Electronic Supplementary Material (ESI) for Analyst.

Supplementary Information for

Rapid separation of cannabinoid isomer sets using differential mobility spectrometry and mass spectrometry

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Experimental and instrumental conditions

Table S1. Instrumental conditions used for the separation of cannabinoid isomers

Source/Gas Conditions			
Ion Source:	TurboSpray	**Temperature:**	34 ºC
Curtain Gas:	20 psi	**Ion Source Gas 1:**	20 psi
Collision Gas:	High	**Ion Source Gas 2:**	0 psi
Polarity:	Negative Mode	**Ion Spray Voltage:**	−4500 V
Compound Conditions			
Declustering Potential:	−100.0 V	**Excitation Energy:**	0.100 V
Collision Energy:	−10.0 V	**CE Spread:**	0.00 V
Entrance Potential:	−10.0 V		
DMS Conditions			
DMS Temperature*:	150 ºC for decarboxylated 225 ºC for acids,	**CV Ramp:**	0.1 V
DMS Offset:	−3.0 V	**Resolving Gas:**	20
Modifier at 1.5% *(v/v*)*:	IPA		

*An equilibration time of 15 min is given when modifying the DMS temperature prior to any experiments being run, or when a modifier is newly introduced.

Mass spectrometric analyses of cannabinoid ions

The cannabinoid derivatives were analyzed in the negative mode to improve the total parent *m/z* ion signal, increasing sensitivity. Protonation of some of the isomers results in lower ionization efficiencies for some derivatives. Product ion scans of Δ^9-THC and CBC in the protonated and deprotonated cases are provided to showcase the relative ionization efficiencies of each parent ion *m/z* peak.

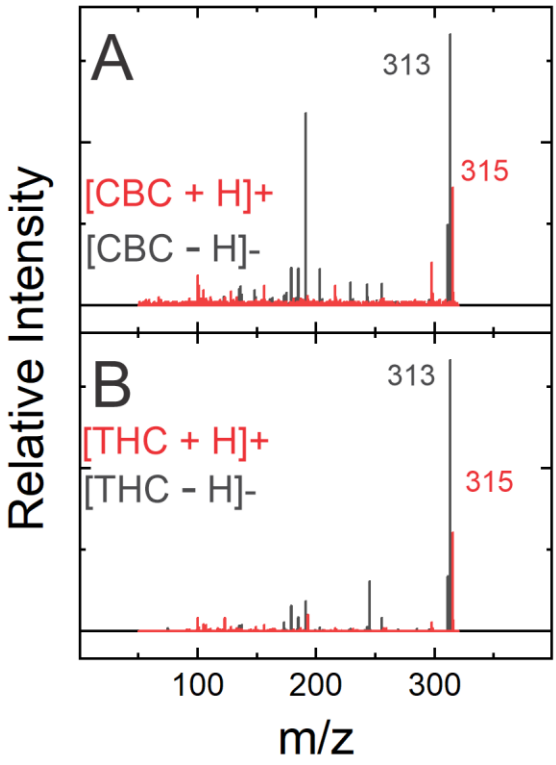

Figure S1. Product ion scans of protonated and deprotonated (**A**) CBC and (**B**) Δ^9-THC.

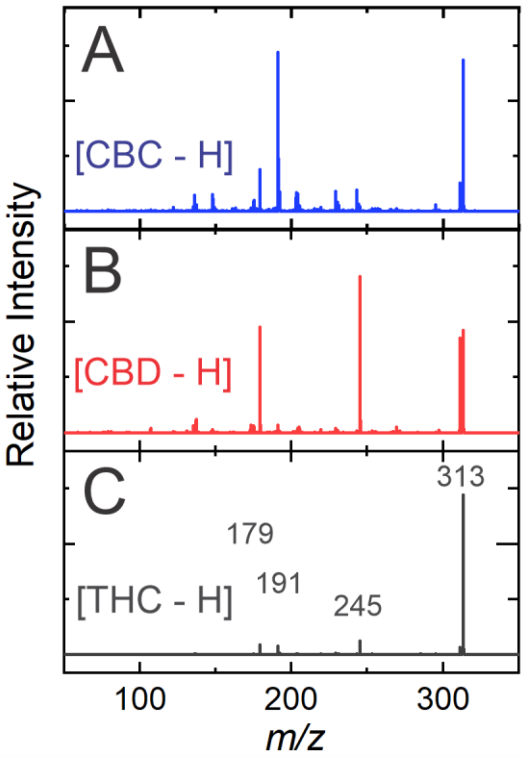

Figure S2. Enhanced product ion scans of (**A**) $[[CBC-H]^-$, (**B**) $[CBD-H]^-$ and (**C**) $[\Delta^9\text{-}THC-H]^-$, using a collision energy of -30 V show similar product ions but variation in product ion relative intensities.

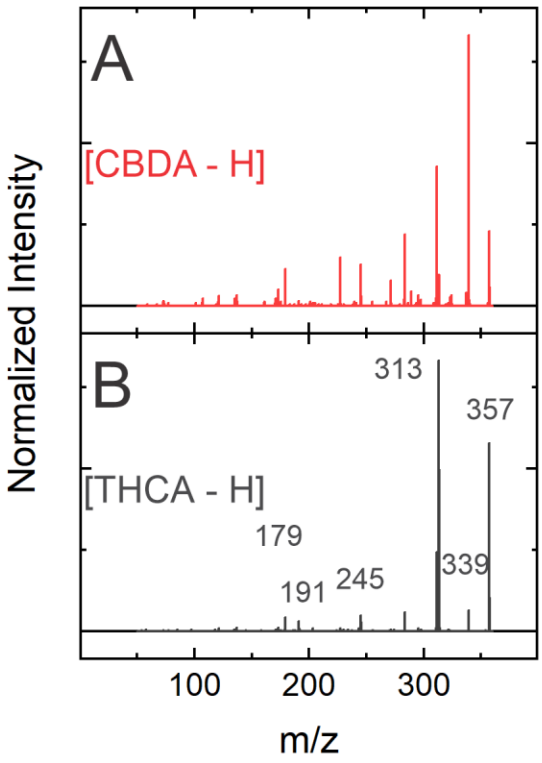

Figure S3. Enhanced product ion scans of (**A**) $[CBDA-H]^-$ and (**B**) $[THCA-H]^-$ using a collision energy of -30 V show similar product ions but variation in product ion relative intensities.

The addition of resolving gas

The resolving gas (DR) is N_2 gas added at a determined flow rate to the end of the DMS cell to extend the ion residence time in the DMS cell, improving the resolution. The flow rate and ion residence time attributed to each DR value are tabulated below.

Table S2. Resolving gas conditions and corresponding flow rate and residence times

DR value:	Flow rate (cm^3/ms):	Ion residence time (ms):
8	0.014966	9.463722
10	0.016833	10.05587
12	0.018617	10.69519
14	0.020283	11.37081
16	0.021883	12.10491
18	0.023367	12.87554
20	0.024900	13.78254
22	0.026333	14.75410

The behavior of cannabinoid derivatives under various modifier conditions

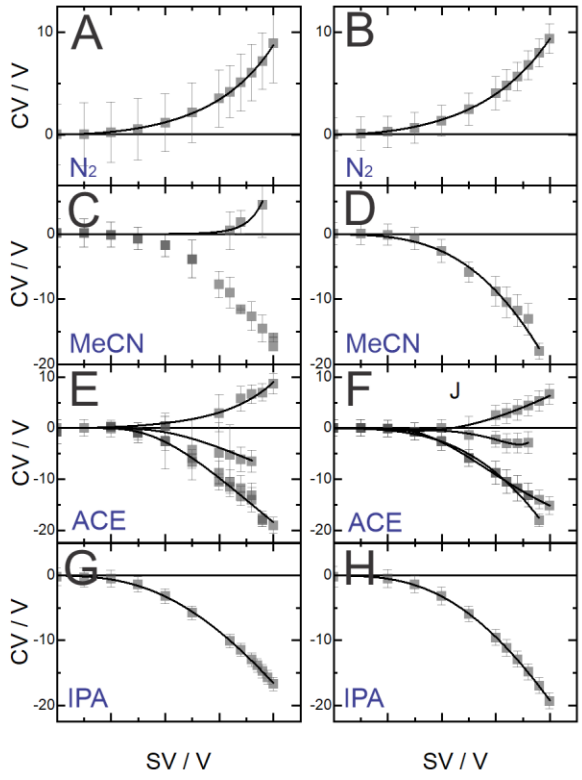

Figure S4. The dispersion plots of CBD (*left*) and CBC (*right*) in (**A**) and (**B**) N_2 conditions, (**C**) and (**D**) MeCN-modified conditions, (**E**) and (**F**) acetone-modified conditions, and (**G**) and (**H**) IPA-modified conditions.

