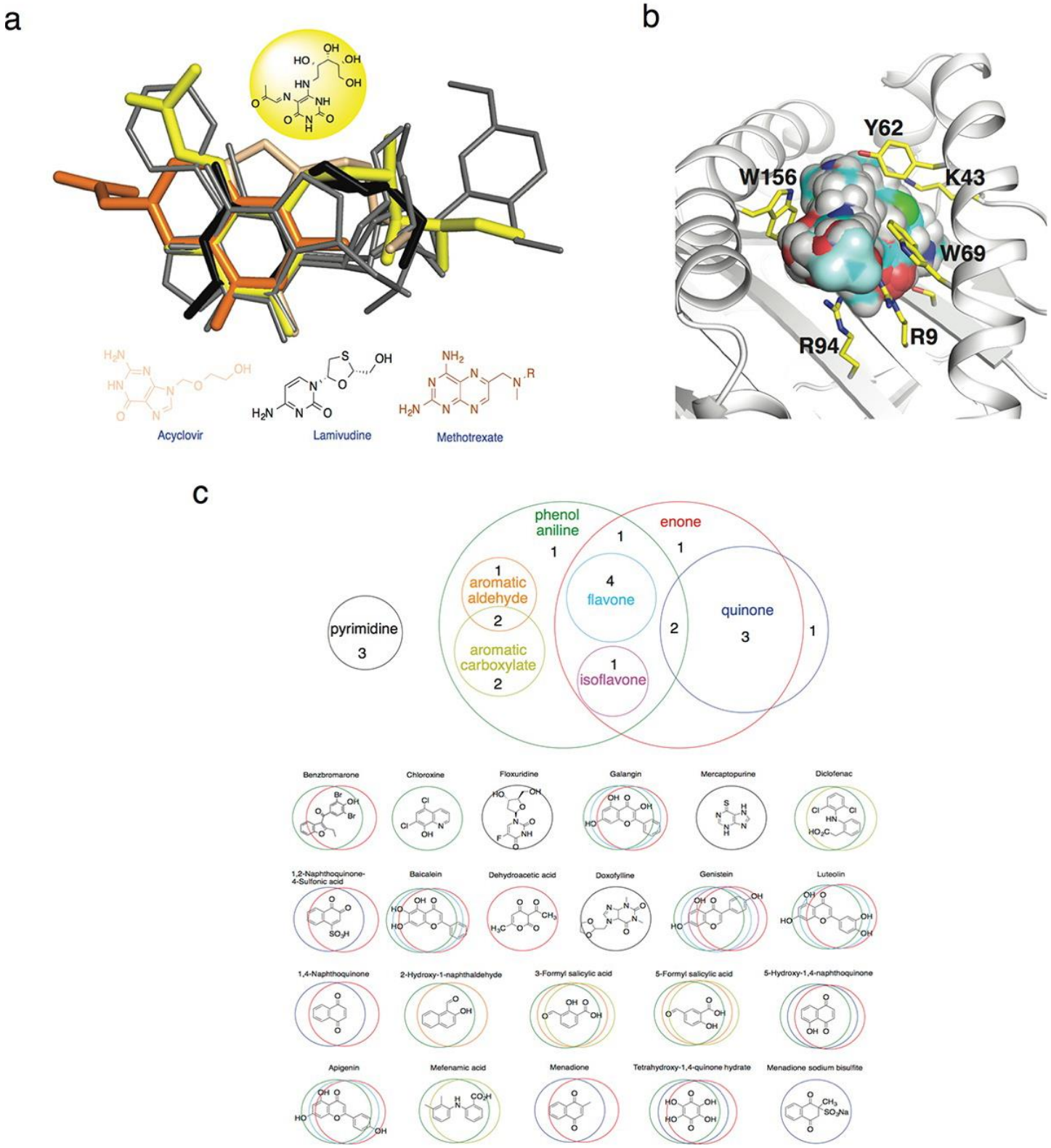
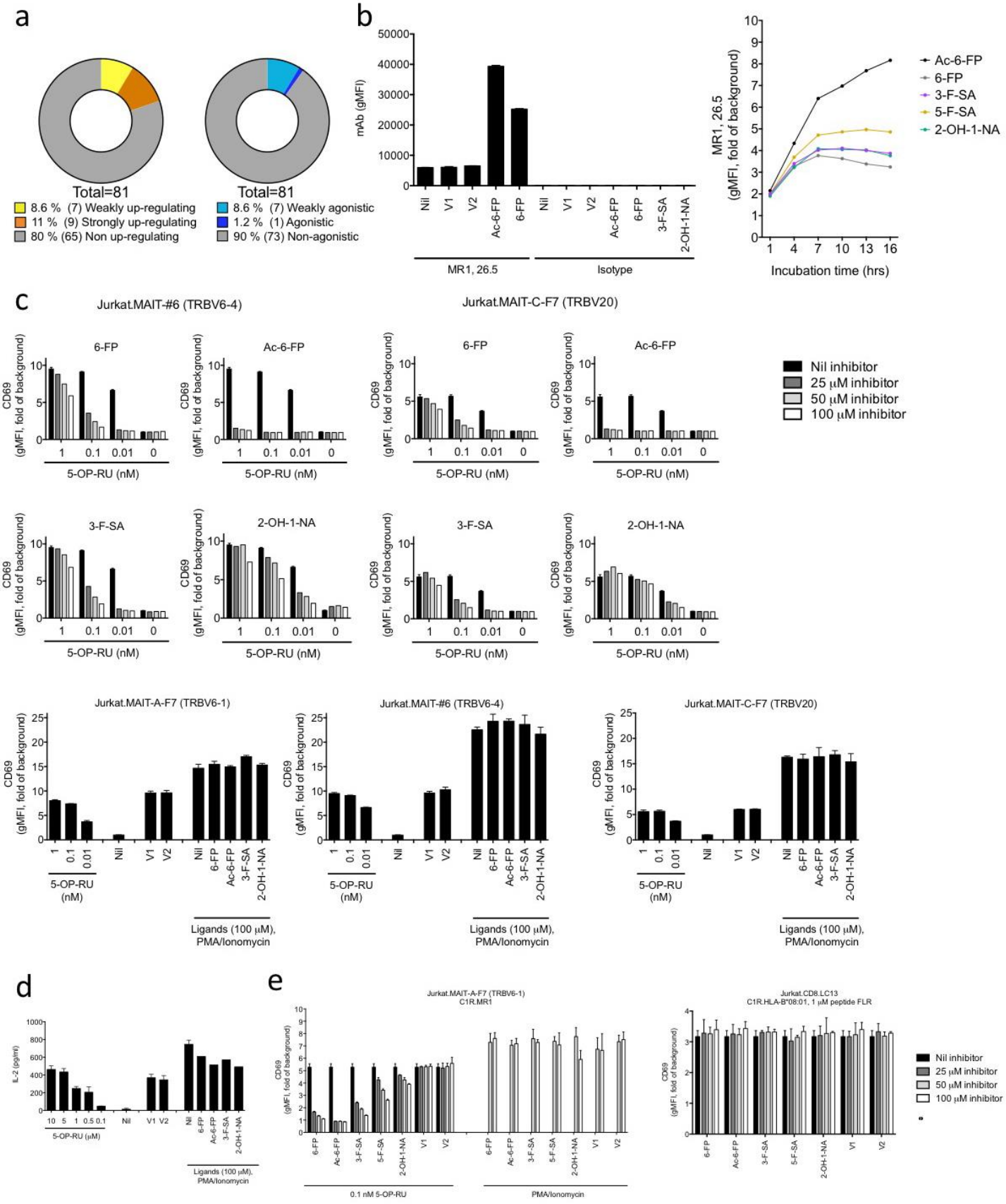


Supplementary Figure 1

***In silico* screening of MR1 ligands.**

a) Superimposition of 9 drugs (sticks) on 5-OP-RU. These drugs are consistent with the shape matching to 6-FP. Colored chemical structures of drugs (e.g. Acyclovir, Lamivudine, Methotrexate) correspond to colored sticks, with other drugs shown in grey. **b)** Side view of all 20 virtual screening drug hits (shown as surfaces) in complementarity with the MR1 binding site. Carbon (white); oxygen (red); nitrogen (blue); chlorine (green); fluorine (cyan). **c)** Classification of twenty-two representative structures of active compounds (including 9 drugs) according to their chemical substructures: pyrimidines (black), phenols/anilines (green), enones (red), aromatic aldehydes (orange), aromatic carboxylates (olive), quinones (dark blue), flavones (light blue), isoflavones (pink).



