

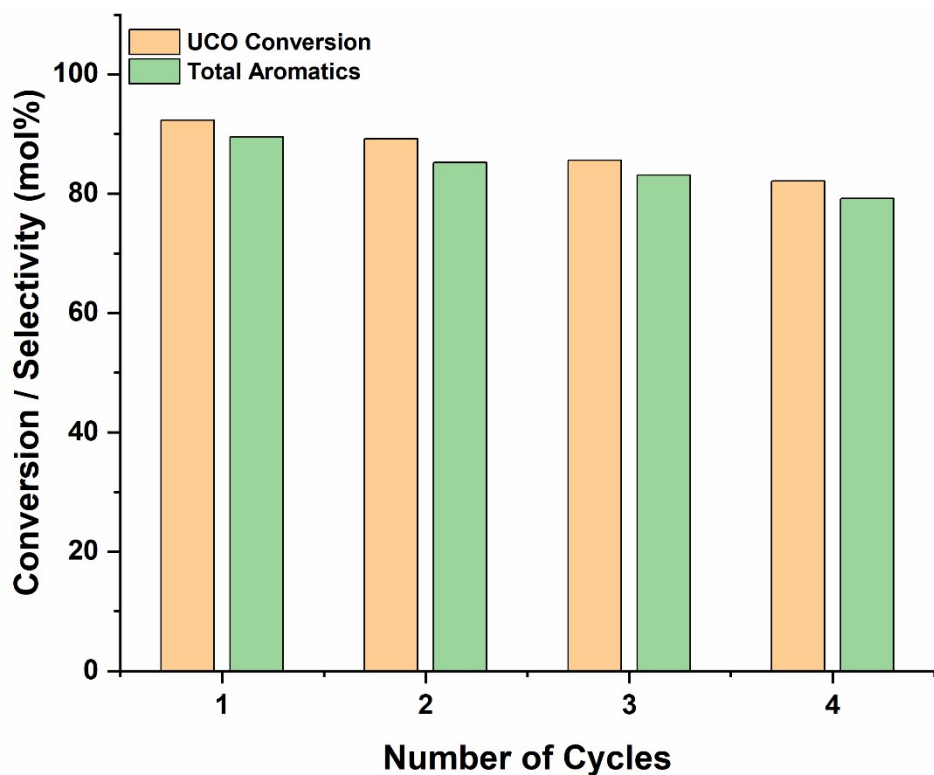


Figure S14. Recyclability of ZnCr/ISZ (imidazole supported zeolite) after several cycle.

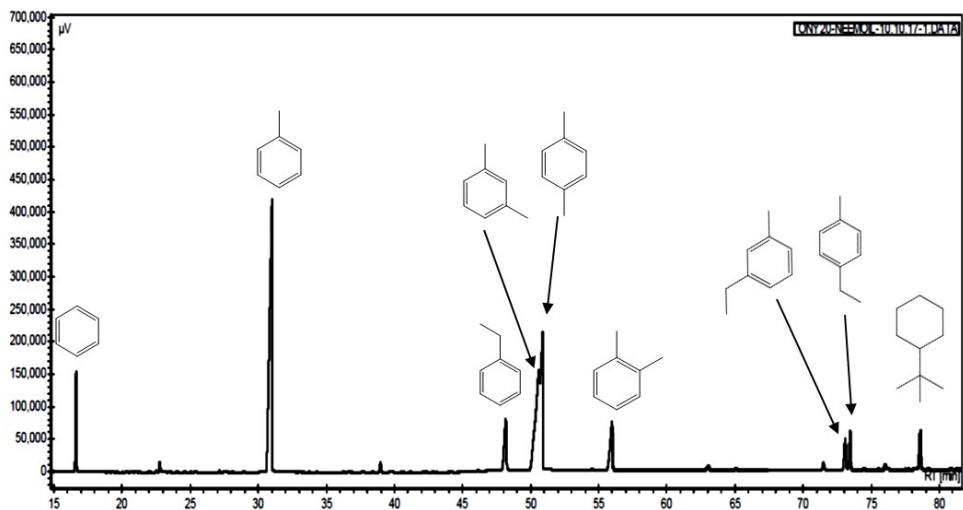


Figure S15. GC- DHA chromatogram of liquid product (as per ASTM D6730), indentation has been done using the relative RT.

Mass balance

WCO Conversion = (weight of converted WCO)/ (weight of the WCO reactant) × 100%

Yield of liquid products = (C atoms in liquid products/C atoms in the starting reactant) × 100%

Weight of WCO reactant(g)=5.46

Weight of liquid product formed(g) =4.89

Total Liquid Yield= (4.89/5.4) *100= 90.5%

Weight of gas product formed=0.1265

Total gases yield= (0.1265/5.46) *100= 2.31%

Weight of solid (carbon deposit on catalyst) =0.0049

$$\text{Carbon Balance (in wt \%)} = \frac{\text{Wt. of liquid} + \text{Gas} + \text{Solid}}{\text{Wt of UCO}} \times 100\% = \frac{5.0214}{5.46} \times 100\% = 92 \pm 3\%$$