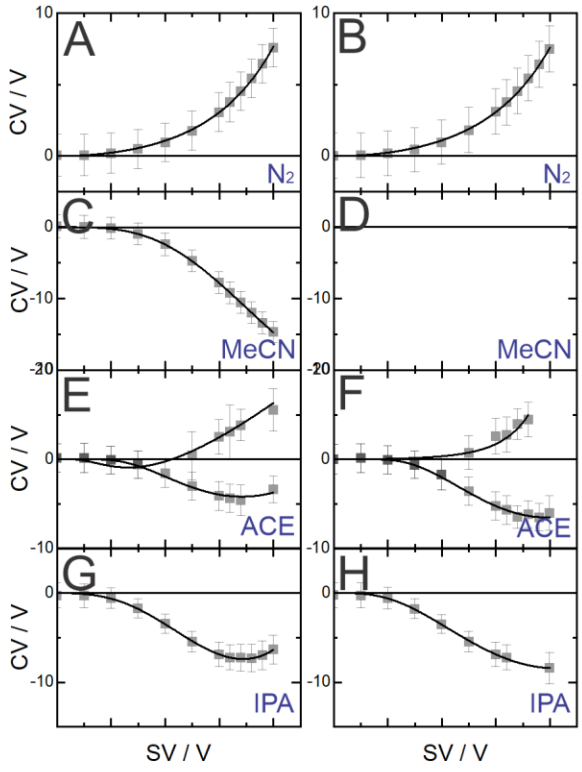

Figure S5. The dispersion plots of CBDA (*left*) and (−)-THCA (*right*) in (**A**) and (**B**) N_2 conditions, (**C**) and (**D**) MeCN-modified conditions, (**E**) and (**F**) acetone-modified conditions, and (**G**) and (**H**) IPA-modified conditions.

Preferential solvation studies observed in acetone modifier conditions

Sample temperature studies for cannabinoid isomers

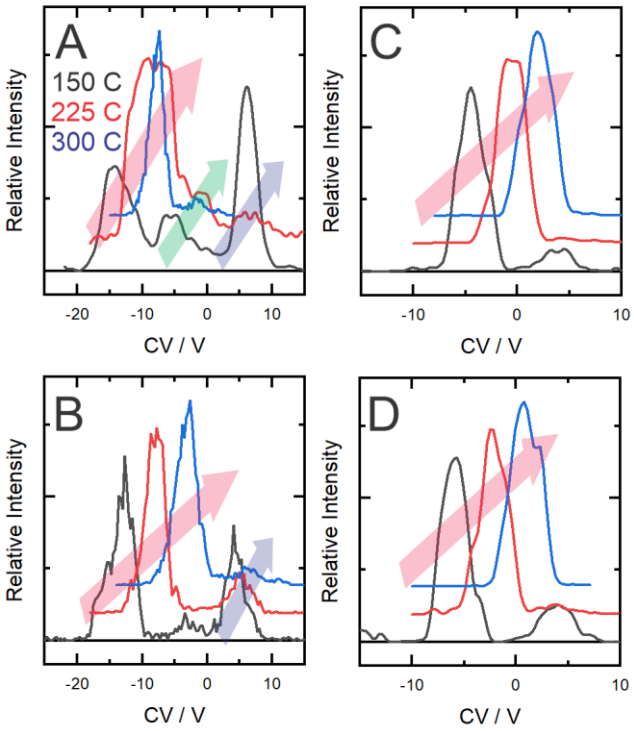

Figure S6. Temperature studies of (**A**) CBD, (**B**) CBC, (**C**) CBDA, and (**D**) THCA anions under N_2 seeded with 1.5% acetone vapor taken at SV = 3600 V.

Precursor ion studies of cannabinoid DMS peaks

Precursor ion scans were taken for each SV/CV pair noted in the previous figures for the decarboxylated anion species. Agreement with solvent studies were found, in which peak I consistently contained a *m/z* 429 peak, pertaining to the deprotonated analyte clustered with 2 acetone molecules. Peak II contained a *m/z* 373 peak, corresponding to the deprotonated analyte clustered with acetic acid. Peak III showed a *m/z* 627 peak, likely indicated a proton-bound dimer of the deprotonated analyte with its neutral counterpart. It is noted that even though solvent studies showed dependence of peak intensity of peaks III and IV on methanol and acetonitrile, respectively, precursor ion scans did not show peaks corresponding to these.

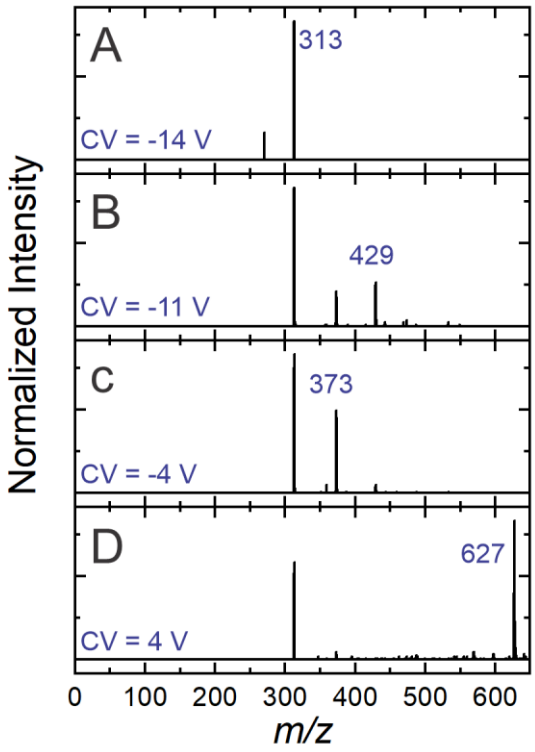

Figure S7. Precursor ion scans of peaks I-IV taken at DcP set to 0 V for $[THC - H]^-$ in an N_2 carrier gas environment seeded with 1.5% (*v/v*) acetone. Ions of interest are labelled.

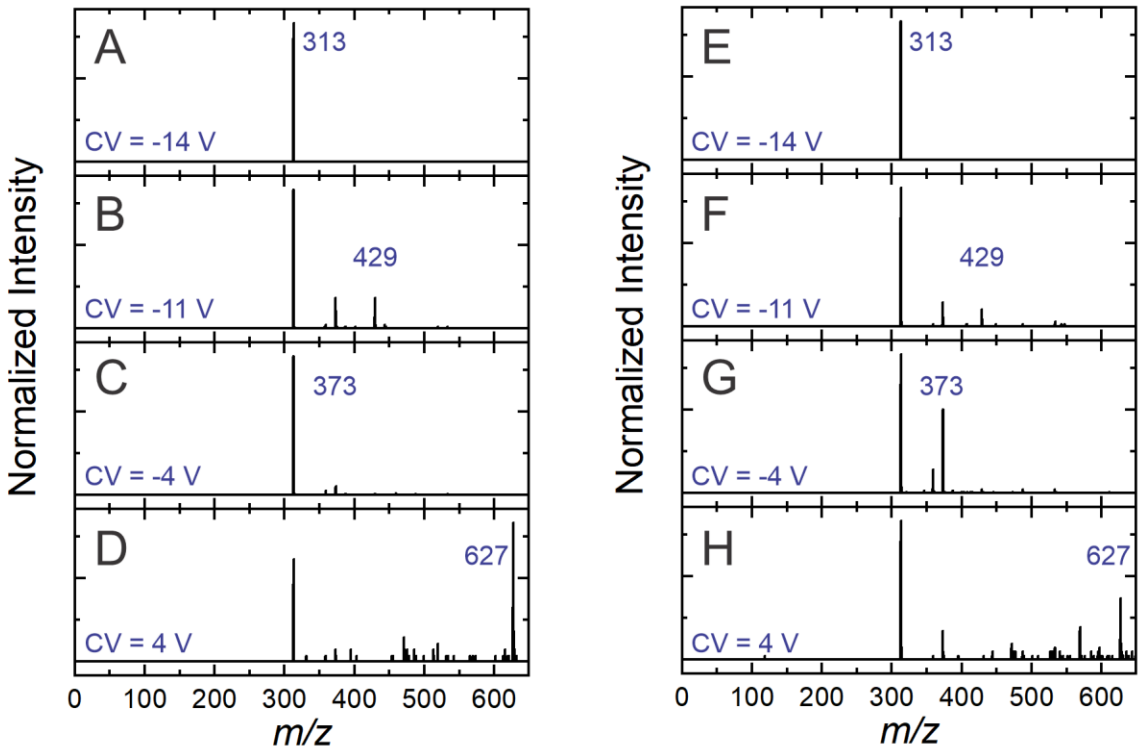

Figure S8. Precursor ion scans of peaks I-IV taken at DcP set to 0 V for $[CBD - H]^-$ (**A – D**) and $[CBC - H]^-$ (**E – H**) in an N_2 carrier gas environment seeded with 1.5% (*v/v*) acetone. Ions of interest are labelled.