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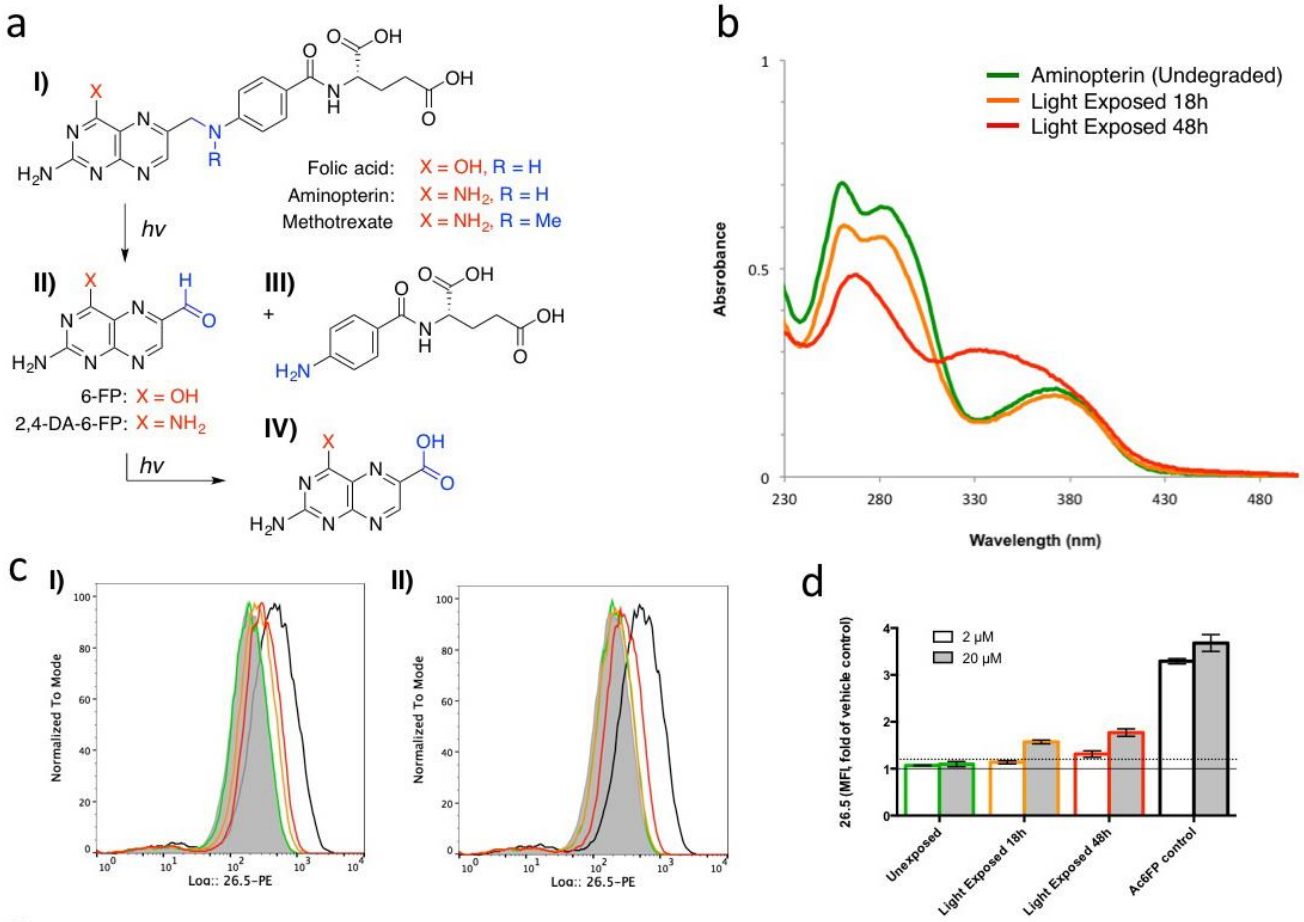
Supplementary Figure 2

Upregulation of MR1 expression and activation of MAIT cells.

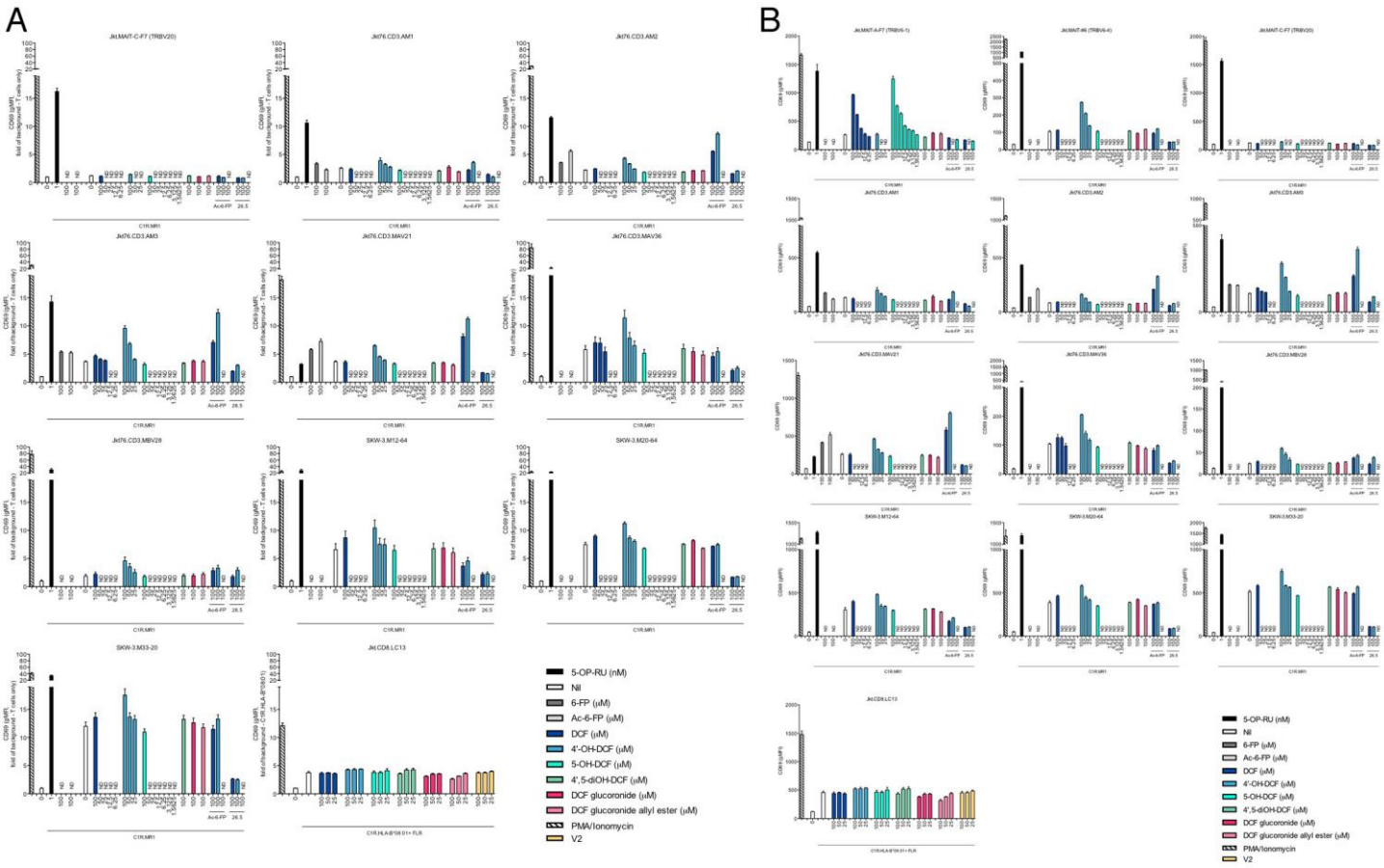
a) Graphical display of percentages MR1 upregulating versus agonistic compounds identified as part of the functional screen in Figure 2a. **b**) gMFI of 26.5 (mean of triplicate samples and SEM) and isotype control (single samples) staining at 7 hours for Nil, vehicle controls (V) and ligands (left panel). Repeat experiment of Figure 2c including 5-F-SA (right panel) showing single samples. **c**) First 2 rows: Drug/small molecule dose dependent inhibition of Jurkat.MAIT-#6 and Jurkat.MAIT-C-F7 activated by 5-OP-RU in the presence of C1R.MR1 cells and assayed by flow cytometric staining for CD69 as a marker of activation. Displayed is gMFI CD69 fold of background control for one representative of three experiments. 5-OP-RU activation with nil inhibitor/activator was assayed in triplicate displaying mean and SEM (error bars). Third row: gMFI of CD69 (mean of triplicate samples and SEM) for Nil (PBS), vehicle controls with maximum concentration of 5-OP-RU, and ligands co-incubated with PMA/Ionomycin are displayed for Jurkat.MAIT-A-F7, Jurkat.MAIT-#6 and Jurkat.MAIT-C-F7. **d**) IL-2 production in the presence of PBS, vehicle controls with maximum concentration of 5-OP-RU, and ligands co-incubated with PMA/Ionomycin. Displayed are mean of triplicate samples except for ligands co-incubated with PMA/Ionomycin where single samples are shown. **e**) Repeat experiment of Figure 2d/f including in addition gMFI of CD69 (mean of triplicate samples and SEM) for vehicle controls with maximum concentration of 5-OP-RU, ligands and ligands co-incubated with PMA/Ionomycin (left panel). In parallel the effect of ligands and vehicles on Jurkat.CD8.LC13 activation by C1R.HLA-B*08:01 in the presence of FLR peptide was tested (right panel).


a
I)
Folic acid: X = OH, R = H
Aminopterin: X = NH2, R = H
Methotrexate X = NH2, R = Me
hv
II)
III)
+
6-FP: X = OH
2,4-DA-6-FP: X = NH2
hv
IV)
b
Aminopterin (Undegraded)
Light Exposed 18h
Light Exposed 48h
Absrobance
Wavelength (nm)
c
I)
II)
Normalized To Mode
Log:: 26.5-PE
d
2 µM
20 µM
26.5 (MFI, fold of vehicle control)
Unexposed
Light Exposed 18h
Light Exposed 48h
Ac6FP control
e
MS extracted refolded sample
191.0677
C7 H7 O N6
% max intensity
180.1833
C4 H20 N8
181.7355
183.7807
185.9921
C8 O3 N3
188.0017
H4 O8 N4
190.1227
C12 H16 O N
192.0713
C2 H8 O3 N8
196.1307
C8 H20 O5
198.4812
200.6519
m/z
Theoretical 2,4-DA-6-FP isotopes
191.0676
C7 H7 O N6
192.0709
C2 H8 O3 N8
194.0752
C3 H10 O4 N6

Supplementary Figure 3

Degradation of 2,4-DA-6-FP.