Carbon deposition rate= (Carbon deposition/ Catalyst amount*Reaction time) = (0.0049/1*4)
=0.0012=1.20*10⁻³

Table S1: Brønsted and Lewis acidic strength of different imidazole supported zeolite catalyst

Catalyst	Brønsted acidic strength (mmol/g)	Lewis acidic strength (mmol/g) ^b	B/L	Total acidity (B+L) (mmol/g)
ISZ	0.36	0.12	3.0	0.48
20Zn/Z	0.28	0.14	2.0	0.42
20Zn3Cr/Z	0.26	0.22	1.08	0.46
20Zn3Cr2B/Z	0.25	0.29	0.86	0.54
20Zn3Cr2Al/Z	0.27	0.23	1.17	0.50
20Zn3Cr2S/Z	0.24	0.28	0.85	0.52
20Zn3Cr2P/Z	0.26	0.25	1.04	0.51
20Zn3Cr/Z ^a	0.29	0.14	2.07	0.43

Brønsted and Lewis acidic site can be calculated using Py-Ir, ^a spent catalyst: recovered after 4 hr time on stream, ^b Standard deviation for acidity ± 0.5

Table S2. XPS peak fitting data for Zn, Al, Cr and Si (Calculated by using Origin software)**Zn-2p**

Metal	Peak	Peak Position	Peak Area	% Fitting
Fresh Catalyst				
Zn (fitted)	2p3/2	1019.5945	2910.0049	96.63 %
	2p1/2	1042.5989	1455.51973	
	Cumulative	-	4365.52463	
Zn Raw	2p3/2	1019.57256	2946.71447	
	2p1/2	1042.64566	1570.74468	
	Cumulative	-	4517.45915	
Spent Catalyst				
Zn (fitted)	2p3/2	1019.28512	5397.22324	99.42%
	2p1/2	1042.28386	2675.92126	
	Cumulative	-	8073.1445	
Zn Raw	2p3/2	1019.27508	5510.90957	
	2p1/2	1042.36089	2608.66946	
	Cumulative	-	8119.57903	

Al-2p

Metal	Peak	Peak Position	Peak Area	% Fitting
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Fresh Catalyst				
Al (fitted)	Peak 1	75.62312	15955.84004	97.16 %
	Peak 2	74.48118	13242.16732	
	Cumulative	-	29168.00736	
Al Raw	Raw	-	30,018.3463	
Spent Catalyst				
Al (fitted)	Peak 1	75.77273	13964.51059	99.09%
	Peak 2	74.55898	15584.44958	
	Cumulative	-	29,548.96017	
Al Raw	Raw data	-	29,819.80916	

Cr-2p

Metal	Peak	Peak Position	Peak Area	% Fitting
Fresh Catalyst				
Cr-2p	Peak 1	575.80361	337.02512	99.07%
	Peak 2	585.50407	168.6196	
	Peak 3	578.05476	265.42322	
	Peak 4	587.74517	124.01506	
	Peak 5	582.80445	174.34465	
	Cumulative	-	1069.42765	
Cr-2p (Raw)	Raw data	-	1079.44794	
Spent Catalyst				
Cr-2p	Peak 1	575.8802	368.80394	99.61%
	Peak 2	585.58485	182.72314	
	Peak 3	578.24806	232.09816	
	Peak 4	587.94773	115.02482	
	Peak 5	582.80635	173.65441	
	Cumulative	-	1072.30447	
Cr-2p (Raw)	Raw data	-	1076.50028	

Si-2p

Metal	Peak	Peak Position	Peak Area	% Fitting
Fresh Catalyst				
Si-2p	Peak 1	101.85179	3223.13608	98.33%
	Peak 2	102.57831	1136.02628	
	Cumulative	-	4359.16236	
Si-2p (Raw)	Raw data	-	4433.09267	
Spent Catalyst				
Si-2p	Peak 1	101.54266	1915.32251	95.42%
	Peak 2	102.41532	2318.04999	
	Cumulative	-	4233.3725	
Si-2p (Raw)	Raw data	-	4436.23349	

Table S3. Detail hydrocarbon analysis (GC-DHA) data of the liquid product, as per ASTM D6730

Carbon No	Saturates		Unsaturated			Aromatics	Oxyg unknown	Total
	Cyclic	Iso	Normal	Cyclic	N + Iso			
4		0.01			0.10			0.11
5		0.13	0.07	0.02	0.25			0.47
6		0.28	0.18	0.21	0.09	15.3		16.06
7	0.02	0.05	0.48		0.25	35.6		36.4
8		0.04	0.57			29.1		29.71
9	0.5	0.7				4.3		5.5
10	1.3	0.12	0.09			3.0		4.51
11		0.47	0.09			1.2	0.36	2.21
12	0.03	0.08	0.4			1.0	0.59	2.1
13			0.11				0.69	0.80
14			0.50				0.50	1.0
15			0.08				0.70	0.78
16							0.35	0.35
17								
18+								
Total	1.85	1.88	2.66	0.23	0.69	89.5	3.19	100

Table S4. Compositions of the gaseous product as per ASTM D7833 (GC-RGA) over ZnCr/ISZ catalyst.