Precursor ion studies of MeCN-modified conditions

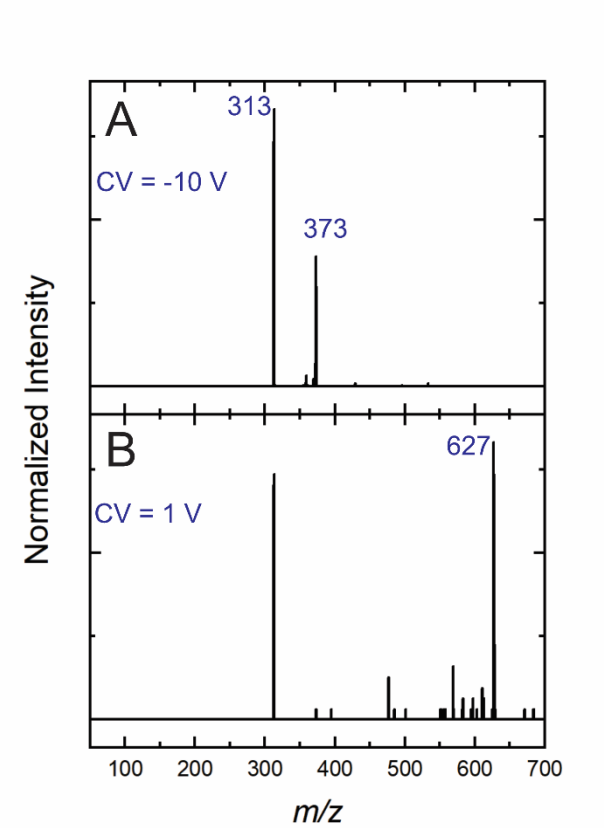

Figure S 9. Precursor ion scans of deprotonated THC in N_2 seeded with 1.5% (*v/v*) MeCN at SV = 3600 V for the ion populations at (**A**) CV = −10 V and (**B**) CV = 1 V. The ion population at CV = −10 V includes an adduct with acetic acid, while the ion population at CV = 1 V includes a THC dimer.

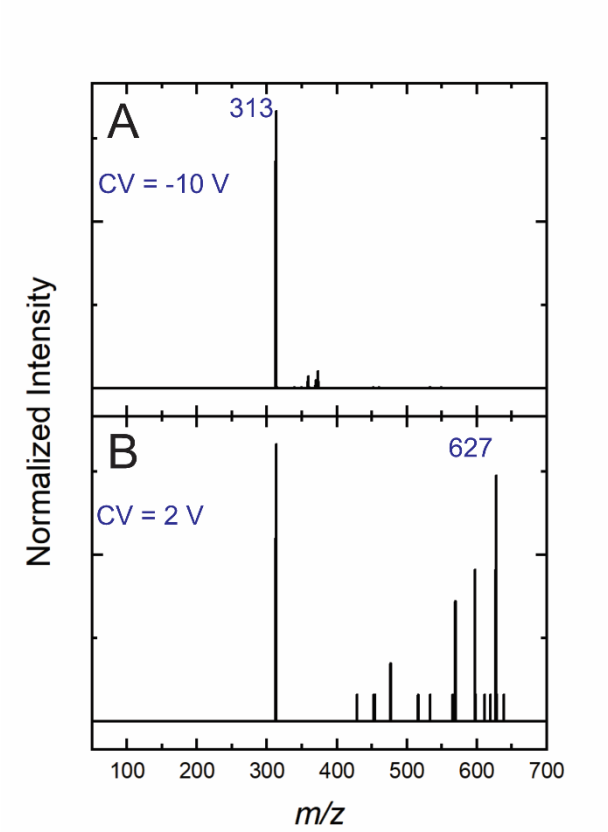

Figure S10. Precursor ion scans of deprotonated CBD in N_2 seeded with 1.5% (*v/v*) MeCN at SV = 3600 V for the ion populations at (**A**) CV = −10 V and (**B**) CV = 2 V. The ion population at CV = 2 V includes a CBD dimer.

IPA modifier studies

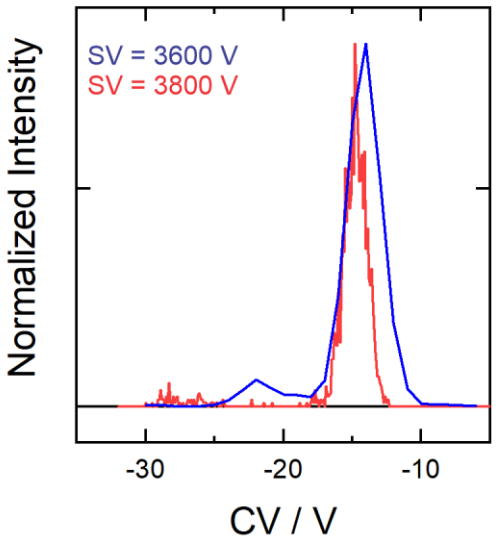

Figure S11. Ionogram of $[\mathrm{THC}-\mathrm{H}]^-$ taken under N_2 gas conditions seeded with 1.5% (*v/v*) IPA at $\mathrm{T} = 150$ °C at SV = 3600 V (*blue*) and SV = 3800 V (*red*) shows the disappearance of the minor ionogram peak with increasing SV.

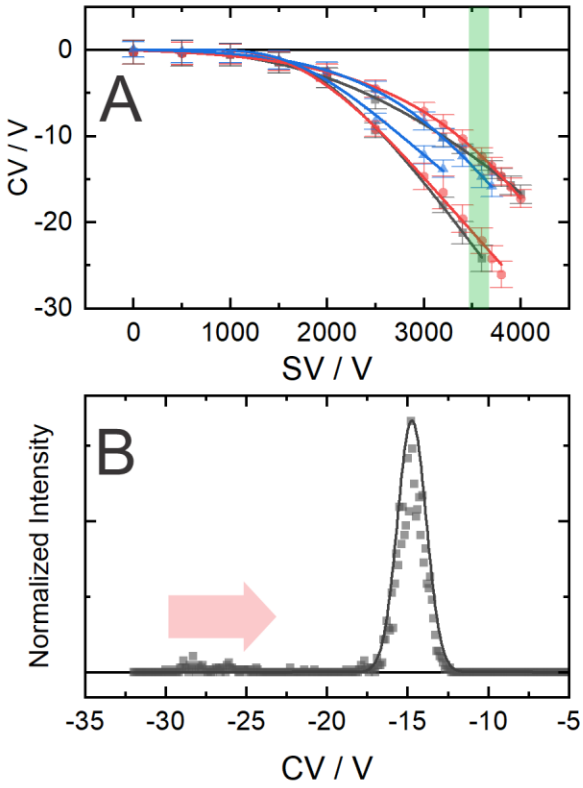

Figure S12. (**A**) Dispersion plots of $[CBD - H]^-$ taken under N_2 gas conditions seeded with 1.5% (*v/v*) IPA at $T = 150$ °C (*black*), $T = 225$ °C (*red*), and $T = 300$ °C (*blue*). (**B**) The ionogram of $[CBD - H]^-$ under N_2 gas conditions seeded with 1.5% (*v/v*) IPA at $T = 150$ °C and SV = 3800 V. As temperature is increased, the dominant peak does not change significantly in DMS behavior, while the minor peak trends towards weaker clustering.

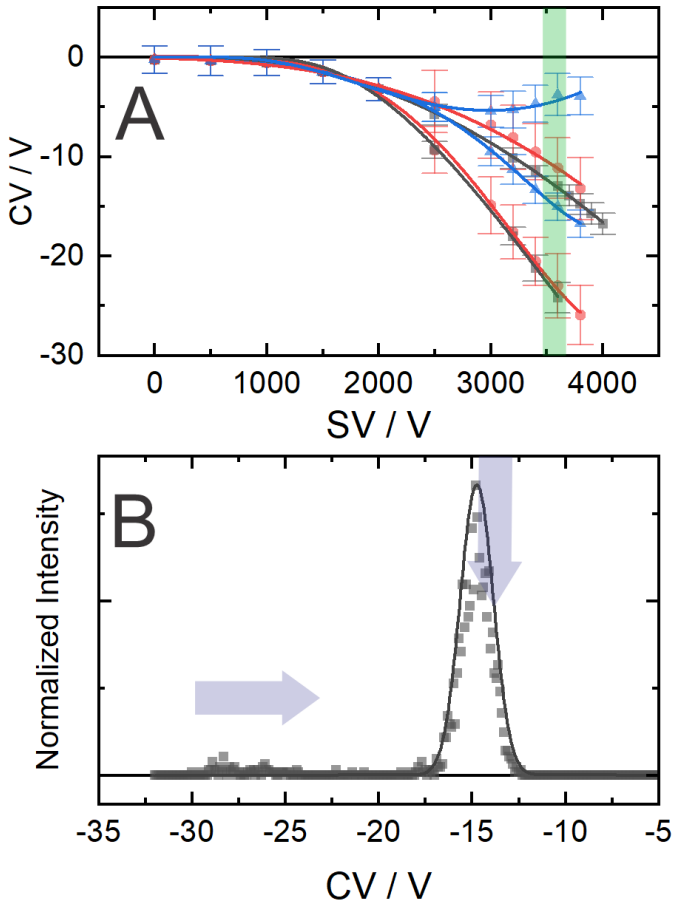

Figure S13. (**A**) Dispersion plots of $[CBD - H]^-$ taken under N_2 gas conditions seeded with 0.6% (*v/v*) IPA (*black*), 0.3% (*v/v*) IPA (*red*), and 1.5% (*v/v*) IPA (*blue*) at T=150 °C. (**B**) The ionogram of $[CBD - H]^-$ under N_2 gas conditions seeded with 1.5% (*v/v*) IPA at T=150 °C and SV = 3800 V. As the concentration of IPA reduces in the carrier gas, the dominant peak decreases in intensity while the minor peak shifts towards weaker clustering.