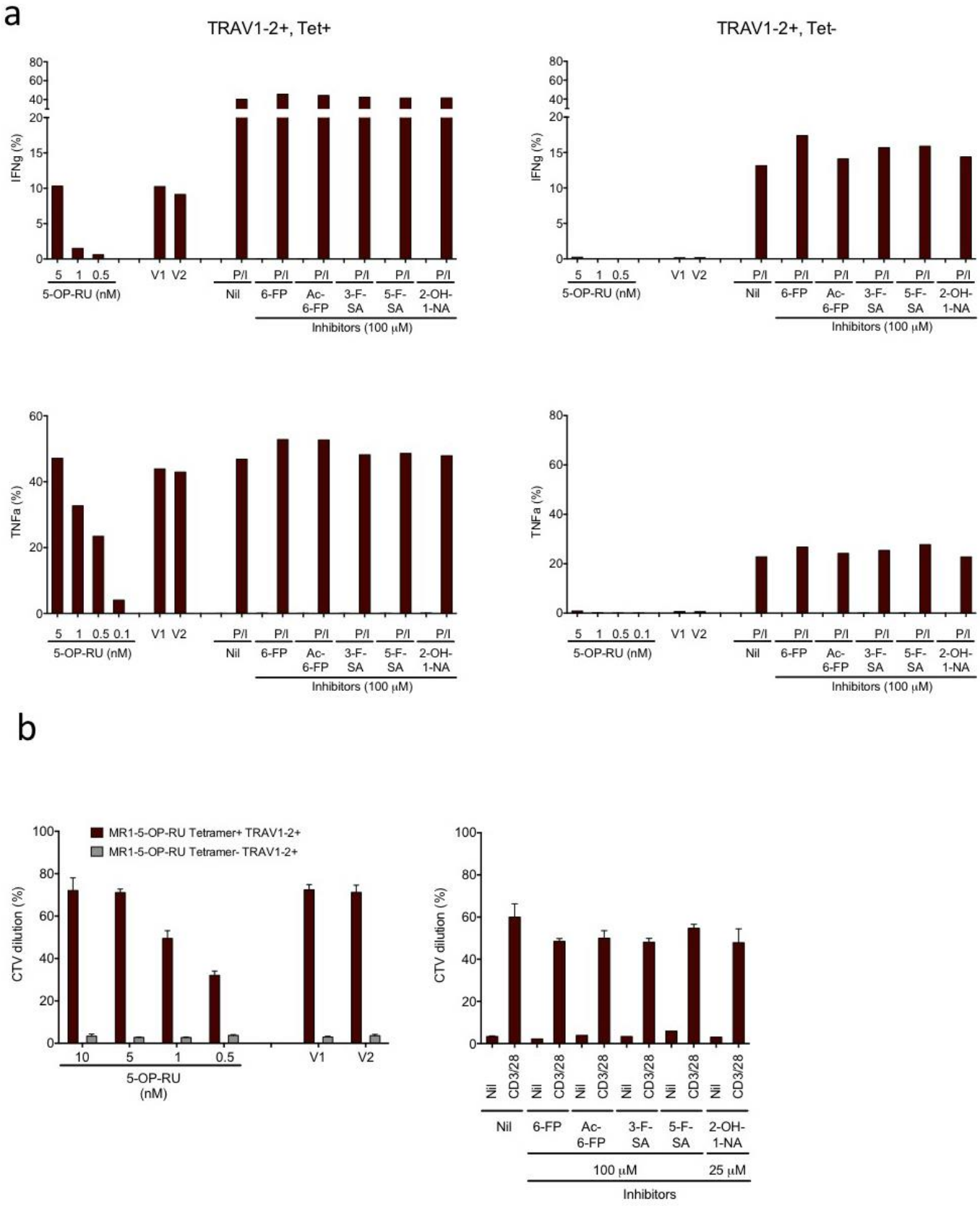
a) Chemical structures of aminopterin/folic acid (I) as they decompose to form respective formyl pterin (II) and aminobenzoylglutamic acid (III). The aldehyde on (II) then further degrades to carboxylic acid (IV). **b)** Absorbance spectra of aminopterin after exposure to a fluorescent lamp for 0h (green), 18h (orange) and 48h (red). **c&d)** MR1 surface upregulation by C1R.MR1 cells treated with 20μM or 2μM of photodegraded aminopterin from (**b**), shown as histogram of 26.5 (**c**) and as MFI 26.5-fold of PBS vehicle control (mean of triplicate samples with SEM). Representative of two separate experiments. **e)** Mass spectra and elemental analysis of compound extracted from MR1 refolded in the presence of photodegraded aminopterin compared with theoretical spectra for 2,4-DA-6-FP.



Supplementary Figure 4

Activation of MR1-restricted T cell lines by DCF and DCF metabolites.

Effect of Diclofenac and its metabolites on MR1 restricted T cell lines and Jurkat.CD8.LC13 activation by C1R.HLA-B*08:01 co-incubated with FLR peptide. Displayed are fold of background MFI CD69 (a) or MFI CD69 (b) for one representative of two experiments.



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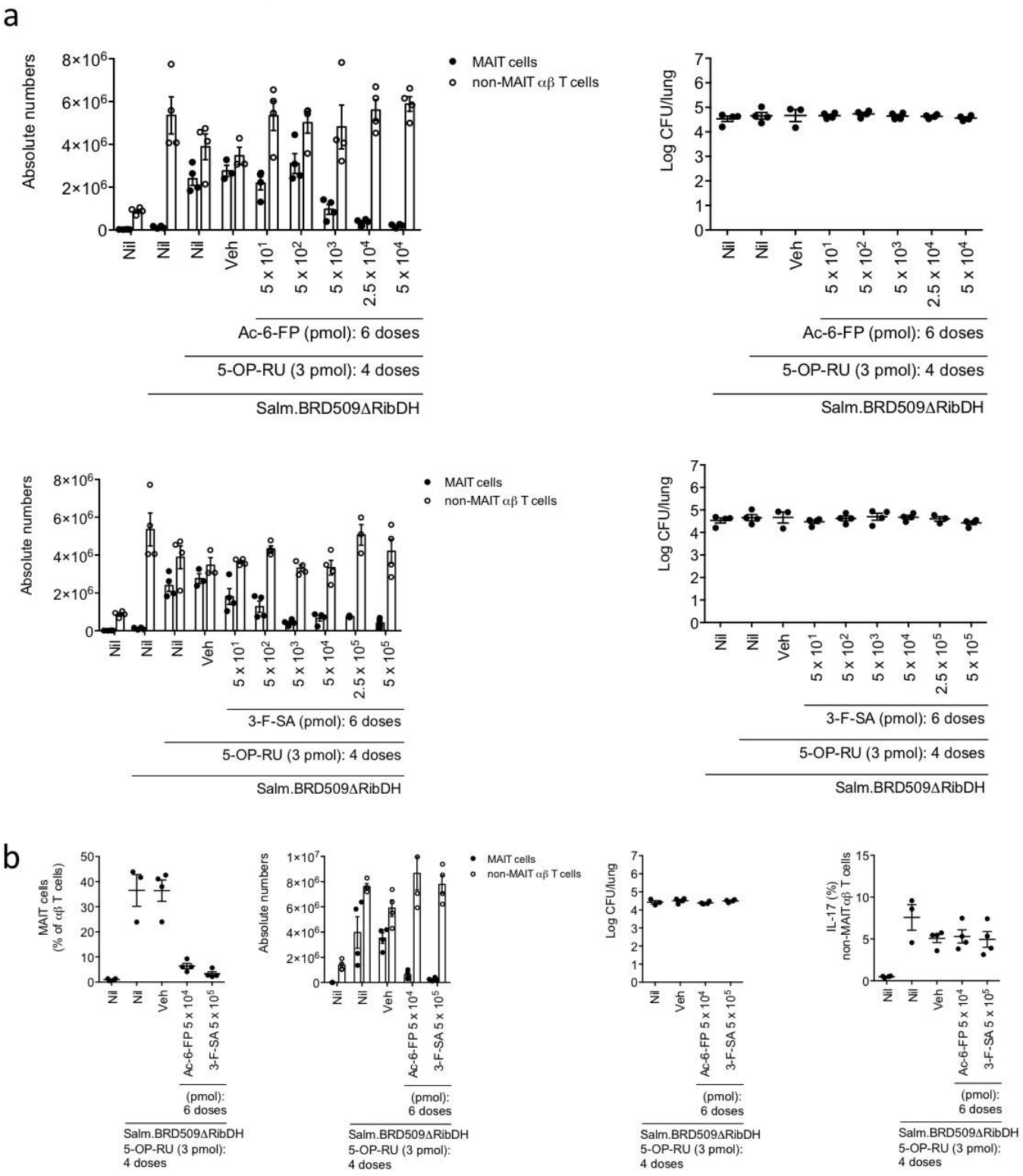
Supplementary Figure 5

Inhibition of the activation of MAIT cells by drugs and drug-related molecules *ex vivo*.

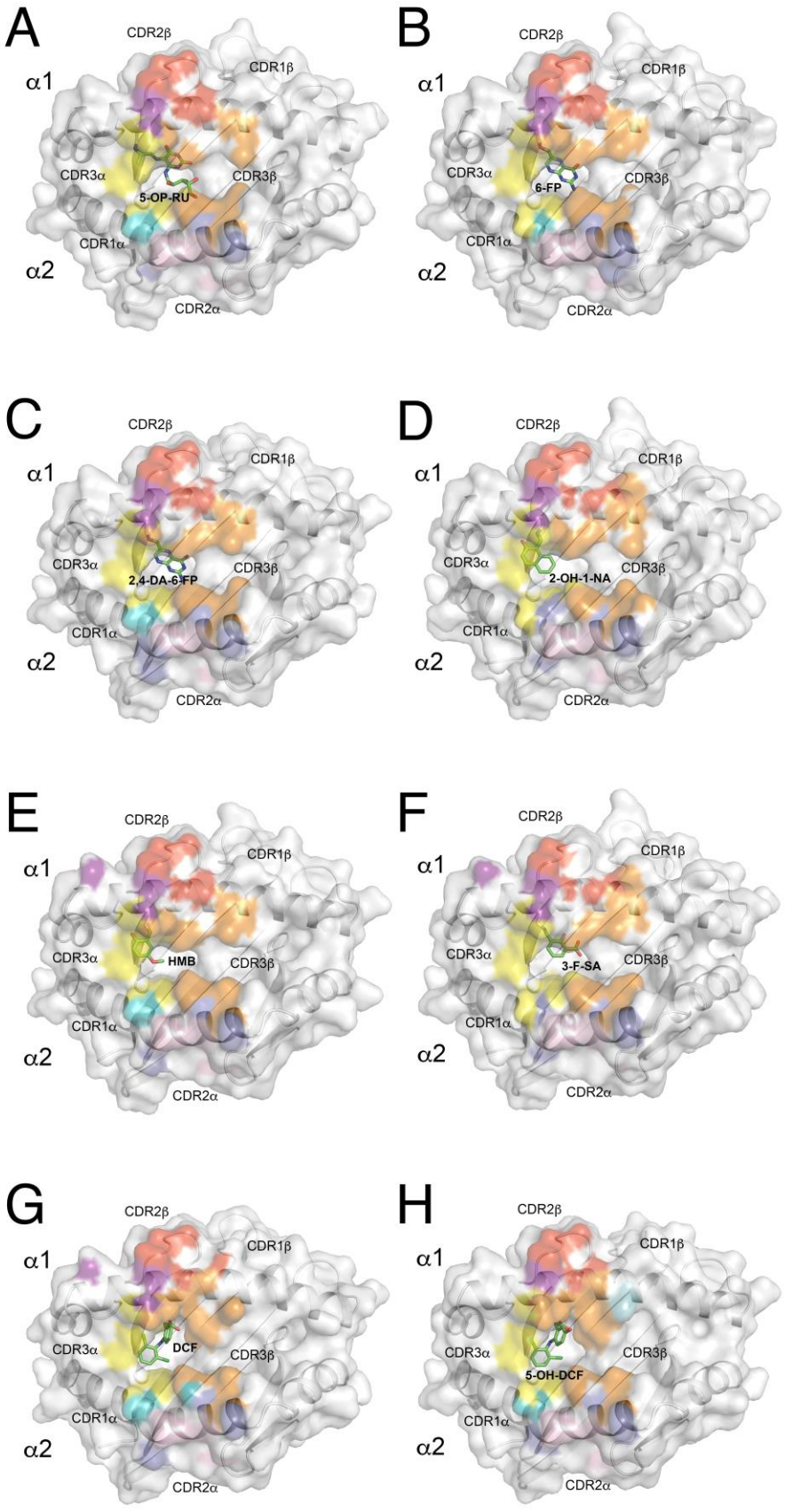
a) % cytokine production gated on live, $CD3^+$, TRAV1-2^+ 5-OP-RU-MR1-tetramer$^-$ (representative of non MAIT T cells) or TRAV1-2^+ 5-OP-RU-MR1-tetramer$^+$ (MAIT cells) cells. Samples include titrating amounts of 5-OP-RU, vehicle controls in the presence of maximum concentration of 5-OP-RU, Nil (PBS), and maximum concentration of inhibitors in the presence or absence of PMA/Ionomycin stimulus. Displayed is data of one representative donor. **b)** % CTV dilution gated on live, $CD3^+$, TRAV1-2^+ 5-OP-RU-MR1-tetramer$^-$ (representative of non MAIT T-cells) or TRAV1-2^+ 5-OP-RU-MR1-tetramer$^+$ (MAIT cells) cells. Samples include titrating amounts of 5-OP-RU (triplicate samples, SEM) and Nil (triplicate samples, SEM), vehicles (triplicate samples, SEM) and maximum concentrations of inhibitors in the presence (triplicate samples, SEM) or absence (single samples) of plate bound CD3/CD28. Displayed is data of one representative donor.