Sr. No.	Product name	Carbon No.	Product (in %)	Total product formed (in mg)
1	Hydrogen	H ₂	8.9	0.0018
2	Carbon dioxide	C ₁	3.1	0.0092
3	Carbon monoxide	C ₁	2.6	0.014
4	Methane	C ₁	4.7	0.023
5	Ethane	C ₂	1.18	0.0061
6	Ethylene	C ₂	11.57	0.0307
7	Propylene	C ₃	22.96	0.0256
8	Iso Butane	C ₄	2.38	0.0532
9	n butane	C ₄	2.04	0.0012
10	Iso-Butene	C ₄	0.75	0.0056
11	2-Pentene	C ₅	1.82	0.0023
12	2-Methyl-2-Butene	C ₅	1.39	0.0009

Table S5. Products distribution from aromatisation of waste cooking oil over a different loading of Zn and Co supported ISZ zeolite catalyst

S/N	Catalyst	Total Conversion (%)	Total aromatics (%)	Total (C6-C8) (%)	Product selectivity						
					Benzen e	Toluen e	o-xylen e	m-xylen e	p-xylen e	total xylene	Ethyl-benzen e
1	Zn ₅ /ISZ	82.3	85.3	51.7	7.1	26.2	2.5	7.0	7.1	16.6	1.8
2	Zn ₁₀ /ISZ	85.1	84.0	57	8.2	28.4	3.2	7.6	7.6	18.4	2.0
3	Zn ₂₀ /ISZ	89.0	91.0	62.6	9.0	30.7	3.8	8.2	8.5	20.5	2.4
4	Zn ₂₀ Cr ₁ /ISZ	89.6	84.6	58.7	10.3	28.9	2.4	7.5	8.0	17.9	1.6
5	Zn ₂₀ Cr ₂ /ISZ	90.3	87.3	61.6	10.9	30.1	2.8	7.9	7.9	18.6	2.0
6	Zn ₂₀ Cr ₃ /ISZ	92.3	89.5	65.9	12.0	32.3	3.2	9.5	7.1	19.8	1.8

Reaction conditions: catalyst wt-1 g (pelletized); reaction temp.-430°C; LHSV-1.5 h-1; GHSV-1200 h-1; time-after 4h. * relative standard deviation (RSD) is ±5%

Table S6. Table for aromatics distribution over time-on-stream

Time	Aromatics (Total)	Mono aromatics	Mono (Branched)	Di- aromatics	Poly- aromatics	Benzene	Toluene	Xylenes			Ethyl benzene
								o	m	p	
4	89.5	65.9	9.2	8.3	6.1	12	32.3	3.2	9.5	7.1	1.8
8	87.2	55	10.3	12.2	9.7	7.2	25.3	3.2	9.2	8	2.1
12	81.5	45.8	12.0	13.5	10.2	5.1	22.3	3	7.4	6.2	1.8
16	74.2	39.8	6.5	15.1	12.8	4.8	19.2	3	6.2	5.1	1.5
20	71.2	37.6	3.6	15.9	14.1	4.2	18.5	2.8	5.8	4.8	1.5

Table S7. Recent Literature survey on waste cooking oil into valuable chemicals

Feed	Catalysts	Temperature (°C)	Reactor and reaction condition	Aromatic selectivity/ yield (%)	Stability	Ref
Nonedible Oils	Zn/HZSM-5	515°C	Catalytic fixed bed	58.56%	3-4 hour	1, 2
Waste cooking oil	HZSM-5 with (CoO, NiO, CaO)	350-550°C	Microwave-assisted catalytic pyrolysis	702.20 mg/ml	-	3, 4
Waste cooking oil	HZSM-5	450°C	Microwave pyrolysis	-	60 min	4, 5
Lignin and waste cooking oil	ZSM-5	500 °C	pyro probe reactor	82.6%	30-60 min	6, 7
Non-edible oil cake's	Al/SBA-15	400 °C,	Hydrothermal reactor at high pressure -25 bar (H ₂)	19.5%	-	8, 9
Rubber seed oil	ZSM-5	550 °C	Fixed bed reactor	78.6%	15 min	10
Camelina (sativa) seed oil	Zn, Na/ZSM-5	500°C	Fixed bed reactor	6.2 %	60 min	11
Used cooking oil (UCO)	Zn,Cr supported Imidazole catalyst	400-550°C	fixed bed continuous flow reactor	89.5%	4 h	Our work

We have compared the catalyst performance with the other catalyst reported in the literature. All the literature reports microwave-assisted pyrolysis of WCO or used WCO along with bio-oil, lignin, plastic etc., for microwave/catalytic fast co-pyrolysis. As an industrial intervention, microwave-assisted pyrolysis of WCO faces challenges related to heating uniformity, energy efficiency, and capital costs and thus requires further research. The use of co-pyrolysis is complex and in a very nascent research stage; therefore needs more time to mature. Thus, the direct conversion of WCO to aromatics is advantageous; in terms of C₆-C₈ selectivity, it shows the best transformation ever reported from WCO.