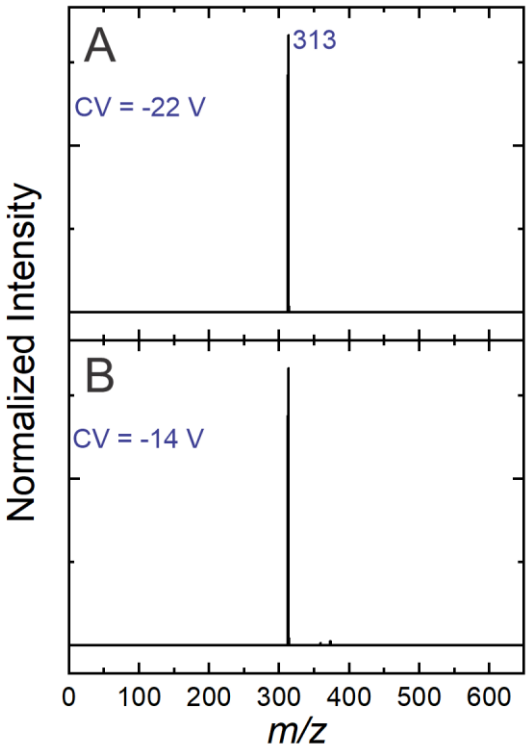

Figure S14. Precursor ion scans of peaks I and II taken at DcP set to 0 V for $[THC - H]^-$ in an N_2 carrier gas environment seeded with 1.5% (*v/v*) IPA at CV = −22 V (**A**) and CV = −14 V (**B**). No *m/z* ion peak other than the parent ion mass is detected.

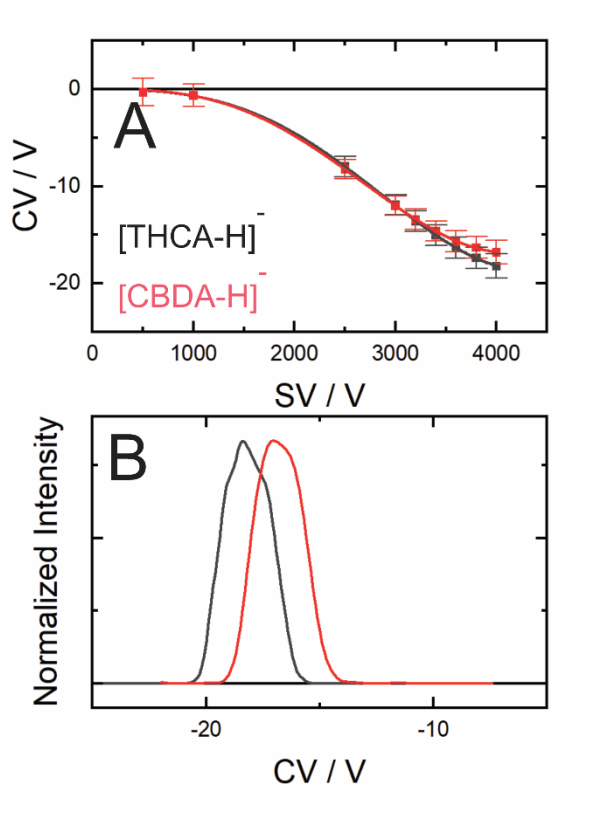

Figure S15. (**A**) Dispersion plots of deprotonated (−)-THCA (*black*) and CBDA (*red*) under an N_2 seeded with 1.5% (*v/v*) IPA at T = 150 °C shows inadequate separation at high SV. (**B**) An ionogram taken at SV = 4000 V of the two isomers with resolving gas shows insufficient separation at these conditions.

Table S3. Computed binding energies ($kJ\ mol^{-1}$) of adducts formed between anionic cannabinoid molecules, $[M-H]^{-1}$, and neutral solvent molecules at T = 298 K.

Cannabinoid	**Binding Energy**				
	MeOH	MeCN	ACE	IPA	AA
Δ^9-THC	32.6	22.7	17.4	34.1	93.0
CBD	37.5	28.7	17.9	43.4	78.3
CBC	35.2	14.3	7.5	49.2	85.6
(−)-THCA	21.6	9.4	5.3	19.6	67.1
CBDA	10.6	10.1	2.3	11.8	37.1

Quantification of Cannabinoid Derivatives

The standard addition method for THCA yielded precise results, allowing for the quantification of THCA using this method. In the case of CBDA, due to the effect of ionization efficiency, the use of an internal standard is better suited for calibration, to account for the ionization efficiency occurring. An internal standard calibration curve is shown for the case of CBDA. Accurate measurements of CBDA were achieved using this method. A calibration plot of CBDA is also provided to determine the LOD and LOQ values using the separation methods employed.

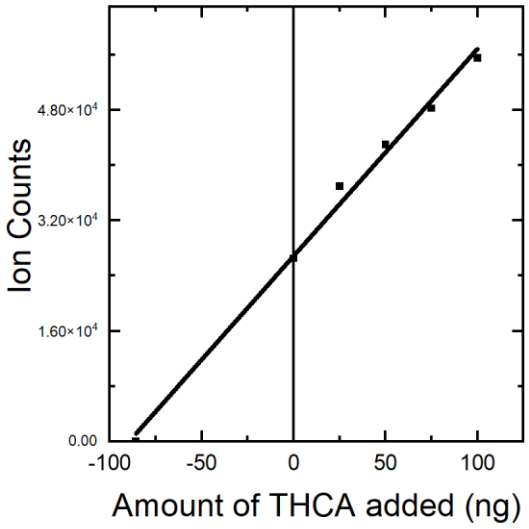

Figure S16. Standard addition calibration curve of THCA in marijuana flower extract Blueberry Haze

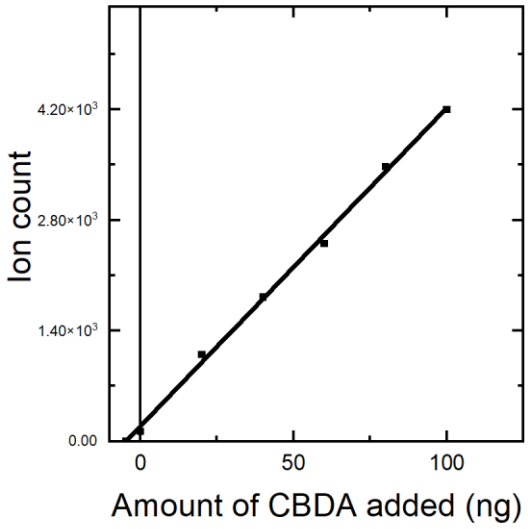

Figure S17. Standard addition calibration curve of CBDA in marijuana flower extract Blueberry Haze

Table S4. LOD and LOQ of the proposed method and accuracy determination

Isomer	LOD (ng/mL)	LOQ (ng/mL)	R^2
(−)-**THCA**	13	41	0.993
CBDA	7	21	0.996

A second marijuana extra (Pure Sun) was acquired and extracted using the methods mentioned previously. A 200 ng/mL concentration of flower to solvent was used in the quantification of THCA and CBDA in the extract. The concentration of the two carboxylated isomers was determined using standard addition.

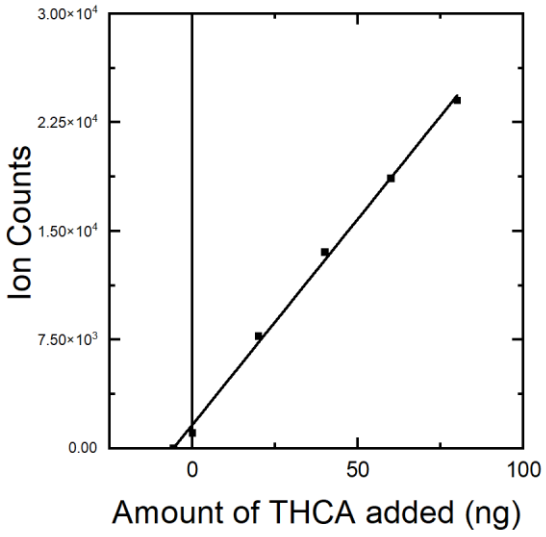

Figure S18. Standard addition calibration curve of THCA in marijuana flower extract Pure Sun