Supplementary Figure 6

Inhibition of the activation of MAIT cells by small molecules *in vivo*.

(a) Inhibitory effect of intranasally administered Ac-6-FP and 3-F-SA on MAIT cell accumulation in the lungs of C57BL/6 mice upon 5-OP-RU and Salm.BRD509Δ*ribDH* stimulus. Matching data in Figure 4c, absolute numbers of MAIT cells and non-MAIT αβ T cells (mean values +/- SEM as error bars of four mice as well as CFU counts in the lungs are shown. (b) Repeat experiment at the maximum inhibitor concentration including in addition IL17 production by non-MAIT αβ T cells in response to Salm.BRD509Δ*ribDH* stimulus in the presence or absence of inhibitors.

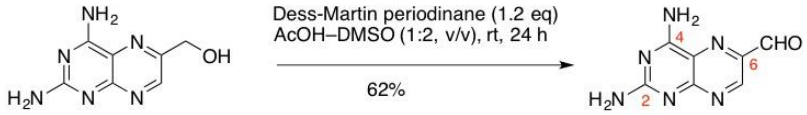

A
CDR2β
CDR1β
α1
CDR3α
5-OP-RU
CDR3β
CDR1α
α2
CDR2α
B
CDR2β
CDR1β
α1
CDR3α
6-FP
CDR3β
CDR1α
α2
CDR2α
C
CDR2β
CDR1β
α1
CDR3α
2,4-DA-6-FP
CDR3β
CDR1α
α2
CDR2α
D
CDR2β
CDR1β
α1
CDR3α
2-OH-1-NA
CDR3β
CDR1α
α2
CDR2α
E
CDR2β
CDR1β
α1
CDR3α
HMB
CDR3β
CDR1α
α2
CDR2α
F
CDR2β
CDR1β
α1
CDR3α
3-F-SA
CDR3β
CDR1α
α2
CDR2α
G
CDR2β
CDR1β
α1
CDR3α
DCF
CDR3β
CDR1α
α2
CDR2α
H
CDR2β
CDR1β
α1
CDR3α
5-OH-DCF
CDR3β
CDR1α
α2
CDR2α

Supplementary Figure 7

TCR contacts with MR1.

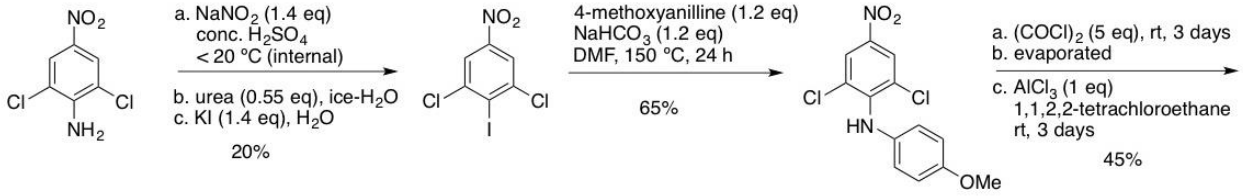
Contact regions of the CDR1α(teal), CDR2α(pink), CDR3α(yellow), CDR1β(cyan), CDR2β(red), CDR3β(orange) and framework residues (slate and deep purple for α- and β-chains, respectively) of A-F7 MAIT TCR on MR1 (white surface), which is presenting 5-OP-RU (A), 6-FP (B), 2,4-DA-6-FP (C), 2-OH-1-NA (D), HMB (E), 3-F-SA (F), DCF (G) or 5-OH-DCF (H).

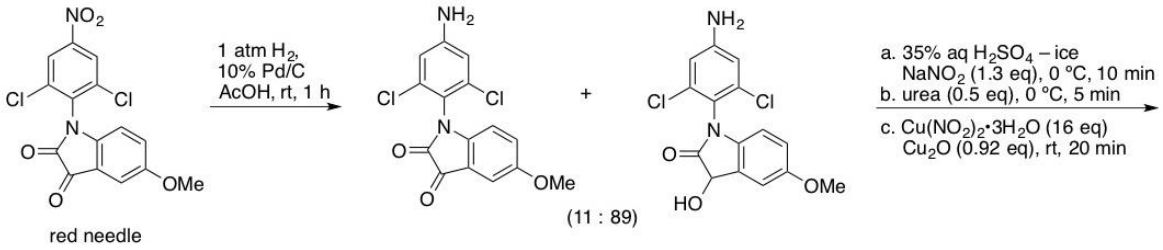
A

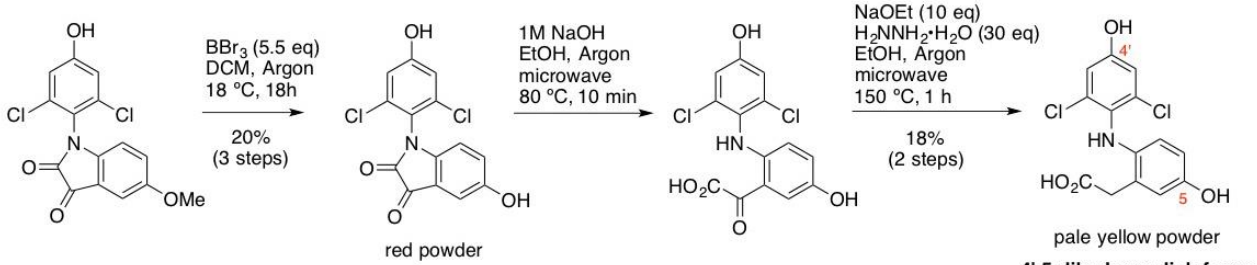


2,4-diamino-6-formylpteridine

B

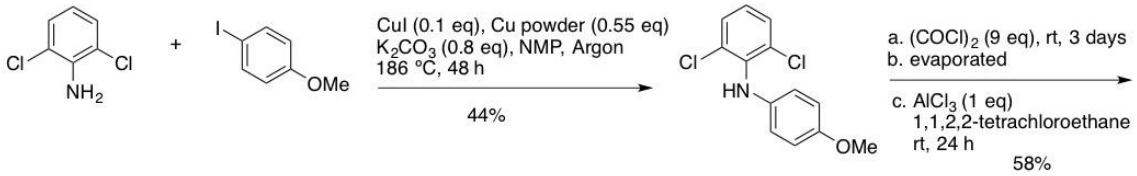


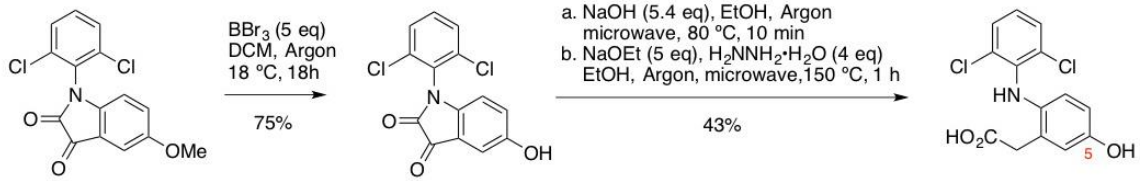




4',5-dihydroxy diclofenac

C





5-hydroxy diclofenac

Supplementary Figure 8

Chemical synthesis of metabolites.

Synthesis of 2,4-diamino-6-formylpteridine (A), 4′,5-dihydroxy diclofenac (B) and 5-hydroxy diclofenac (C).

Supplementary Table 1. Summary of *in silico* hits (147) from fragment based screening.