Table S8. Py-probe data of ¹²C Methyl oleate with catalyst

Ret. time	Area (%)	Compound
1.905	0.06	CH ₃ C(O)O(CH ₂) ₃ CH=CH ₂
2.179	0.12	Formic acid, hexyl ester
2.262	0.21	2-Hexene
2.337	0.18	2-Propenoic acid, methyl ester
2.55	0.16	1,3-Cyclohexadiene
2.644	0.08	Cyclopentene, 3-methyl-
2.747	0.28	Benzene
3.03	0.24	Cyclopentane, 1,2-dimethyl-
3.13	0.48	Heptane
3.319	0.08	Methyl 3-butenolate
3.434	0.06	Methyl 11-(2-cyclopenten-1-yl)undecanoate
3.709	0.24	3-Methylenecyclohexene
3.794	0.04	Bicyclo[4.1.0]hept-2-ene
3.909	0.13	Cyclopentane, ethylidene-
4.109	1.03	Toluene
4.21	0.03	Cyclopentane, 1,3-bis(methylene)-
4.462	0.2	Cyclopropane, pentyl-
4.63	0.83	Hexanal
4.683	0.03	1,3,5-Cycloheptatriene
4.754	0.06	4-Pentenoic acid, methyl ester
4.847	0.04	Silicone caulk
5.007	0.06	Methyl valerate
5.04	0.05	1,3-Octadiene
5.347	0.06	1,3-Cyclohexadiene, 5,6-dimethyl-
5.403	0.06	1-Propylcyclopentene
5.518	0.04	1-Ethyl-2-trifluoroacetoxycyclohexane
5.678	0.41	Ethylbenzene
5.892	0.93	p-Xylene
6.155	0.12	2-Heptanone
6.21	0.25	Cyclopropane, 1-methyl-2-pentyl-
6.256	0.13	Cyclohexanone
6.313	0.08	3-Nonene, (E)-

6.384	0.29	Heptanal
6.424	0.07	2-Cyclopenten-1-one, 2-methyl-
6.453	0.07	2-Nonene, (E)-
6.539	0.13	5-Hexenoic acid, methyl ester
6.764	0.2	Hexanoic acid, methyl ester
6.805	0.07	1,3-Nonadiene, (E)-
6.91	0.03	2-Cyclohexen-1-one
7.191	0.05	Cyclopentene, 1-butyl-
7.315	0.16	Benzene, propyl-
7.354	0.05	2-Heptenal, (Z)-
7.451	0.07	3-Oxatricyclo[3.2.2.0(2,4)]nonane
7.511	0.32	Benzene, 1-ethyl-4-methyl-
7.697	0.03	1-Octen-3-one
7.771	0.06	1,1,3,3,5,5,7,7-Octamethyl-7-(2-methylpropoxy)tetrasiloxan-1-ol
7.803	0.06	Phenol
7.961	0.18	1-Decene
8.037	0.22	Mesitylene
8.162	0.22	Octanal
8.349	0.37	6-Heptenoic acid, methyl ester
8.51	0.38	Heptanoic acid, methyl ester
8.549	0.03	5-Decyne
8.674	0.03	(E)-4-Oxohex-2-enal
8.749	0.15	Indane
8.907	0.09	1H-Indene, 1-chloro-2,3-dihydro-
8.992	0.03	Benzoic acid, cyclohexylmethyl ester
9.084	0.43	Cyclohexane, 1,3-butadienylidene-
9.22	0.03	Ethyl (Z)-non-3-enyl carbonate
9.398	0.06	3-Cyclopentylpropionic acid, 2-methylphenyl ester
9.518	0.03	Acetic acid, 2,4,4-trimethylpentyl ester
9.555	0.03	Bicyclo[2.2.2]octane, 2-methyl-
9.634	0.16	E-11,13-Tetradecadien-1-ol
9.676	0.06	4-Nonenal, (E)-
9.719	0.16	5-Undecene, (E)-
9.858	0.29	Nonanal
9.983	0.22	3-Octenoic acid, methyl ester, (Z)-

10.178	0.92	Octanoic acid, methyl ester
10.209	0.13	Cycloundecene(E)
10.285	0.04	7-Tetradecen-1-ol, (Z)-, TMS derivative
10.377	0.04	2,5-Dimethylphenyl methyl carbinol
10.479	0.03	1H-Indene, 2,3-dihydro-5-methyl-
10.518	0.05	5-Undecene, 3-methyl-, (E)-
10.552	0.03	p-Toluic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester
10.649	0.07	1H-Indene, 3-methyl-
10.734	0.31	2-Decyn-1-ol
10.825	0.04	Cyclooctylidene-(2-phenylaziridin-1-yl)amine
11.096	0.03	(3E,5Z)-1,3,5-Undecatriene
11.201	0.24	1-Dodecene
11.274	0.06	4-Undecene, (E)-
11.415	0.1	Decanal
11.529	0.19	8-Nonenoic acid, methyl ester
11.659	0.18	Nonanoic acid, methyl ester
11.715	0.25	4-Dodecen-1-ol
11.875	0.06	2-Ethyl-2,3-dihydro-1H-indene
11.984	0.05	4-Oxononanal
12.036	0.03	11-Tridecyn-1-ol
12.088	0.04	5,7-Dodecadiene, (E,E)-
12.27	0.4	2-Decenal, (E)-
12.324	0.09	13,16-Octadecadiynoic acid, methyl ester
12.375	0.13	6-Nonynoic acid, methyl ester
12.753	0.16	Formic acid, 10-chlorodecyl ester
12.851	0.1	Naphthalene, 1-methyl-
13.1	0.15	10-Hydroxydecanoic acid, methyl ester
13.178	0.25	Decanoic acid, methyl ester
13.256	0.05	Methyl 8-oxooctanoate
13.69	0.14	2-Undecenal
13.74	0.11	2-Undecenal
13.855	0.15	2-Undecenal
14.545	0.29	Nonanoic acid, 9-oxo-, methyl ester
14.57	0.23	Nonanoic acid, 9-oxo-, methyl ester
14.652	0.7	Nonanoic acid, 9-oxo-, methyl ester