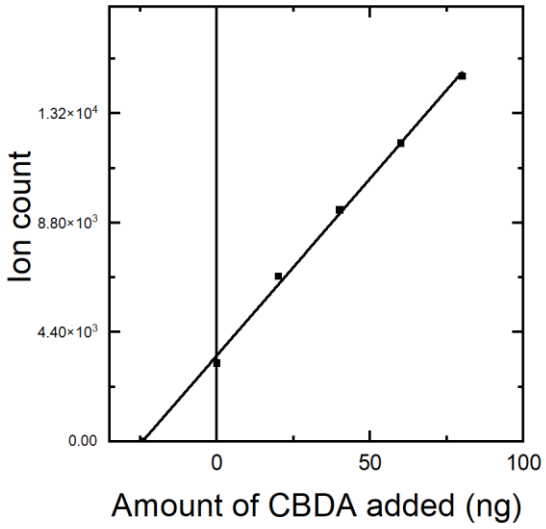

Figure S19. Standard addition calibration curve of CBDA in marijuana flower extract Pure Sun

Table S5. Calculated results from quantification of Pure Sun Marijuana extract

Isomer	Expected (*w*/w) Percentage (%)	Calculated (*w*/w) Percentage (%)	R^2
(−)-**THCA**	0-2	2.8 ± 0.06	0.997
CBDA	10-15	12.1 ± 0.2	0.997

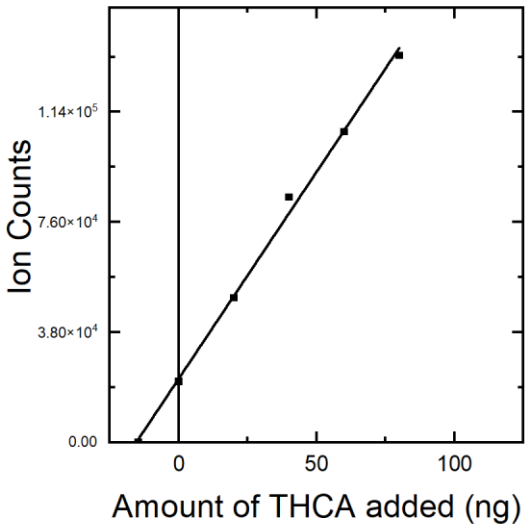

Figure S20. Standard addition calibration curve of THCA in marijuana flower extract Skunky Haze

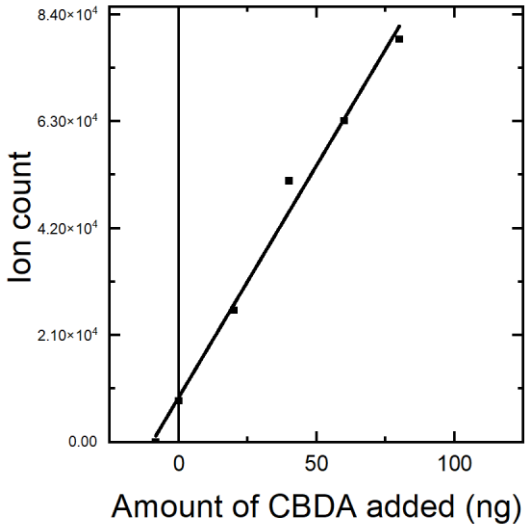

Figure S21. Standard addition calibration curve of CBDA in marijuana flower extract Skunky Haze

Table S6. Calculated results from quantification of Skunky Haze Marijuana extract

Isomer	Expected (*w*/w) Percentage (%)	Calculated (*w*/w) Percentage (%)	R^2
(−)-**THCA**	7-12	7.3 ± 0.06	0.995
CBDA	7-12	4.2 ± 0.04	0.987

Quantification of the decarboxylated isomer sets

The amounts of THC, CBD, and CBC were negligible in the marijuana flower extract tested, as expected. To test the accuracy of quantifying these isomers using the developed method, a 1:1:1 standard mixture of a predetermined concentration of each isomer was measured in the DMS and quantified via standard addition. A summary of the accuracy of the quantification step is provided in Table S7.

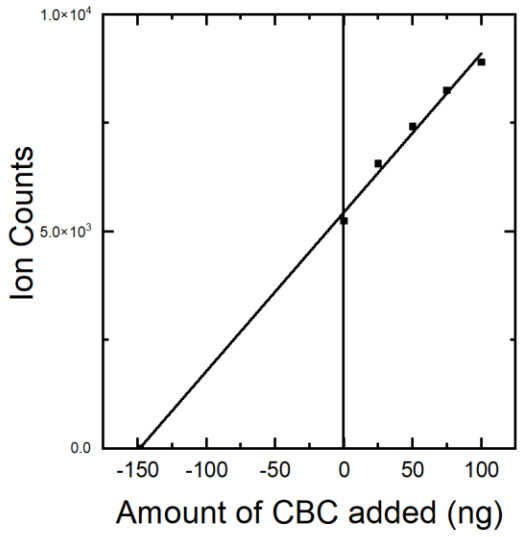

Figure S22. Standard addition calibration curve of CBC in standard mixture

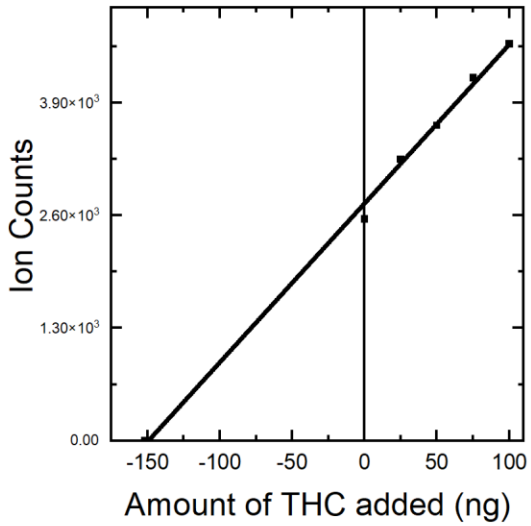

Figure S23. Standard addition calibration curve of THC in standard mixture

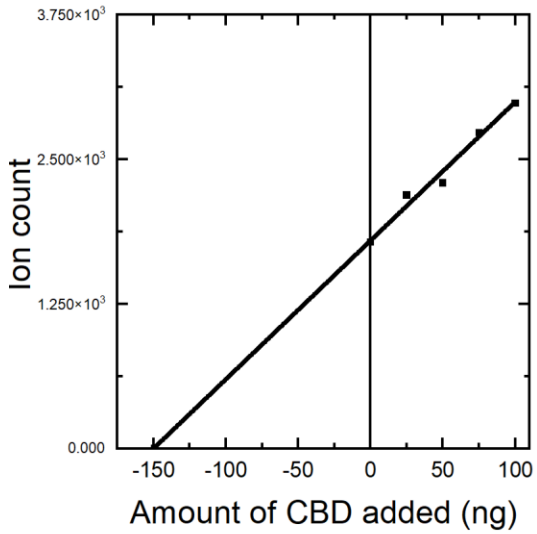

Figure S24. Standard addition calibration curve of CBD in standard mixture

Table S7. Calculated results from quantification of THC, CBD, and CBC standard mixture

Isomer	Concentration in Sample (ng/mL)	Measured Concentration (ng/mL)	LOD (ng/mL)	LOQ (ng/mL)	R^2
THC	150	152.0	7	23.9	0.990
CBD	150	149.0	18.9	57.2	0.978
CBC	150	148.2	18.4	55.7	0.982

XYZ coordinates of optimized cannabinoid molecule structures

[THC – H]$^-$ Bare Ion

O	-0.61031800	-1.98794800	0.61960700
O	-0.26015400	1.65800400	-2.51377800
C	-2.50404000	-0.51109900	0.58916700
C	-1.95818700	0.27847300	-0.61287300
C	-2.05078600	-1.98283200	0.53781300
C	-4.00602300	-0.23558200	0.72896200
C	-0.49269000	-0.03453000	-0.84837800
C	-4.23120600	1.24928900	1.06761400
C	-2.27550800	1.74925500	-0.41274400
C	-3.29508300	2.18880800	0.33403500
C	0.09633100	-1.13201000	-0.22821500
C	-2.48963200	-2.76451000	1.77912000
C	-2.48939500	-2.72201000	-0.73620300
C	0.27445300	0.73834500	-1.81534400
C	1.44595000	-1.46880300	-0.40013300
C	2.23271400	-0.68137000	-1.25092700
C	-3.57989900	3.65902600	0.51434800
C	1.66267100	0.38522200	-1.93485800
C	3.70852700	-0.99636900	-1.42366700
C	4.65712800	0.02950200	-0.76883100
C	4.53304000	0.10947000	0.75583200
C	5.44700700	1.16459700	1.38886300
C	5.32805200	1.23386600	2.91512000
H	-2.01258200	-0.10570900	1.48506100
H	-2.51797300	-0.02886400	-1.51457000
H	-4.46412000	-0.85818600	1.50476000
H	-4.51069500	-0.47739400	-0.21414600
H	-4.10887400	1.40211300	2.15180700
H	-5.27345400	1.52778600	0.85435500
H	-1.63721700	2.43599100	-0.95755800
H	-2.22833000	-2.21735400	2.68907200
H	-3.56685800	-2.94922900	1.77518200
H	-1.97375100	-3.72806100	1.80092200
H	-3.57913600	-2.71341300	-0.83950000
H	-2.05255200	-2.26297900	-1.62403000
H	-2.15410800	-3.76217100	-0.69186700
H	1.84609800	-2.33490200	0.11471200
H	-3.55031900	3.94477400	1.57526100
H	-4.58207000	3.92268700	0.14862100
H	-2.85128500	4.27088100	-0.02188300
H	3.91967200	-1.99074600	-1.01025700
H	3.94738200	-1.04643300	-2.49336700
H	4.45386100	1.01775000	-1.19735500
H	5.69481800	-0.22041600	-1.03473900
H	3.49085300	0.32128700	1.01642200
H	4.76126300	-0.87404400	1.19038700
H	5.20856300	2.14648200	0.96170900
H	6.49047300	0.95874000	1.11420100
H	5.59235500	0.27556600	3.37528700
H	5.98653000	1.99975000	3.33852800
H	4.30300500	1.47013300	3.21726300
H	2.25169100	0.97508000	-2.63310300