Name	CAS No.	MW
1-Amino-2-naphthol-4-sulfonic acid	116-63-2	239.25
1,2-Naphthoquinone-4-sulfonic acid sodium salt	521-24-4	260.20
1,2,4-Benzenetricarboxylic acid	528-44-9	210.14
1,3,5-Benzenetricarboxylic acid	554-95-0	210.14
1,4-Benzodioxan-6-carboxaldehyde	29668-44-8	164.16
1,4-Benzoquinone	106-51-4	108.09
1,4-Naphthoquinone	130-15-4	158.15
2-Acetamidobenzoic acid	89-52-1	179.17
2-Acetyl-1-methylpyrrole	932-16-1	123.15
2-Acetyl-5-methylfuran	1193-79-9	124.14
2-Acetylthiophene	88-15-3	126.18
2-Amino-3,5-dibromobenzaldehyde	50910-55-9	278.93
2-Amino-6-mercaptopurine (Thioguanine)[a]	154-42-7	167.19
2-Aminonicotinic acid	5345-47-1	138.12
2-Aminopyrimidine	109-12-6	95.10
2-Anilino-1,4-naphthoquinone	6628-97-3	249.27
2-Anisaldehyde	135-02-4	136.15
2-Anisic acid	579-75-9	152.15
2-Benzoylbenzoic acid	85-52-9	226.23
2-Biphenylcarboxaldehyde	1203-68-5	182.22
2-Biphenylcarboxylic acid	947-84-2	198.22
2-Carbethoxy-5,7-dihydroxy-4'-methoxyisofavone	15485-76-4	356.33
2-Carboxybenzaldehyde	119-67-5	150.13
2-Chloro-3-nitrobenzoic acid	3970-35-2	201.56
2-Chloro-4-nitrobenzoic acid	99-60-5	201.56
2-*Cis*,4-*trans*-abscisic acid	14375-45-2	264.32
2-furyl methyl ketone	1192-62-7	110.11
2-Hydroxy-1-naphthaldehyde	708-06-5	172.18
2-Hydroxy-1,4-naphthoquinone	83-72-7	174.15
2-Hydroxy-4-methoxybenzaldehyde	673-22-3	152.15
2-Hydroxy-5-methoxybenzaldehyde	672-13-9	152.15
2-Hydroxyphenylacetic acid	614-75-5	152.15
2-Methyl-1,4-naphthoquinone (Menadione)[a]	58-27-5	172.18
2-Pyrazinecarboxylic acid	98-97-5	124.10
2-Quinoxalinecarboxylic acid	879-65-2	174.16
2,3-Pyridinedicarboxylic acid	339155-13-4	167.12
2,4-Diamino-6-formylpteridine	4261-17-0	190.16
2,5-Dimethyl-p-benzoquinone	137-18-8	136.15
2,6-Dichloroquinone-4-chloroimide	101-38-2	210.45
2,6-Pyridinedicarboxylic acid	499-83-2	167.12
3-Acetylbenzonitrile	6136-68-1	145.16
3-Acetylcoumarin	3949-36-8	188.18
3-Amino-2-naphthoic acid	5959-52-4	187.19
3-Anisaldehyde	591-31-1	136.15
3-Benzyloxy-4-methoxybenzaldehyde	6346-05-0	242.27
3-Chloro-2-nitrobenzoic acid	4771-47-5	201.56
3-Chlorosalicylic acid	1829-32-9	172.57
3-Ethoxy-4-hydroxybenzaldehyde	121-32-4	166.17
3-Formylsalicylic acid	610-04-8	166.13
3-Hydroxy-4-methyl-2-nitrobenzoic acid	6946-15-2	197.14
3-Hydroxybenzoic acid	99-06-9	138.12
3-Hydroxyflavone	577-85-5	238.24
3,4-Dichlorobenzaldehyde	6287-38-3	175.01
3,4-Pyridinedicarboxylic acid	490-11-9	167.12
3,4,5-Trihydroxybenzaldehyde	13677-79-7	154.12
4-Acetamidobenzaldehyde	122-85-0	163.17
4-Acetylpyridine	1122-54-9	121.14
4-Aminouracil	873-83-6	127.10
4-Anisaldehyde	123-11-5	136.15
4-Benzyloxy-3-methoxybenzaldehyde	2426-87-1	242.27
4-Biphenylacetic acid	5728-52-9	212.24
4-Biphenylcarboxaldehyde	3218-36-8	182.22
4-Biphenylcarboxylic acid	92-92-2	198.22
4-Chloro-3-nitrobenzaldehyde	16588-34-4	185.56
4-Formylbenzoic acid	619-66-9	150.13
4-Guanidinobenzoic acid	16060-65-4	179.18
4-Hydroxy-3-methoxybenzaldehyde (isovanillin)	621-59-0	152.15
4-Hydroxy-3-methoxyphenylacetic acid	1131-94-8	182.17
4-Hydroxy-3-nitrobenzoic acid	616-82-0	183.12
4-Hydroxyphenylacetic acid	156-38-7	152.15
4-Phenoxybenzoic acid	2215-77-2	214.22
5-Aminonaphthalene-2-sulfonic acid	119-79-9	223.25
5-Aminosalicylic acid	89-57-6	153.14
5-Bromo-2'-deoxyuridine (Broxuridine)	59-14-3	307.10
5-Bromosalicylaldehyde	1761-61-1	201.02
5-Bromouracil	51-20-7	190.98

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5-Chlorosalicylic acid	321-14-2	172.57
5-Formylsalicylic acid	616-76-2	166.13
5-Hydroxy-1,4-naphthoquinone	481-39-0	174.15
5,8-Dihydroxy-1,4-naphthoquinone	475-38-7	190.15
6-Aminonicotinic acid	7418-65-7	138.12
6-Chloro-4-hydroxycoumarine	19484-57-2	196.59
6-Chloropurine	87-42-3	154.56
7-Hydroxyflavone	6665-86-7	238.24
8-Aminonaphthalene-2-sulfonic acid	119-28-8	223.25
8-Hydroxyquinoline-2-carboxylic acid	1571-30-8	189.17
8-Hydroxyquinoline-5-sulfonic acid	207386-92-3	225.22
9-Anthraldehyde	642-31-9	206.24
Acridone	578-95-0	195.22
Adenine	73-24-5	135.13
Adenosine	58-61-7	267.24
Alloxan	50-71-5	142.07
Alpha-Ionone	127-41-3	192.30
Anthraflavic acid	84-60-6	240.21
Anthranilic acid	118-92-3	137.14
Anthraquinone-2-sulfonic acid sodium salt	131-08-8	310.26
Apigenin (4',5,7-trihydroxyflavone)	520-36-5	270.24
Baicalein (5,6,7-trihydroxyflavone)	491-67-8	270.24
Benzalacetone (4-phenyl-3-buten-2-one)	122-57-6	146.19
Benzbromarone	3562-84-3	424.08
Benzofuran-2-carboxylic acid	496-41-3	162.14
Biochanin A (5,7-dihydroxy-4'methoxyisoflavone)	491-80-5	284.26
Bumetanide	28395-03-1	364.42
Calconcarboxylic acid	3737-95-9	438.41
Chelidamic acid	138-60-3	183.12
Chromone-2-carboxylic acid	4940-39-0	190.15
Chrysin (5,7-Dihydroxyflavone)	480-40-0	254.24
Coumarin[a]	91-64-5	146.14
Dehydroacetic acid	520-45-6	168.15
Di-furan-2-yl-methanone	17920-86-4	162.14
Dicumarol (3,3'-methylenebis[4-hydroxycoumarin])	66-76-2	336.29
Duroquinone (tetramethyl-p-benzoquinone)	527-17-3	164.20
Galangin (3,5,7-trihydroxyflavone)	548-83-4	270.24
Gallocyanine (7-dimethylamino-4-hydroxy-3-oxo-phenoxazine-1-carboxylic acid)	1562-85-2	336.73
Genistein (4',5,7-trihydroxyisoflavone)	446-72-0	270.24
Homogentisic acid (2,5-dihydroxyphenylacetic acid)	451-13-8	168.15
Hypoxanthine (6-hydroxypurine)	68-94-0	136.11
Indole-2-carboxylic acid	1477-50-5	161.16
Indole-3-carboxaldehyde	487-89-8	145.16
Isophorone	78-59-1	138.21
Isophthalaldehyde	626-19-7	134.13
Isoquinoline-1-carboxylic acid	486-73-7	173.17
Isovanillic acid (3-hydroxy-4-methoxybenzoic acid)	645-08-9	168.15
Kaempferol (3,4',5,7-tetrahydroxyflavone)	520-18-3	286.24
Khellin	82-02-0	260.24
Kinetin (6-Furfurylaminopurine)	525-79-1	215.21
Kojic acid	501-30-4	142.11
Leucopterin (2-amino-4,6,7-trihydroxypteridine)	492-11-5	195.14
Luteolin (3',4',5,7-tetrahydroxyflavone)	491-70-3	286.24
Menadione sodium bisulfite	130-37-0	276.24
Morin hydrate (1',3,3',5,7-pentahydroxyflavone)	654055-01-3	302.24
Myricetin (3,3',4',5,5',7-hexahydroxyflavone)	529-44-2	318.24
Naringenin (4',5,7-trihydroxyflavanone)	67604-48-2	272.25
Phloroglucinol carbaldehyde (2,4,6-trihydroxybenzaldehyde)	487-70-7	154.12
Picramic acid (2-amino-4,6-dinitrophenol)	96-91-3	199.12
Quercetin (3,3',4',5,7-pentahydroxyflavone)	117-39-5	302.24
Rhodizonic acid	118-76-3	170.08
Tenofovir	147127-20-6	287.22
Tetrachloro-o-benzoquinone	2435-53-2	245.88
Tetrahydroxy-1,4-quinone	319-89-1	172.09
Theobromine	83-67-0	180.16
Theophylline (1,3-dimethylxanthine)	58-55-9	180.16
Thiamine hydrochloride (vatamin B1)	67-03-8	337.27
Toluquinone	553-97-9	122.12
Uridine	58-96-8	244.20
Vanillan (4-hydroxy-3-methoxybenzaldehyde)	121-33-5	152.15
Xanthopterin	119-44-8	179.14

[a] also identified as FDA drug hits in Supplementary Table 2.

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Supplementary Table 2. Summary of screened and tested FDA approved drugs.