14.748	0.58	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester
15.715	0.99	Dodecanoic acid, methyl ester
15.74	0.38	Dodecanoic acid, methyl ester
15.796	0.54	Dodecanoic acid, methyl ester
15.829	1.42	Dodecanoic acid, methyl ester
16.42	0.08	7-Hexadecenoic acid, methyl ester, (Z)-
16.517	0.28	9-Hexadecenoic acid, methyl ester, (Z)-
16.655	0.03	7-Hexadecenoic acid, methyl ester, (Z)-
16.854	0.04	Tridecanoic acid, methyl ester
16.9	0.03	12-Tridecynoic acid, methyl ester
17.005	0.04	Dodecanoic acid, 10-methyl-, methyl ester
17.595	0.23	Tridecanoic acid, 12-methyl-, methyl ester
17.715	0.42	Methyl 12-oxo-9-dodecenoate
17.745	0.1	9-Octadecenoic acid (Z)-, methyl ester
17.891	0.98	Methyl myristoleate
18.133	3.35	Methyl tetradecanoate
18.173	0.72	Methyl tetradecanoate
18.225	0.9	Tridecanoic acid, 12-methyl-, methyl ester
18.246	0.54	Methyl tetradecanoate
18.3	2.27	Methyl tetradecanoate
18.587	0.12	Tridecanoic acid, 4,8,12-trimethyl-, methyl ester
18.62	0.06	Tridecanoic acid, 4,8,12-trimethyl-, methyl ester
18.835	1.51	Pentadecanoic acid, methyl ester
18.865	0.27	Tridecanoic acid, 12-methyl-, methyl ester
18.9	0.38	Pentadecanoic acid, methyl ester
18.921	0.27	Tetradecanoic acid, 12-methyl-, methyl ester
18.945	1.19	Tridecanoic acid, 12-methyl-, methyl ester
19.092	2.18	Pentadecanoic acid, methyl ester
19.325	0.89	Pentadecanoic acid, methyl ester
19.986	2.62	9-Hexadecenoic acid, methyl ester, (Z)-
20.295	5.8	Hexadecanoic acid, methyl ester
20.357	1.52	Hexadecanoic acid, methyl ester
20.414	0.6	Tridecanoic acid, methyl ester

20.435	3.28	Z-11-Tetradecen-1-ol difluoroacetate
20.625	1.59	Hexadecanoic acid, methyl ester
20.793	0.2	Hexadecanoic acid, 14-methyl-, methyl ester
20.955	0.89	Cyclopropaneoctanoic acid, 2-hexyl-, methyl ester
21.026	0.68	Cyclopropaneoctanoic acid, 2-hexyl-, methyl ester
21.063	0.27	Pentacosanoic acid, methyl ester
21.1	0.36	11-Hexadecenoic acid, 15-methyl-, methyl ester
21.159	0.63	10-Undecenoic acid, methyl ester
21.195	0.22	Methyl 18-methylcosanoate
21.242	0.44	cis-10-Heptadecenoic acid, methyl ester
21.27	0.26	cis-10-Heptadecenoic acid
21.314	0.53	1,19-Eicosadiene
21.366	0.31	Hexadecanoic acid, 14-methyl-, methyl ester
21.405	1.35	Hexadecanoic acid, 14-methyl-, methyl ester
22.245	6.37	9-Octadecenoic acid, methyl ester, (E)-
22.34	1.77	9-Octadecenoic acid (Z)-, methyl ester
22.491	2.97	9-Octadecenoic acid, methyl ester, (E)-
22.57	1.8	9-Octadecenoic acid, methyl ester, (E)-
22.797	5.47	9-Octadecenoic acid, methyl ester, (E)-
22.851	1.39	9-Octadecenoic acid, methyl ester, (E)-
22.884	1.01	6-Octadecenoic acid, methyl ester, (Z)-
22.91	0.75	9-Octadecenoic acid, methyl ester, (E)-
22.95	1.23	9-Octadecenoic acid, methyl ester, (E)-
23.047	4.17	9-Octadecenoic acid, methyl ester, (E)-
23.124	0.33	Methyl 9-cis,11-trans-octadecadienoate
23.17	0.61	1-Tetradecanol
23.208	1.18	1-Tetradecanol
23.293	0.44	Methyl 9-cis,11-trans-octadecadienoate
23.348	0.52	Methyl hexadec-9-enoate
23.426	0.03	Nonadecanoic acid, methyl ester
23.529	0.06	8,11,14-Eicosatrienoic acid, (Z,Z,Z)-
23.636	0.17	9-Octadecynoic acid, methyl ester
23.685	0.09	Butanoic acid, 4-(2-hydroxycyclohexyl)-, methyl ester
23.846	1.26	Oxiraneoctanoic acid, 3-octyl-, methyl ester, cis-
23.994	1.56	Cyclopropaneoctanoic acid, 2-hexyl-, methyl ester