[CBD – H]$^-$ Bare Ion

O	-1.01488400	-1.27162600	-1.64537300
O	-0.01983700	0.21378700	2.77759800
C	-2.22284500	1.24928900	-0.40857000
C	-1.94670300	0.13844000	0.66767300

C	-3.70997800	1.30789300	-0.78431300
C	-4.23688900	-0.05784400	-1.23318300
C	-2.98399800	-0.96126500	0.68161500
C	-0.56616000	-0.49798600	0.56824200
C	-3.99561400	-1.10672300	-0.17596200
C	-1.64336400	2.59192900	0.01244100
C	-0.13696800	-1.18235000	-0.56257800
C	0.31497100	-0.40876600	1.72207700
C	-4.90983000	-2.30191700	-0.17466900
C	-0.16559400	2.61475200	0.31980400
C	2.00613800	-1.68662600	0.42943900
C	1.12931600	-1.77109000	-0.66562700
C	1.60517100	-1.03501200	1.58214300
C	3.40765300	-2.24905100	0.30191700
C	-2.37092800	3.71142800	0.11767400
C	4.31496200	-1.41139700	-0.62367000
C	4.51749300	0.02647800	-0.13907500
C	5.36772100	0.87580200	-1.08813700
C	5.55935400	2.31304100	-0.59291100
H	-1.68298100	0.95237100	-1.31419800
H	-1.95869400	0.60811800	1.65826400
H	-3.86045600	2.04879000	-1.57779900
H	-4.29740200	1.63693200	0.08152200
H	-3.74623500	-0.36203700	-2.16952200
H	-5.31113800	0.01176900	-1.45356000
H	-2.81102200	-1.72008400	1.44231600
H	-5.95976100	-2.00666300	-0.04072600
H	-4.64913500	-3.00876500	0.61768900
H	-4.85522400	-2.83586700	-1.13376500
H	0.40695700	2.08688800	-0.44874200
H	0.20253100	3.64201200	0.39798000
H	0.03329400	2.10045700	1.26541400
H	1.41981200	-2.28939000	-1.57735000
H	2.27623600	-0.95498700	2.43265500
H	3.86806800	-2.30785600	1.29491100
H	3.36441200	-3.27463700	-0.08739300
H	-1.90549400	4.64794900	0.41137300
H	-3.43834800	3.74273600	-0.06279000
H	3.87236400	-1.39031200	-1.62711100
H	5.29207300	-1.90615500	-0.72143100
H	3.53780500	0.49524700	-0.00130500
H	4.98506700	0.01122400	0.85499000
H	-0.56487800	-1.76037700	-2.34042900
H	4.89191400	0.89134800	-2.07696900
H	6.34861600	0.40171700	-1.22906700
H	6.16224000	2.90628000	-1.28851400
H	4.59407000	2.81403900	-0.47149800
H	6.05962700	2.32780600	0.38127800

[CBC – H]$^{-}$ Bare Ion

O	2.09657200	-0.53537400	-1.54912800
O	1.35677900	-3.02510600	2.48830800
C	3.27290400	0.14059300	-1.02734300
C	2.85141500	1.57177400	-0.60414000
C	3.90481200	-0.64419700	0.10140300
C	1.26705000	-1.21927400	-0.67311000
C	4.21925200	0.22719000	-2.22949900
C	1.87488400	1.63724100	0.58333900
C	1.78202300	-1.75705500	0.51303200
C	-0.92607100	-2.06939300	-0.18056800
C	3.16960000	-1.51845000	0.81453400
C	-2.40133200	-2.12840300	-0.51895600

C	-0.06177800	-1.35950400	-1.04619600
C	-3.12719200	-0.80793000	-0.20486000
C	0.92864600	-2.51658700	1.41491500
C	-0.45203300	-2.62734000	0.99167300
C	-4.62289400	-0.83408900	-0.52950800
C	1.37492900	3.02988100	0.83204200
C	-5.33620700	0.48605700	-0.21862200
C	0.11158500	3.46984500	0.75262100
C	-6.83252100	0.45770800	-0.54586200
C	-0.23331100	4.91409400	1.02927800
C	-1.07477500	2.60716700	0.39740700
H	3.75721200	2.14772600	-0.36895100
H	2.38510300	2.04369300	-1.47773700
H	4.95233300	-0.45354200	0.31471500
H	3.74100800	0.76653100	-3.05237600
H	5.14083800	0.74865900	-1.95341700
H	4.47179200	-0.77909300	-2.56928400
H	2.38495600	1.25827900	1.47591300
H	1.04638800	0.95651500	0.40235800
H	3.58710000	-2.06631000	1.65350300
H	-2.53328800	-2.35811000	-1.58511600
H	-2.87823600	-2.94071700	0.04170200
H	-0.41300300	-0.91741300	-1.97175500
H	-2.64543900	0.00348400	-0.76214200
H	-2.98272100	-0.57420000	0.85659200
H	-1.12068200	-3.16961700	1.65492400
H	-4.76145700	-1.07739800	-1.59216300
H	-5.10482100	-1.64593400	0.03252400
H	2.14299800	3.76057200	1.09336300
H	-4.85242200	1.29565300	-0.77877700
H	-5.19665000	0.72760000	0.84217500
H	-7.34413700	-0.32399800	0.02586100
H	-7.31699200	1.41176200	-0.31441800
H	-6.99779300	0.24832400	-1.60825000
H	-0.94830800	4.99494500	1.85840700
H	0.65070600	5.50443100	1.28416300
H	-0.71441100	5.37715400	0.15774800
H	-0.80962900	1.57695400	0.16334300
H	-1.79718100	2.58733700	1.22304800
H	-1.60398900	3.02458100	-0.46887600

[THCA – H]$^-$ Bare Ion

O	1.19558100	-2.19954300	-0.57129900
O	0.59803700	2.30299800	0.90289900
O	-1.56221700	3.41709700	0.66005000
O	-3.30689800	2.42286100	-0.28337000
C	3.22740000	-1.02246300	-0.06925200
C	2.47205100	0.21135200	0.45543100
C	2.42959600	-2.31311500	0.17718700
C	4.66787600	-0.98002900	0.44939400
C	1.00919300	0.14412000	0.06292300
C	5.39398500	0.23450500	-0.15428900
C	3.21400800	1.45488500	-0.00006900
C	4.52436500	1.46946500	-0.26547900
C	0.46929000	-1.03041000	-0.43629300
C	3.11200300	-3.53815100	-0.43090600
C	2.09889700	-2.56165900	1.65477500
C	0.13244600	1.25573600	0.30111800
C	-0.86923800	-1.11693400	-0.83971400
C	-1.72334800	-0.02824900	-0.71228500
C	5.23664600	2.71760000	-0.71997800
C	-1.24795100	1.17396600	-0.13046500

C	-3.15838800	-0.23567500	-1.15817100
C	-4.11406800	-0.51882800	0.01299700
C	-2.13134800	2.36578200	0.06388300
C	-5.57232800	-0.64275700	-0.43365800
C	-6.53971700	-0.93789600	0.71688800
C	-8.00007700	-1.04543200	0.26584600
H	3.26716700	-0.92884000	-1.16352500
H	2.52110600	0.21184200	1.55712900
H	5.21637200	-1.89354400	0.20062800
H	4.65677300	-0.89978800	1.54254300
H	5.76493800	-0.02133900	-1.15889100
H	6.29132300	0.46894900	0.43494900
H	2.62568200	2.36134400	-0.06543000
H	3.40041200	-3.34019100	-1.46651000
H	4.00159600	-3.81823000	0.13779400
H	2.41568500	-4.38020200	-0.42332400
H	3.01443500	-2.61723900	2.25076000
H	1.47108800	-1.76416800	2.05385900
H	1.55640500	-3.50497900	1.75728500
H	-1.22412500	-2.05956000	-1.24033600
H	5.71623600	2.56470600	-1.69638800
H	6.03507000	2.99738100	-0.01965700
H	4.54907000	3.56160300	-0.80721000
H	-3.51785600	0.64420000	-1.69141300
H	-3.18493100	-1.08771500	-1.84905200
H	-4.02870500	0.29661700	0.73471300
H	-3.79952100	-1.44109500	0.51943700
H	-0.58506800	3.14178900	0.86873900
H	-5.86920000	0.29291500	-0.92382600
H	-5.66269400	-1.43345700	-1.19279800
H	-6.44597600	-0.14755800	1.47111300
H	-6.23937400	-1.87014200	1.21243900
H	-8.33267400	-0.11364900	-0.20356000
H	-8.12574700	-1.84705100	-0.47046100
H	-8.67127600	-1.25478800	1.10543700