Name	CAS No.	MW	Use
Acyclovir	59277-89-3	225.21	antiviral
Amrinone	60719-84-8	187.20	pyridine phosphodiesterase 3 inhibitor
Aspirin	50-78-2	180.16	anti-inflammation, antipyretic
Azacytidine	320-67-2	244.21	antineoplastic
Azathiopurine	446-86-6	277.27	immunosuppressive antimetabolite
Chlorothiazide	58-94-6	295.72	a thiazide diuretic
Chloroxine	773-76-2	214.05	antibacterial
Coumarin[a]	91-64-5	146.14	perfumes and fabric conditioners,
Diclofenac	15307-86-5	296.15	NSAID
Diflunisal	22494-42-4	250.20	NSAID
Doxofylline	69975-86-6	266.25	treatment of asthma
Dyphylline	479-18-5	254.24	broncho- and vasodilator
Fenoprofen	31879-05-7	242.27	anti-inflammatory
Floxuridine	50-91-9	246.19	antineoplastic antimetabolite
Flucytosine	2022-85-7	129.09	antifungal
Flufenamic acid[a]	530-78-9	281.23	analgesic, anti-inflammatory
Ketorolac	74103-06-3	255.27	NSAID
Lamivudine	134678-17-4	229.26	a reverse transcriptase inhibitor
Mefenamic acid	61-68-7	241.29	NSAID
Menadione[a]	58-27-5	172.18	precursor of vitamin K2
Mercaptopurine	50-44-2	152.18	antimetabolite
Methaqualone	72-44-6	250.30	sedative-hypnotic drug
Methotrexate	59-05-2	454.44	antineoplastic
Methoxamine	390-28-3	211.26	alpha-adrenergic agonist
Methoxsalen	298-81-7	216.19	natural product targeting DNA
Nalidixic acid	389-08-2	232.24	antimicrobial
Phenazopyridine	94-78-0	213.24	used in urinary tract disorders
Phenylephrine	59-42-7	167.21	α-adrenergic receptor agonist
Pipemidic acid	51940-44-4	303.32	antibacterial
Pyrimethamine	58-14-0	248.71	folic acid antagonist
Quinethazone	73-49-4	289.74	diuretic
Salsalate	552-94-3	258.23	NSAID
Thioguanine	154-42-7	167.19	antineoplastic, antimetabolite
Triameterene[a]	396-01-0	253.26	a pteridine diuretic
Trimethoprim	738-70-5	290.32	antibacterial
Trichloromethiazide	133-67-5	380.66	A thiazide diuretic
Diclofenac Metabolites and other NSAIDs[b]			
4'-hydroxydiclofenac	64118-84-9	312.15	Metabolite of diclofenac
5-hydroxydiclofenac	69002-84-2	312.15	Metabolite of diclofenac
4',5-dihydroxydiclofenac	69002-86-4	328.15	Metabolite of diclofenac
Diclofenac Acyl-β-D-glucuronide	64118-81-6	472.27	Metabolite of diclofenac
Diclofenac Acyl-β-D-glucuronide allyl ester	698358-10-0	512.34	Metabolite of diclofenac
Celecoxib	169590-42-5	381.37	NSAID
Etodolac	41340-25-4	287.35	NSAID
Flunixin	38677-85-9	296.24	NSAID
Flurbiprofen	5104-49-4	244.26	NSAID
Indomethacin	53-86-1	357.79	NSAID
Meloxicam	71125-38-7	351.4	NSAID
Rofecoxib	162011-90-7	314.36	NSAID
Piroxicam	36322-90-4	331.35	NSAID
Tenoxicam	59804-37-4	337.37	NSAID

[a] Drugs not approved in US, but approved in other countries.

[b] Metabolites of Diclofenac and COX-2 inhibitors. The latter were included after identification of diclofenac as an MR1 ligand. Note: Some drugs are no longer approved in USA but are still prescribed in other countries. E.g. Coumarin is sold in India (Dipodem), Argentina (Esberiven), Brazil (Venalot), Taiwan (Venalot Depot). Flufenamic acid is sold in Japan (Fenazol 5%), Taiwan (Flufemin). Trychloromethiazide is sold in Japan (Flutria), Taiwan (Eazide). Pipemidic acid is sold in Brazil (Balurol), Italy (Diperpen). Menadione (vitamin K3) is approved for veterinary use in countries like Germany (Vita Men), Australia (Solquin), Italy (Izokappa), Chile (Katin). (Information obtained from www.drugs.com)

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Supplementary Table 3. Small molecule screening

Colour coding as in Figure 2a

Compounds		Normalized Jurkat.MAIT activation		Normalized MR1 upregulation	
Name	**Use/Origin**	**100 µM**	**10 µM**	**100 µM**	**10 µM**
1,2-Naphthoquinone-4-sulfonic acid	Colourimetric determination. Synthesis of anticancer agents.	-0.48	-0.97	10.31	2.98
1,4-Benzodioxan-6-carboxaldehyde	Intermediate.	-4.20	-1.95	1.41	0.88
1,4-Naphthoquinone	Derivatives have pharmacological properties.	7.43	0.48	-4.02	35.63
2-Amino-6-mercaptopurine	Incorparates into DNA and inhibits synthesis. Treatment of leukaemia.	-4.08	3.29	-0.43	-3.26
2-Carboxybenzaldehyde	Intermediate. Metabolite of ampicillin phthalidyl ester.	-1.06	-2.69	3.06	2.12
2-Furyl methyl ketone	Intermediate. Used in the production of the antibiotic Cefuroxime.	-0.40	-2.16	-0.46	-1.39
2-Hydroxy-1-naphthaldehyde	Intermediate. Active core of sirtinol.	-0.11	4.98	125.12	107.76
2-Pyrazinecarboxylic acid	Analogue is a urate retaining drug. Metabolite of Pyrazinamide.	-3.34	-1.77	-1.54	0.32
3-Acetylcoumarin	Intermediate.	-3.23	-3.25	0.22	1.41
3-Formylsalicylic acid	Analogue of salicylic acid.	-4.07	-3.51	124.44	51.13
4-Biphenylacetic acid	Anti-inflammatory, used in the treatment of rheumatoid arthritis.	-0.15	0.76	-0.86	-0.52
4-Guanidinobenzoic acid hydrochloride	Intermediate. Aminobenzoic acid derivatives treat inflammation.	-2.25	0.78	-2.06	-7.02
5-Aminosalicylic acid	Treatment of ulcerative colitis etc.	-1.06	-2.69	3.06	2.12
5-Bromouracil	Major chemical mutagen.	-2.95	-0.27	-6.67	-3.86
5-Chlorosalicylic acid	Intermediate.	-3.15	-2.44	0.59	0.66
5-Formylsalicylic acid	Analogue of salicylic acid.	3.68	1.86	149.23	64.85
5-Hydroxy-1,4-naphthoquinone	Colouring matter isolated from walnut shells. Used in herbal remedies.	-20.19	1.45	-34.35	38.54
6-Chloro-4-hydroxy coumarine	Coumarin is from plants.	-0.06	0.87	-6.34	1.74
7-Hydroxyflavone	Intermediate. Antifungal, analgesic.	3.07	-0.48	-12.11	-0.90
Acridone	Intermediate. Derivatives show potential as antimalarial drugs.	-5.69	-2.58	-11.03	-5.47
Acyclovir	Acyclic nucleoside used in the treatment of viral infections.	-3.41	-3.58	-2.30	-0.42
Amrinone	Phosphodiesterase inhibitor. Cardiac stimulant and vasodilator.	-2.79	-0.52	-0.54	1.02
Anthranilic acid	Dyes, drugs, perfumes and pharmaceuticals.	-3.23	-2.35	0.36	0.45
Apigenin	Wool dye. Induces autophagy in leukaemia cells. Inhibits CYP2C9.	-2.10	-2.91	75.45	28.78
Azacitidine	Antineoplastic agent. Treats acute myeloid leukaemia.	-4.88	3.32	-18.75	-17.79
Azathioprine	Immunosuppressant and antieoplastic agent - treats leukaemia.	5.22	5.30	-10.17	-2.83
Baicalein	Lipoxygenase inhibitor. Anti-inflammatory agent. In the herbal supplement Sho-Saiko-To.	4.36	-1.45	41.93	5.13
Benzbromarone	Anti-gout medication. Inhibitor of CYP2C9. Causes hepatotoxicity.	18.90	0.00	-22.68	-3.46
Biochanin A	A phytoestrogen, has putative benefits in dietary cancer prophylaxis.	0.65	-0.16	-15.50	-2.62
Bumetanide	A loop diuretic. Used in the tratment of heart failure.	-4.20	-3.94	-0.77	-1.05
Celecoxib	Analgesic and anti-inflammatory - rheumatoid and osteo-arthrisis.	-2.23	-3.16	-2.74	-3.08
Chlorothiazide	Used in the treatment of oedema.	-4.76	-5.52	1.06	1.84
Chloroxine	Treatment of amoebiasis, bacterial dysentary and skin infections.	24.14	-2.33	-17.76	-0.66
Coumarin	Perfumes. Used in the treatment of asthma and lymphedema.	-5.63	-4.83	-10.76	0.54
Dehydroacetic acid	Fungicide and bactericide. Used in processed fruit and vegetables.	-4.20	-2.26	14.24	1.54
Diclofenac	Anti-inflammatory used to treat pain and other afflictions such as gout.	80.39	4.22	-12.20	6.27
Dicumarol	Anticoagulant drug related to warfarin.	-5.73	-3.86	-2.02	4.00
Diflunisal	Analgesic, anti-inflammatory and antipyretic.	2.06	-0.67	-13.73	-1.31
Doxofylline	Used in the treatment of asthma, a bronchodilator.	-4.44	-3.13	19.88	6.08
Dyphylline	Adenosine antagonist, exhibits strong activity as a bronchodilator.	-5.04	-4.85	1.14	-0.45
Etodolac	Analgesic, anti-inflammatory and antipyretic - rheumatoid disorders.	-9.30	-3.62	-6.50	-2.40
Fenoprofen	Analgesic and anti-inflammatory - rheumatoid and osteoarthrisis.	3.11	-2.27	-3.58	-2.69
Floxuridine	Antineoplastic agent, inhibits DNA and RNA synthesis.	14.56	10.77	-0.36	-1.63
Flucytosine	Antifungal agent used in the treatment of urinary tract infections.	-4.55	-4.29	0.60	0.90
Flufenamic acid	Analgesic and anti-inflammatory. Used in rheumatic disorders.	-0.15	-3.49	-5.95	1.75
Flunixin	Anti-inflammatory used by veterinarians.	-8.50	-4.50	-14.93	-4.57
Flurbiprofen	Analgesic, anti-inflammatory and antipyretic - rheumatoid disorders.	0.63	-3.66	-5.50	-2.81
Galangin	Flavonol found in galanga root. Growth inhibitor of breast tumor cells. Antiviral, antibacetrial.	15.19	4.20	-15.41	-6.60
Genistein	Phytoestrogen; tyrosine kinase inhibitor. Antioxidant and anthelmintic.	-1.68	4.32	38.44	9.32
Indomethacin	Analgesic with anti-inflammatory and antipyretic action.	3.48	5.22	-11.39	-6.85
Kaempferol	Flavone, antioxidant. Possible cancer treatment.	2.04	6.13	-22.02	-10.51
Ketorolac	Analgesic. Inhibits synthesis of prostaglandins.	-5.89	-4.21	-8.69	-1.73
Khellin	Vasodilator (asthma treatment). Induces skin pigmentation via UV light.	-4.99	-2.83	-5.04	-2.78
Kojic acid	Antibiotic.	-3.39	-1.62	-0.80	6.00
Kabetalol	Antihypertensive agent with beta-adrenoreceptor blocking properties.	-2.97	0.61	-3.12	-1.79
Lamivudine	Antiviral used in the treamtent of AIDS and hepatitis B.	-4.21	-2.65	-2.27	-3.45
Luteolin	Flavone; antioxidant, anti-inflammatory, anti-allergic and anti-cancer.	-3.66	3.18	20.31	-4.98
m-Hydroxybenzoic acid	Intermediate for plasticisers, resins, pharmaceuticals etc.	-1.43	0.04	-2.12	-1.79
Mefenamic acid	Anti-inflammartory. Relief from pain. Used in rheumatic disorders.	-3.19	-3.23	-2.55	25.78
Meloxicam	Analgesic and anti-inflammatory. Inhibits cyclooxygenase.	-2.69	-6.02	-6.57	-3.97
Menadione	Nutritional supplement. Treatment of hypoprothrombinemia.	-11.55	-4.38	14.33	47.01
Menadione sodium bisulfite	Reduces blood clotting time. Treatment for hyperprothrombinaemia.	21.16	-0.48	20.43	129.16
Mercaptopurine	Antineoplastic agent - treatment of leukaemia. Adenine analog.	17.51	14.14	-3.52	-3.37
Methaqualone	A hypnotic, used to be used for the treatment of insomnia.	-2.34	-0.43	-3.60	-2.22
Methoxamine	A pressor agent in hytotensive states.	-0.82	-0.87	-2.58	-2.42
Methoxsalen	Increases the formation of melanin following exposure to UV light.	-4.63	-3.47	2.58	1.34
Nalidixic acid	Bactericide used in the treatment of urinary-tract infections.	-3.77	-4.57	0.42	0.64
Phenazopyridine	Used in pain relief for conditions such as cystitis and urethritis.	-2.08	-0.89	-8.57	-0.67
Phenylephrine	Treatment of hypotensive states and the relief of nasal congestion.	-5.02	-4.66	-0.84	1.61
Pipemidic acid	Intermediate. A quinolone (synthetic broad-spectrum antibacterial).	-4.45	-8.50	-16.15	-14.36
Piroxicam	Analgesic, anti-inflammatory and antipyretic - rheumatoid disorders.	-0.93	-3.58	-6.05	-3.79
Pyrimethamine	Antimalarial drug and dihydrofolate reductase inhibitor.	-5.40	-5.40	-20.14	-15.35
Quinethazone	Thiazide-like diuretic used to treat hypertension.	-3.72	-1.13	-3.02	-2.12
Rofecoxib	Analgesic and anti-inflammatory. Inhibits sysnthesis of prostaglandins.	-4.97	-2.23	-4.01	-3.29
Salsalate	Anti-inflammatory, used in the treament of arthritis.	-2.42	2.10	1.47	-0.75
Tenofovir	Anti-retroviral, blocks reverse transcriptase.	-4.59	-4.34	-2.50	-4.21
Tenoxicam	Anti-inflammatory - treats rheumatoid arthristis, osteoarthristis etc.	-1.94	-3.37	-1.85	-1.12
Tetrahydroxy-1,4-quinone hydrate	Systemic keratolytic.	11.20	0.94	33.47	4.02
Theobromine	Vasodilator, diuretic and heart stimulant.	0.41	2.69	-9.49	-10.00
Triamterene	Diuretic used in the treatment of hypertension and edema.	6.14	3.49	-3.82	-3.41
Trichlormethiazide	Antihypertensive. Diuretic used to treat oedema.	-1.62	-1.13	-5.31	-2.58
Trimethoprim	Antibacterial.	0.65	-1.29	-4.92	-1.78