24.053	0.44	Methyl 7-oxopentadecanoate
24.133	0.38	Methyl 18-methylnonadecanoate
24.245	0.03	1,2-Cyclohexanedicarboxylic acid, heptyl 4-methoxyphenyl ester
24.369	0.76	Cyclohexane, [6-cyclopentyl-3-(3-cyclopentylpropyl)hexyl]-
24.439	0.06	Pentanoic acid, 2-methyl-, anhydride
24.522	0.14	(1R,2R,3S,5R)-(-)-2,3-Pinandediol
24.605	0.04	9-Octadecenoic acid, methyl ester, (E)-
24.687	0.05	Octadecanoic acid, 9,10-dihydroxy-, methyl ester
24.871	0.14	Heptadeca-7,10-dione
24.988	0.3	Cedrol
25.095	0.04	1-Ethyltricyclo[5.2.1.1(2,6)]undec-8-en-11-ol
25.434	1.58	Cyclopropaneoctanoic acid, 2-octyl-, methyl ester
25.547	0.1	Docosanoic acid, methyl ester
25.735	0.03	trans-9-Octadecenoic acid, pentyl ester
25.774	0.03	11-Dodecen-1-ol difluoroacetate
26.032	0.03	Butyl 9,12-octadecadienoate
26.112	0.09	cis-11-Eicosenoic acid, methyl ester
26.279	0.03	Tricosanoic acid, methyl ester
26.46	0.04	Decyl oleate
26.517	0.05	Methyl 18-methylcosanoate
26.595	0.08	Benzene, 1-iodo-3-(trifluoromethyl)-
26.628	0.08	Oxalic acid, 2-ethylhexyl octadecyl ester
26.719	0.08	Oleic diethanolamide
26.781	0.07	(4aS,5S,8aS)-5-Isopentyl-1,1,4a-trimethyl-6-methylenedecahydronaphthalene
26.804	0.08	Triacontane
26.861	0.19	15-Tetracosenoic acid, methyl ester, (Z)-
27.023	0.03	Tetracosanoic acid, methyl ester
27.174	0.03	9-Octadecenoic acid (Z)-, hexadecyl ester
27.205	0.03	Methyl 18-methylcosanoate
27.275	0.03	2H-3,9a-Ethanocyclopent[b]oxocin-2-one, octahydro-5,5,7,11-tetramethyl-, (3S,6aS,7R,9aS,11R)-
27.3	0.04	Hexadecanoic acid, decyl ester
27.418	0.06	9-Octadecenamide, (Z)-
27.643	0.11	Squalene

28.103	0.03	Lubricant (grease)
28.216	0.11	Hexacosane, 1-iodo-
28.541	0.11	9-Octadecenoic acid (Z)-, octadecyl ester
28.598	0.04	Tetracontane-1,40-diol
28.628	0.04	13-Docosen-1-ol, (Z)-
28.741	0.05	Oleic anhydride
28.875	0.04	Triacontane, 1-bromo-
29.168	0.03	11-Hexacosyne
29.407	0.15	Docosanedioic acid, dimethyl ester
29.459	0.03	Nonacosan-14-one
29.559	0.06	Triacontane
29.883	0.03	Vitamin E
29.929	0.06	Cholesterol
30.049	0.03	Hexadecanoic acid, tetradecyl ester
30.216	0.05	1-Decanol, 2-hexyl-
30.308	0.05	Cholest-4-en-6-one
30.995	0.03	Cholest-4-en-3-one
31.044	0.08	16-Hentriacontanone
31.163	0.05	Dotriacontane
31.268	0.04	Cholest-7-en-3-ol, 14-methyl-, (3.beta.)-
31.382	0.03	E,E,Z-1,3,12-Nonadecatriene-5,14-diol
31.61	0.17	.gamma.-Sitosterol
31.794	0.12	1-Decanol, 2-hexyl-
32.145	0.05	Olean-12-ene
33.175	0.09	Nonacosan-14-one
33.312	0.03	Dotriacontane
33.726	0.03	Oleyl oleate
33.92	0.08	9-Hexadecenoic acid, eicosyl ester, (Z)-
34.184	0.06	Hexadecanoic acid, octadecyl ester