[CBDA – H]$^-$ Bare Ion

O	-1.07284100	-1.61220700	-0.96564300
O	-0.42483300	1.35279400	2.66512400
O	2.68290900	-3.18883900	-0.76476200
O	0.68463100	-3.11859000	-1.72701700
C	-2.38769100	1.14152000	-0.70450900
C	-2.19936000	0.40783400	0.65408500
C	-3.87126500	1.52656000	-0.85966800
C	-4.75093600	0.27271200	-0.91762900
C	-3.25271700	-0.66850900	0.82576700
C	-0.79032300	-0.12509000	0.83087000
C	-4.39957700	-0.74001800	0.14750100
C	-1.45403100	2.32328200	-0.86933200
C	-0.29070900	-1.14026200	-0.05231800
C	0.05310700	0.36905600	1.80616200
C	-5.38054700	-1.86678700	0.33308700
C	1.89964700	-1.04408900	1.09481700
C	1.07625700	-1.60653200	0.09265400
C	-1.56978500	3.46037300	0.11673400
C	1.37383500	-0.07621500	1.94634600
C	3.37282600	-1.36968300	1.26595400
C	-0.54248500	2.34023700	-1.84550500
C	4.26533900	-0.71742900	0.18960800
C	4.17912300	0.81078300	0.14673800
C	1.56283800	-2.69190900	-0.81818400
C	5.05674500	1.43499300	-0.94226300

C	4.94993800	2.96259600	-0.99499700
H	-2.14783900	0.41070100	-1.47997400
H	-2.36687800	1.13701800	1.45399900
H	-4.18406300	2.14556300	-0.00956400
H	-4.01038900	2.12917700	-1.76429600
H	-5.81071600	0.55113300	-0.82888600
H	-4.64985400	-0.20742200	-1.90239500
H	-3.01957000	-1.43605300	1.56003200
H	-5.51301700	-2.42275200	-0.60455300
H	-5.04476000	-2.57301600	1.09640000
H	-6.37242000	-1.49287100	0.62115000
H	-0.89006100	4.27700100	-0.14007200
H	-2.58872300	3.86216800	0.14840900
H	-1.32507400	3.11583100	1.12603100
H	2.00568000	0.36669400	2.71258100
H	3.52900700	-2.44687700	1.23047700
H	3.69035500	-1.00888100	2.25294900
H	-0.42868900	1.50139000	-2.52368400
H	0.13976200	3.17603800	-1.97326100
H	5.30633500	-1.01786200	0.37208300
H	3.98897300	-1.13496700	-0.78117500
H	3.13748300	1.10893400	-0.01490700
H	4.46484800	1.22697000	1.12407500
H	-0.18614200	-2.57097600	-1.57306700
H	0.28735900	1.58608800	3.26789700
H	6.10344800	1.14462500	-0.78136500
H	4.77035300	1.01443400	-1.91373900
H	5.57983600	3.38821200	-1.78324100
H	5.25677100	3.41057400	-0.04326000
H	3.91769900	3.27332800	-1.18577300

[THC – H]$^-$ ⋯ IPA

O	0.85926600	-2.41161800	0.10367300
O	0.22505500	2.11022800	-1.40005000
C	2.78361400	-0.99962600	0.36481000
C	2.02263600	0.24858800	-0.10955100
C	1.83772700	-1.98067200	1.07759500
C	4.03667800	-0.55459100	1.12514100
C	0.71813300	-0.13868600	-0.77801700
C	4.99037300	0.17315400	0.16136500
C	2.95149000	1.09000300	-0.96238200
C	4.28250100	1.06474700	-0.83826100
C	0.21547600	-1.42987800	-0.64062500
C	2.54523900	-3.27546300	1.47809500
C	1.11593400	-1.36953800	2.28633500
C	-0.08806800	0.85919700	-1.44134500
C	-0.99231900	-1.83316100	-1.22411900
C	-1.73063900	-0.90609500	-1.96366700
C	5.18669400	1.91252400	-1.69609700
C	-1.27486300	0.40283200	-2.08475200
C	-3.08513300	-1.29078200	-2.52675600
C	-4.25411600	-0.57094100	-1.82217100
C	-4.29448400	-0.80738000	-0.31030600
C	-5.44352000	-0.07626000	0.38927400
C	-5.42470500	-0.25735300	1.91024800
H	3.11441700	-1.53870000	-0.53443600
H	1.77341000	0.86422500	0.76898500
H	4.55765200	-1.40154600	1.58284100
H	3.74486700	0.12157100	1.93664300
H	5.58877300	-0.56710100	-0.39288600

H	5.71904200	0.76722400	0.73074100
H	2.47056800	1.76019400	-1.66518100
H	3.10518200	-3.68180100	0.63155600
H	3.23224200	-3.10925200	2.31110900
H	1.80046000	-4.01457900	1.78390100
H	1.83718300	-1.02143200	3.03136100
H	0.49652800	-0.52370000	1.98885500
H	0.46992800	-2.12133600	2.74756500
H	-1.34307400	-2.84569600	-1.06095400
H	5.89879500	1.29061600	-2.25632900
H	5.78622800	2.60025800	-1.08422300
H	4.61546100	2.50608000	-2.41345500
H	-3.12545500	-1.05710500	-3.59799900
H	-3.22442500	-2.37476100	-2.43517400
H	-5.20399800	-0.89272700	-2.27239600
H	-4.16861200	0.50606200	-2.00654100
H	-4.36923000	-1.88490400	-0.10836900
H	-3.34107800	-0.48546400	0.12045900
H	-6.40363100	-0.42634700	-0.01321500
H	-5.38420400	0.99251900	0.15023200
H	-4.49084700	0.12519300	2.33329200
H	-6.25289400	0.27138100	2.39338200
H	-5.49832500	-1.31632500	2.18063600
H	-1.86273900	1.15039200	-2.60949600
C	-1.47587000	1.89284100	2.96848700
H	-2.39304400	1.34754200	3.21427000
H	-1.55474800	2.91008400	3.36660200
H	-0.63281100	1.39909600	3.45943100
C	-1.25357000	1.93987300	1.46038000
H	-1.16953000	0.90839800	1.08505600
C	-2.41546200	2.60954400	0.72195000
H	-2.19863000	2.63149400	-0.34802200
H	-3.35076700	2.06198700	0.88020400
H	-2.54148300	3.63794400	1.07822200
O	-0.03256400	2.63006400	1.23254500
H	0.16224800	2.56385100	0.26019100

[CBD – H]$^{-}$ ⋯ IPA

O	1.28628600	-2.41861000	-1.47343300
O	0.48990900	1.70481000	0.76934800
C	2.87318600	-1.36751800	0.99977900
C	2.40287700	-0.25789600	0.02051300
C	4.39721200	-1.24067200	1.20253600
C	5.14170400	-1.48116800	-0.11580900
C	3.30702100	-0.19772800	-1.19162100
C	0.93409200	-0.35225300	-0.34487400
C	4.52777800	-0.73290100	-1.27732400
C	2.12230800	-1.36373400	2.31765600
C	0.40924400	-1.41253300	-1.07479200
C	0.05057200	0.70278900	0.08559000
C	5.35850100	-0.66639300	-2.53179200
C	2.07021300	-0.07296700	3.09384700
C	-1.81555200	-0.48055700	-1.01248800
C	-0.94430600	-1.50123200	-1.41742600
C	-1.32582200	0.59209100	-0.28334400
C	-3.29549900	-0.58783000	-1.31190100
C	1.52935600	-2.47603000	2.76299700
C	-4.08018500	-1.28726300	-0.18798300

C	-5.58024700	-1.40098400	-0.47303000
C	-6.36575200	-2.09365600	0.64536000
C	-7.86564000	-2.20178200	0.35270500
H	2.68797900	-2.32970900	0.51345800
H	2.49186800	0.70900700	0.52990600
H	4.73503900	-1.95144000	1.96482100
H	4.63295800	-0.23542000	1.57072400
H	5.15141400	-2.55728700	-0.34901500
H	6.19735900	-1.19283300	-0.00979300
H	2.89658500	0.33020800	-2.04982400
H	6.31731400	-0.16162500	-2.35137600
H	4.83852500	-0.13451800	-3.33270600
H	5.59979200	-1.67467000	-2.89596800
H	1.60119100	-0.21846400	4.07054100
H	3.07512000	0.33477800	3.25419500
H	1.50207200	0.68232300	2.53849100
H	-1.31001800	-2.35224400	-1.98863700
H	-1.98926400	1.38996400	0.03569500
H	-3.71330000	0.41442900	-1.46395400
H	-3.44939200	-1.13858400	-2.24907300
H	0.99702600	-2.49722900	3.70953100
H	1.52977200	-3.39013900	2.17734800
H	-3.92069500	-0.73572200	0.74539500
H	-3.65673500	-2.28622600	-0.02797200
H	-5.99568500	-0.39728900	-0.63650200
H	-5.73310800	-1.94891500	-1.41343100
H	0.78278100	-3.06128900	-1.98134000
H	-6.21311300	-1.54557200	1.58291900
H	-5.95031300	-3.09576100	0.80900000
H	-8.31063600	-1.21043200	0.21637000
H	-8.04645200	-2.77174700	-0.56508800
H	-8.40289100	-2.69962500	1.16620800
C	-0.71712900	4.16264300	-1.30270600
H	-1.80165600	4.10617800	-1.44609200
H	-0.31010400	3.15380800	-1.39096200
H	-0.28908200	4.78901700	-2.09509600
C	-0.40383200	4.73276200	0.08607300
H	0.69367700	4.80224600	0.18220600
C	-0.99403500	6.12871800	0.27384100
H	-2.08509600	6.08230900	0.18976100
H	-0.74676800	6.51287600	1.26733800
H	-0.61400900	6.82637600	-0.48050600
O	-0.92158700	3.90880800	1.11126900
H	-0.44540100	3.02971500	1.05112000