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Supplementary Table 4. IC50 values of the inhibitors tested

T cell line	Inhibitor	Conc. 5-OP-RU	IC50 (μM)	R^2 of IC50
Jurkat.MAIT-A-F7 (TRBV6-1)	6-FP	1 nM	71.40	0.97
		0.1 nM	8.86	1.00
		0.01 nM	ND	
	Ac-6-FP	1 nM	3.91	0.99
		0.1 nM	ND	
		0.01 nM	ND	
	3-F-SA	1 nM	90.34	0.98
		0.1 nM	12.25	1.00
		0.01 nM	ND	
	2-OH-1-NA	1 nM	ND	
		0.1 nM	134.00	0.90
		0.01 nM	26.85	0.87
Jurkat.MAIT-#6 (TRBV6-4)	6-FP	1 nM	122.20	0.99
		0.1 nM	12.86	1.00
		0.01 nM	0.29	0.98
	Ac-6-FP	1 nM	0.36	1.00
		0.1 nM	ND	
		0.01 nM	ND	
	3-F-SA	1 nM	150.20	1.00
		0.1 nM	18.01	1.00
		0.01 nM	8.47	0.98
	2-OH-1-NA	1 nM	ND	
		0.1 nM	106.90	0.98
		0.01 nM	17.24	0.94
Jurkat.MAIT-C-F7 (TRBV20)	6-FP	1 nM	145.80	0.98
		0.1 nM	13.04	1.00
		0.01 nM	0.33	0.94
	Ac-6-FP	1 nM	0.42	0.99
		0.1 nM	ND	
		0.01 nM	ND	
	3-F-SA	1 nM	ND	
		0.1 nM	12.62	0.98
		0.01 nM	8.87	1.00
	2-OH-1-NA	1 nM	ND	
		0.1 nM	555.10	1.00
		0.01 nM	24.01	0.90
Bw58.CD3.MAIT-Vβ8.2	6-FP	10 μM	101.30	0.98
		5 μM	166.80	0.99
		1 μM	93.35	0.89
	Ac-6-FP	10 μM	31.46	0.98
		5 μM	17.52	1.00
		1 μM	13.94	0.94
	3-F-SA	10 μM	113.50	0.89
		5 μM	77.66	0.99
		1 μM	27.02	1.00
	2-OH-1-NA	10 μM	36.30	1.00
		5 μM	34.20	1.00
		1 μM	31.28	1.00

ND: Not determined when non-linear regression did not converge or was ambiguous.

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Supplementary Table 5. Data collection and refinement statistics

	A-F7 TCR: MR1(HMB)	A-F7 TCR: MR1(DCF)	A-F7 TCR: MR1(2,4-DA-6-FP)	A-F7 TCR: MR1(2-H-1-NA)	A-F7 TCR: MR1(3-F-SA)	A-F7 TCR: MR1(5-OH-DCF)
Data collection						
Temperature	100K	100K	100K	100K	100K	100K
Space group	*C2*	*C2*	*C2*	*C2*	*C2*	*C2*
Cell dimensions						
a, *b*, *c* (Å)	216.2, 69.7, 142.4	212.6. 69.5, 142.9	215.3, 69.7, 142.4	216.4, 69.9, 143.1	217.1, 70.5, 143.4	213.1, 69.6, 142.4
□□□□α, β, γ□ (°)	90, 104.3, 90	90, 103.4, 90	90, 104.0, 90	90 104.4, 90	90.0, 104.8, 90.0	90, 103.7, 90
Resolution (Å)	52.37-2.20 (2.24-2.20)	49.0-2.70 (2.78-2.70)	45.35-2.10 (2.14-2.10)	75.15-2.10 (2.14-2.10)	53.97-1.90 (1.93-1.90)	57.87-2.50 (2.56-2.50)
R_{pim}[1]	4.8 (27.3)	8.1 (50.7)	6.5 (57.8)	5.8 (36.7)	4.5 (38.1)	4.4 (28.8)
$CC_{1/2}$	99.6 (86.0)	98.0 (71.0)	99.5 (59.7)	99.3 (82.1)	99.7 (74.6)	99.6 (87.4)
I/σ_1	10.4 (2.3)	6.6 (1.3)	8.0 (1.4)	7.9 (2.1)	11.1 (1.8)	12.3 (2.3)
Completeness (%)	99.7 (97.8)	98.6 (99.2)	100.0 (100.0)	99.8 (100)	97.6 (94.2)	98.7 (97.8)
Total N$^{o.}$ observations	448364 (19719)	154771 (12941)	524584 (25862)	445269 (22402)	722223 (35045)	273724 (14991)
N$^{o.}$ unique observations	104381 (5091)	55489 (4567)	119864 (5891)	120949 (6014)	161424 (7648)	69625 (4403)
Multiplicity	4.3 (2.9)	2.8 (2.8)	4.4 (4.4)	3.7 (3.7)	4.5 (4.6)	3.9 (3.4)
Refinement statistics						
R_{factor}[2] (%)	18.4	18.8	18.0	17.3	18.1	17.3
R_{free}[3] (%)	22.8	23.8	22.6	21.9	22.5	23.1
No. atoms						
• Protein	12788	12825	12816	12799	12855	12762
• Ligand	32	70	91	60	37	42
• Water	1067	172	882	1217	1429	437
Ramachandran plot (%)						
• Most favoured	97.0	97.0	98	98	98.0	97.5
• Allowed region	2.9	2.9	2	2	1.9	2.5
B-factors (Å^2)						
• Protein	35.1	54.4	40.4	34.4	35.3	45.9
rmsd bonds (Å)	0.011	0.004	0.009	0.010	0.008	0.06
rmsd angles (°)	1.27	0.85	1.19	1.22	1.13	0.97

[1] $R_{p.i.m} = \Sigma_{hkl} [1/(N-1)]^{1/2} \Sigma_i | I_{hkl,i} - \langle I_{hkl} \rangle | / \Sigma_{hkl} \langle I_{hkl} \rangle$

[2] $R_{factor} = (\Sigma | |F_o| - |F_c| |) / (\Sigma |F_o|)$ - for all data except as indicated in footnote 3.