Table S9. Pyro-probe data of ¹²C methyl linoleate with catalyst

Ret time	Area, %	Compound name
1.883	0.4	2-Methyl-1-butene
2.188	0.23	1-Pentene, 2-methyl
2.276	0.63	2-Hexene
2.344	0.38	Allyl isocyanate
2.557	0.39	1,4-Cyclohexadiene
2.653	0.22	Cyclopentene, 4-methyl-
2.749	0.91	Benzene
3.03	0.15	1-Heptene
3.174	0.48	Cyclopropane, trimethylmethylene-
3.314	0.05	3-Ethylheptanoic acid
3.44	0.05	Cyclopentane, ethylidene-
3.7	0.23	3-Methylenecyclohexene
3.909	0.16	Cyclopentane, ethylidene-
4.093	2.15	Toluene
4.452	0.1	Cyclopropane, pentyl-
4.607	0.19	1-Heptanol, 2-propyl-
4.752	0.07	Cyclohexene, 3-ethyl-
5.303	0.11	2,4-Dimethyl-1-heptene
5.669	0.82	Benzene, 1,1'-[oxybis(methylene)]bis-
5.868	1.87	p-Xylene
6.202	0.26	Resin (Styrene, 2-EHA)
6.407	0.06	Spiro[4.4]nonan-1-one
6.45	0.06	4-Nonene
6.984	0.05	1-Undecene, 8-methyl-
7.309	0.32	Benzeneethanol, .alpha.-(phenylmethyl)-
7.414	0.23	Octane, 2,2,6-trimethyl-
7.5	0.69	m-Ethylaniline
7.952	0.08	1-Decene
8.02	0.3	2,6-Xylidine
8.11	0.12	m-Toluic acid, 3-phenylpropyl ester
8.318	0.19	E-10-Dodecen-1-ol propionate
8.484	0.06	1-Pentanol, 2-ethyl-4-methyl-

8.73	0.1	1H-Indole, 2,3-dihydro-
8.893	0.11	1H-Indene, 1-chloro-2,3-dihydro-
8.97	0.06	1,3-Benzodioxole, 3a,7a-dihydro-2,2,4-trimethyl-
9.069	0.4	Tricyclo[4.2.2.0(1,5)]dec-7-ene
9.627	0.16	5-Tetradecene, (E)-
9.697	0.05	Cyclohexane, 1,1-dimethyl-2-propyl-
9.83	0.09	Nonanal
9.955	0.1	E-10-Dodecen-1-ol propionate
10.168	0.12	Z-1,6-Undecadiene
10.531	0.09	4-(3-Pentyl)pyridine
10.623	0.09	1H-Indene, 1-methyl-
10.71	0.22	Diazodiamantane
11.18	0.25	2-Decanone
11.507	0.06	E-10-Dodecen-1-ol propionate
11.635	0.06	Nonanoic acid, methyl ester
11.695	0.13	6-Dodecyne
12.233	0.13	Bicyclo[3.3.1]nonan-3-ol, 7-methylene-
12.837	0.09	Naphthalene, 2-methyl-
13.691	0.07	3,7-Dimethylenebicyclo[3.3.1]nonane
14.761	0.09	1,5-Cyclododecadiene, (E,E)-
14.878	0.05	Cyclopentene, 1-octyl-
15.059	0.08	Bicyclo[3.3.1]nonan-3-ol, 7-methylene-
15.509	0.05	7,9-Di-tertbutyl-1-oxaspiro[4,5]deca-6,9-dien-8-one
16.017	0.11	9,12-Tetradecadien-1-ol, (Z,E)-
16.134	0.1	1,16-Hexadecanediol
16.298	0.05	4-Octylaniline
16.351	0.24	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, [1S-(1.alpha.,3.beta.,5.alpha.)]-
17.576	0.3	Bicyclo[3.3.1]nonan-3-ol, 7-methylene-
18.522	0.06	3-Eicosyne
19.815	0.06	.alpha.-Phellandrene, dimer
19.949	0.11	cis-13-Eicosenoic acid
20.91	0.15	cis-10-Heptadecenoic acid, methyl ester
20.955	0.3	cis-10-Heptadecenoic acid, methyl ester
21.05	0.17	cis-10-Nonadecenoic acid

21.15	0.37	cis-10-Heptadecenoic acid, methyl ester
22.454	44.32	Oxacyclohexadecan-2-one
22.521	5.51	Cyclopropaneundecanal, 2-nonyl-
22.722	18	Oleyl alcohol, trifluoroacetate
22.762	6.5	Tetradecanenitrile
22.832	2.55	Oleic Acid
22.904	0.37	Methyl 9-cis,11-trans-octadecadienoate
22.93	0.34	1-Dodecanol, 2-octyl-, acetate
22.99	0.88	Linoleic acid ethyl ester
23.046	0.34	18-Nonadecenoic acid
23.08	0.12	Tetrapentacontane, 1,54-dibromo-
23.201	0.07	10-Undecenoic acid, 2-methoxy-, methyl ester
23.546	0.25	4H-1,3-Benzodioxin-4-one, 2-(1,1-dimethylethyl)hexahydro-5-methyl-4a-(2-propenyl)-, [2s-(2.alpha.,4a.alpha.,5.beta.,8a.beta.)]-
23.587	0.19	Oxiraneoctanoic acid, 3-octyl-, methyl ester, cis-
23.627	0.14	Vinyl caprylate
23.698	0.24	Oxiraneoctanoic acid, 3-octyl-, methyl ester
23.759	0.89	2-Furanoctanoic acid, 5-hexyltetrahydro-, methyl ester
23.913	0.2	9-Hydroxypentadecanoic acid, methyl ester
24.162	0.66	Dodecane, 1,12-di(2-nitro-3-ethoxyphenoxy)-
24.274	0.1	Fumaric acid, 2-octyl tridec-2-yn-1-yl ester
24.371	0.07	Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy-
24.577	0.05	Octadecanoic acid, 9,10-dihydroxy-, methyl ester
24.756	0.09	Heptadeca-7,10-dione
24.88	0.2	Epicedrol
25.183	0.05	Octadecanoic acid, 9,10-dihydroxy-, methyl ester
25.314	1.07	13-Docosenoic acid, methyl ester, (Z)-
27.376	0.06	9-Octadecenamide, (Z)-
31.578	0.06	(3S,8S,9S,10R,13R,14S,17R)-17-((2R,5R)-5-Ethyl-6-methylheptan-2-yl)-3-methoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,1

Table S10. Pyro-probe data of ¹²C methyl palmitate with catalyst

Ret time	Area, %	Compound name
1.883	0.95	Propane, 1,2-dimethoxy-
2.19	0.13	Propanedioic acid, propyl-
2.274	0.76	Ethane, 1,2-diethoxy-
2.552	0.31	2-(1-Methylcyclopentyloxy)-tetrahydropyran
2.649	0.11	2-Propanamine, N,N-dimethyl-
2.743	0.78	Benzene
3.127	0.1	1,3-Bis(hydroxymethyl)urea
3.695	0.22	8-Nonyn-1-ol tetrahydropyran-2-yl ether
4.077	2.28	Mepivacaine
4.597	0.24	1,3-Bis(hydroxymethyl)urea
4.838	0.13	Cyclotrisiloxane, hexamethyl-
5.659	0.6	Piperidine, 1-ethyl-
5.843	2.63	2,3-Dihydro-6-hydroxy-3-oxo-2-(piperidinomethyl)pyridazine
6.197	0.13	2-(5-Amino-[1,3,4]thiadiazol-2-ylsulfanyl)-1-pyrrolidin-1-yl-ethanone
6.343	0.09	1-Nitro-2-propanol
7.301	0.17	3-Piperidino-1,2-propanediol
7.486	0.82	Ribitol, 1,3:4,5-di-O-(ethylboranediyl)-2-deoxy-
8.015	0.15	3,12-Dibora-2,4,11,13-tetraoxatricyclo[12.4.0.0(5,10)]octadecane, 3,12-diethyl-
8.101	0.16	Ethanol, 2,2'-[methylenebis(thio)]bis-
9.058	0.29	Ribitol, 1,3:4,5-di-O-(ethylboranediyl)-2-deoxy-
9.619	0.11	d-Galactose oxime
9.824	0.13	Nonanal
10.702	0.1	Boroxin, ethyldimethyl-
11.186	0.14	1-Methoxy-3-(trimethylsilyloxymethyl)nonane
12.763	0.21	dl-Threitol
12.83	0.1	6-Methoxynicotinic acid
14.023	0.23	Methoxyamine, TBDMS derivative
15.243	0.1	Methoxyamine, TBDMS derivative
15.415	0.09	dl-Threitol
15.465	0.09	Methoxyamine, TBDMS derivative

19.062	0.12	Propanoic acid, 2-(ethylthio)-, ethyl ester
20.255	50.02	Bis(dimethylamino)methylphosphine
20.365	6.55	Bis(dimethylamino)methylphosphine
20.45	1.73	Bis(dimethylamino)methylphosphine
20.49	2.24	O-Ethylhydroxylamine, TBDMS derivative
20.54	0.98	Bis(dimethylamino)methylphosphine
20.57	0.72	O-Ethylhydroxylamine, TBDMS derivative
20.605	0.78	O-Ethylhydroxylamine, TBDMS derivative
20.665	1.86	Bis(dimethylamino)methylphosphine
20.861	0.12	Bis(dimethylamino)methylphosphine
21.143	0.21	O-Ethylhydroxylamine, TBDMS derivative
21.898	18.84	cis-9-Octadecenoic acid, propyl ester
22.092	1.29	1-Methyl-1-(4-methylpentyl)oxy-1-silacyclobutane
22.252	0.18	9,12-Octadecadienoic acid (Z,Z)-, methyl ester
22.66	0.35	trans,trans-9,12-Octadecadienoic acid, propyl ester
23.406	0.09	Undec-10-ynoic acid, octadecyl ester
23.468	0.16	Methyl 2-hydroxydodecanoate
23.649	0.51	15-Tetracosenoic acid, methyl ester, (Z)-
24.084	0.35	2-Butyl-3-methyl-5-(2-methylprop-2-enyl)cyclohexanone
25.299	0.26	13-Docosenoic acid, methyl ester, (Z)-
26.53	0.13	1,1'-Biphenyl-3,4,4'-trimethoxy-6'-formyl-
29.896	0.16	Cholesterol

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