[3] 5% of data was used for the R_{free} calculation

Values in parentheses refer to the highest resolution bin.

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Supplementary Table 6: Buried surface area calculations of MR1-Ag:MAIT TCR interaction

		Contribution (as % of total BSA)									
	Total (Å^2)	α-Chain	β-Chain	CDR1α	CDR2α	CDR3α	α-framework	CDR1β	CDR2β	CDR3β	β-framework
A-F7 TCR: MR1(DA-6-FP)	1170.2	52.3	47.7	5.8	10.5	21.9	14.0	1.2	13.1	24.8	8.6
A-F7 TCR:MR1(2-OH-1-NA)	1235.6	48.2	51.8	7.3	10.5	19.3	11.1	0.7	12.0	28.8	10.4
A-F7 TCR:MR1(HMB)	1143.0	51.2	48.8	7.6	10.9	20.8	11.9	0.9	13.7	23.6	10.7
A-F7 TCR:MR1(3-F-SA)	1210.0	48.5	51.5	7.1	10.7	20.1	10.6	0.7	11.8	27.8	11.1
A-F7 TCR:MR1(DCF)	1206.5	49.4	50.6	8.3	11.2	18.2	11.8	2.2	12.4	25.9	10.1
A-F7 TCR:MR1(5-OH-DCF)	1161.0	48.3	51.7	7.0	11.2	18.5	11.6	4.2	13.5	25.1	8.9

Determined using the CCP4 implementation of AreaiMol

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Supplementary Table 7. MAIT TCR (A-F7) contacts with MR1(DCF)

CDR	TCR	MR1	Bond
CDR1α	Gly28α	Glu160	VDW
	Phe29α^{N}	Glu160^{Oε2}	H-bond
	Phe29α	Glu160, Asn155	VDW
	Asn30α	Trp156, Tyr152, Glu160	VDW
CDR2α	Val50α	Tyr152, Asn155	VDW
	Leu51α	Leu151, Asn155	VDW
CDR2α framework	Tyr48α	His148, Tyr152	VDW
	Glu55α^{Oε1}	His148^{Nε2}	H-bond
TCR framework	Arg66α^{Nη1}	Asn155^{Oδ1}	H-bond
	Arg66α	Asn155, Glu159	VDW
CDR3α	Ser93α	Tyr62, Glu160, Trp164	VDW
	Asn94α^{O}	Arg61^{Nε}	H-bond
	Asn94α^{O}	Arg61^{Nη2}	H-bond
	Asn94α^{Oη}	Tyr62^{Oη}	H-Bond
	Asn94α	Arg61, Tyr62, Trp164	VDW
	Tyr95α^{Oη}	Trp156^{Nε1}	H-bond
	Tyr95α	Arg61, Tyr62, Leu65, Tyr152, Trp156	VDW
	Asn96α	Arg61	VDW
	Gln96α	Arg61	VDW
CDR1β	Asn30β	Met72	VDW
CDR2β	Ala50β	Gln64	VDW
	Ser51β	Gly68, Arg67	VDW
	Gly53β	Arg41	VDW
	Thr54β^{Oγ}	Gln64^{Oε1}	H-bond
	Thr54β	Gln64, Arg67	VDW
	Thr55β	Gln64	VDV
CDR2β framework	Tyr48β^{Oη}	Arg61^{Nη1}	H-bond
	Tyr48β	Arg61	VDW
	Thr55β	Gln64	VDW
	Asp56β	Gln64	VDW
CDR3β	Trp96β	Leu65, Gly68, Trp69, Met72	VDW
	Thr97β	Arg61, Leu65	VDW
	Glu99β	Arg9, Trp69, Tyr152	VDW
	Glu99β ^{Oε1}	Trp69 ^{Nε1}	H-Bond
	Glu99β ^{Oε2}	Arg9^{Nη1}, Trp69 ^{Nε1}	H-Bond
	Gly100β	Glu149, Tyr152	VDW
	Ser101β^{Oβ2}	Glu149 ^{Oε1}, Glu149^{N}	H-Bond
	Ser101β	His148, Glu149	VDW

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	DCF	**MR1**	**Bond**
	C	Tyr7, Ser24, Leu66	VDW
	C1	Tyr62, Leu66	VDW
	C2	Arg9, Tyr62	VDW
	C3	Try62	VDW
	C4	Tyr7	VDW
	C5	Tyr7	VDW
	C6	Tyr7, Trp164	VDW
	C7	Leu5, Tyr7, Trp156	VDW
	C8	Tyr7, Trp156	VDW
	C9	Tyr7	VDW
	C10	Tyr62	VDW
	C11	Arg9, Tyr62	VDW
	C12	Arg9, Trp69	VDW
	C13	Arg9, Tyr62	VDW
	Cl	Tyr7, Tyr62	VDW
	Cl1	Tyr7, Arg9	VDW
	N	Tyr7, Tyr62	VDW
	O	$Arg^{N\varepsilon}$, $Arg^{N\eta 2}$	H-bond
	O	Tyr7, Arg9, Ser24, Leu66	VDW
	O1	$Ser24^{O\gamma}$	H-Bond
	O1	Tyr7, Ser24, Leu66	VDW
	DCF	**TCR**	**Bond**
	C10	Tyr95α	VDW
	C11	Glu99β, Tyr95α	VDW
	C12	Glu99β	VDW

- Atomic contacts determined using the CCP4i implementation of *CONTACT* and a cutoff of 4Å.
- Van der Waals interactions defined as non-hydrogen bond contact distances of 4Å or less.
- Hydrogen bond interactions are defined as contact distances of 3.3Å or less.
- Salt bridge interactions are defined as contact distances of 4.5Å or less.

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Supplementary Table 8

MAIT TCR (A-F7) contacts with MR1(5-OH-DCF)

CDR	TCR	MR1	Bond
CDR1α	Gly28α	Glu160	VDW
	Phe29α^{N}	Glu160^{Oε2}	H-bond
	Phe29α^{O}	Asn155^{Nδ2}	H-bond
	Phe29α	Glu160	VDW
	Asn30α	Tyr152, Trp156, Glu160	VDW
CDR2α	Val50α	Leu151, Tyr152, Asn155	VDW
	Leu51α	Leu151, Lys154, Asn155	VDW
CDR2α framework	Tyr48α	His148, Tyr152	VDW
	Glu55α^{Oε1}	His148^{Nε2}	H-bond
	Glu55α	His148	VDW
TCR framework	Arg66α^{Nη1}	Asn155^{Oδ1}	H-bond
	Arg66α	Asn155, Glu159	VDW
CDR3α	Ser93α^{Oγ}	Glu160^{Oε1}	H-bond
	Ser93α	Tyr62, Glu160, Trp164	VDW
	Asn94α^{Oδ1}	Tyr62^{Oη}	H-bond
	Asn94α^{O}	Arg61^{Nε}	H-bond
	Asn94α	Arg61, Tyr62, Trp164	VDW
	Tyr95α^{Oη}	Trp156^{Nε1}	H-bond
	Tyr95α^{O}	Arg61^{Nη2}	H-bond
	Tyr95α	Arg61, Tyr62, Tyr152, Trp156	VDW
	Gln96α	Arg61	VDW
CDR2β	Ala50β	Gln64	VDW
	Ser51β	Arg67, Gly68	VDW
	Gly53β	Arg41	VDW
	Thr54β^{Oγ1}	Gln64^{Oε1}, Arg67^{Nη1}	H-bond
	Thr54β	Gln64, Arg67	VDW
CDR2β framework	Tyr48β^{Oη}	Arg61^{Nη1}	H-bond
	Tyr48β	Arg61, Gln64	VDW
	Thr55β	Gln64	VDW
	Asp56β	Gln64	VDW
CDR3β	Trp96β	Leu65, Gly68, Trp69, Met72	VDW
	Thr97β	Arg61, Leu65	VDW
	Gly98β	Leu65	VDW
	Glu99β^{Oε1}	Trp69^{Nε1}	H-bond
	Glu99β^{Oε2}	Arg9^{Nη2}, Trp69^{Nε1}	H-bond
	Glu99β	Arg9, Trp69, Tyr152	VDW
	Gly100β	Glu149, Tyr152	VDW
	Ser101β^{N}	Glu149^{Oε2}	H-bond
	Ser101β	His148, Glu149	VDW

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	5-OH-DCF	**MR1**	**Bond**
	CL1	Tyr7, Lys43, Tyr62	VDW
	C9	Tyr7	VDW
	C8	Trp164	VDW
	C7	Tyr7, Trp164	VDW
	C6	Tyr7, Trp156	VDW
	C5	Tyr7, Trp156	VDW
	CL	Tyr7, Ile96, Trp156	VDW
	C4	Tyr7	VDW
	N	Tyr7	VDW
	C3	Tyr62	VDW
	C10	Tyr62, Tyr95α	VDW
	C11	Arg9, Tyr62, Tyr95α, Glu99β	VDW
	C12	Arg9, Tyr62, Glu99β	VDW
	O2	$Trp69^{N\varepsilon 1}$, $Glu99\beta^{O\varepsilon 1}$, $Glu99\beta^{O\varepsilon 2}$	H-bond
	O2	Arg9, Leu65, Trp69, Glu99β	VDW
	C13	Arg9, Tyr62	VDW
	C2	Arg9, Tyr62	VDW
	C1	Tyr62, Leu66	VDW
	C	Tyr7, Ser24, Leu66	VDW
	O1	$Ser24^{O\gamma}$	H-bond
	O1	Tyr7, Ser24, Leu66	VDW
	O	$Arg9^{N\eta 2}$, $Ser24^{O\gamma}$	H-bond
	O	Tyr7, Arg9, Leu66	VDW
	5-OH-DCF	**TCR**	**Bond**
	O2	$Glu99\beta^{O\varepsilon 1}$ $Glu99\beta^{O\varepsilon 2}$	H-bonds
	O2	Glu99β	VDW
	C11	Glu99β, Tyr95α	VDW
	C12	Glu99β	VDW

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- Van der Waals interactions defined as non-hydrogen bond contact distances of 4Å or less.
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