[CBC – H]$^{-}$ ··· IPA

O	1.903227	-0.780290	-2.261968
O	1.092651	-2.788847	2.027352
C	3.132367	-0.127903	-1.831672
C	2.810091	1.369862	-1.594339
C	3.731897	-0.793680	-0.621800
C	1.067188	-1.347539	-1.316799
C	4.068063	-0.263022	-3.038946
C	1.932531	1.636314	-0.360926
C	1.560565	-1.785983	-0.092730
C	-1.153456	-2.079747	-0.744264
C	2.954628	-1.569616	0.201562
C	-2.638821	-2.099006	-1.048567

C	-0.279958	-1.475736	-1.676453
C	-3.334978	-0.813042	-0.567005
C	0.685202	-2.411984	0.873312
C	-0.687674	-2.544039	0.464650
C	-4.840602	-0.788761	-0.837217
C	1.363275	3.030745	-0.320087
C	-5.529319	0.480012	-0.323930
C	0.096101	3.383420	-0.295883
C	-7.032587	0.513804	-0.614100
C	-0.324837	4.839317	-0.234184
C	-1.074119	2.419229	-0.309565
H	3.751449	1.928954	-1.508577
H	2.298636	1.731336	-2.494365
H	4.770869	-0.617508	-0.409025
H	3.622721	0.208849	-3.919742
H	5.030989	0.212673	-2.831901
H	4.236060	-1.319088	-3.255889
H	2.527712	1.454232	0.538272
H	1.125470	0.908285	-0.337536
H	3.360670	-2.015484	1.089287
H	-2.806531	-2.214828	-2.126316
H	-3.105833	-2.961593	-0.556536
H	-0.618686	-1.102970	-2.628268
H	-2.861145	0.049190	-1.049170
H	-3.149454	-0.696384	0.506664
H	-1.366581	-2.999818	1.185025
H	-5.018847	-0.884652	-1.917063
H	-5.309287	-1.667313	-0.373709
H	2.118362	3.830101	-0.304694
H	-5.047729	1.357951	-0.770876
H	-5.364322	0.563170	0.756637
H	-7.222005	0.470405	-1.691697
H	-7.539349	-0.343909	-0.159427
H	-7.502031	1.424998	-0.229365
H	-0.963415	5.102779	-1.084833
H	-0.909505	5.042624	0.670359
H	0.539496	5.508213	-0.238128
H	-1.744917	2.644051	-1.146079
H	-0.771432	1.376229	-0.394365
H	-1.670678	2.521732	0.603239
C	-0.634342	0.148527	3.132942
H	-1.167443	0.911255	2.554287
H	-0.895660	0.255353	4.190839
H	-0.960738	-0.833820	2.787561
C	0.880470	0.280520	2.956380
H	1.105252	0.152553	1.892430
C	1.395249	1.644281	3.399976
H	1.184797	1.797430	4.464199
H	2.477327	1.699851	3.254055
H	0.924955	2.445355	2.822626
O	1.575468	-0.712947	3.698278
H	1.468457	-1.559360	3.200650

[THCA – H]$^-$ ··· IPA

O	-0.27372200	2.93361500	0.01782700
O	-0.45678000	-1.82022300	-0.32821100
O	1.56159300	-3.11507300	-0.88487100
O	3.50802400	-2.13263600	-1.27738900

C	-2.48844000	2.02116400	-0.15160800
C	-1.97195400	0.57262100	-0.11746400
C	-1.57609500	2.95488400	0.65899200
C	-3.97848300	2.01282600	0.20337600
C	-0.47101900	0.53406100	-0.32004000
C	-4.76496700	1.25829800	-0.88458600
C	-2.77431700	-0.23719800	-1.11864700
C	-4.03299900	0.06105600	-1.45403500
C	0.27434700	1.70300100	-0.27625300
C	-2.00656600	4.41703300	0.55336700
C	-1.42042100	2.54344300	2.12816500
C	0.21887000	-0.70756100	-0.46622200
C	1.65123900	1.70404600	-0.52672100
C	2.33105000	0.52146100	-0.78930700
C	-4.82055700	-0.77190500	-2.43129000
C	1.63134700	-0.71317100	-0.75146200
C	3.82369300	0.63696000	-1.03278000
C	4.66142600	0.28931100	0.20941000
C	2.32259300	-2.01998800	-0.99257800
C	6.16604500	0.32875800	-0.06601300
C	7.01917100	-0.00031700	1.16302200
C	8.52427200	0.02625100	0.87777300
H	-2.39418900	2.37358900	-1.18815700
H	-2.18669700	0.14817700	0.87504100
H	-4.37788300	3.02650000	0.30323400
H	-4.11468300	1.51703400	1.17087600
H	-4.99820800	1.94451900	-1.71306300
H	-5.73925400	0.93794800	-0.49073500
H	-2.29085000	-1.11347700	-1.53136400
H	-2.16670900	4.69421800	-0.49178800
H	-2.92672900	4.59756400	1.11341100
H	-1.22054800	5.05655800	0.96208500
H	-2.39223200	2.53814200	2.62957000
H	-0.98251700	1.54874200	2.21711700
H	-0.76588800	3.25253800	2.64127900
H	2.17619900	2.65201400	-0.49938700
H	-5.17420100	-0.16489700	-3.27536800
H	-5.71340400	-1.19840500	-1.95507200
H	-4.22303100	-1.59502300	-2.82897900
H	4.12507000	-0.01980000	-1.84836400
H	4.04450400	1.66989100	-1.32890700
H	4.38494500	-0.71205700	0.54688600
H	4.41206500	0.98827300	1.01864400
H	0.62259800	-2.79877100	-0.63373100
H	6.39508800	-0.38579800	-0.86653800
H	6.44820400	1.32150400	-0.44586400
H	6.73429200	-0.99025900	1.53856600
H	6.78553100	0.70985800	1.96657800
H	8.78678600	-0.69885300	0.10030800
H	8.84000100	1.01447300	0.52538000
H	9.11164200	-0.21347200	1.77024000
C	-3.10287100	-3.79803100	0.41484700
H	-4.07817800	-4.08821100	0.00763700
H	-2.65618000	-4.66376300	0.91451100
H	-2.45025700	-3.50621400	-0.41086100
C	-3.24497700	-2.63692900	1.40232200
H	-3.72336700	-1.79889000	0.87133600
C	-4.10771300	-3.00207500	2.60570200

H	-3.65757600	-3.83980400	3.14782700
H	-4.17793700	-2.15287900	3.29093500
H	-5.11787500	-3.28670800	2.29335200
O	-1.98055000	-2.22604600	1.90280400
H	-1.38309100	-2.06933900	1.13427800

[CBDA – H]$^{-}$ ⋯ IPA

O	-0.80419500	-0.41082600	-1.53325800
O	-1.19839500	-0.31129200	3.18489200
O	1.32474800	-0.39889800	-2.63422600
O	3.24507100	-0.11866500	-1.55417300
C	-3.04320600	1.04059400	-0.03245600
C	-2.55785300	-0.25428800	0.68966400
C	-4.56232100	0.94310500	-0.25823000
C	-4.90344500	-0.23030200	-1.18555500
C	-3.13987200	-1.49196200	0.03198900
C	-1.04563900	-0.33770300	0.80882400
C	-4.18799000	-1.50627800	-0.80109800
C	-2.61102700	2.29709700	0.71151500
C	-0.22696500	-0.38501300	-0.36642700
C	-0.41519200	-0.33939800	2.04441800
C	-4.68050600	-2.76763000	-1.46283800
C	1.80883300	-0.40021700	1.04335400
C	1.21996300	-0.37464300	-0.24719400
C	-1.37264700	2.97547900	0.18034600
C	0.98310900	-0.37895300	2.16581100
C	3.29608500	-0.55240300	1.31677000
C	-3.26767700	2.77064600	1.78051800
C	3.73466500	-2.02035800	1.55163900
C	3.44471500	-2.98662900	0.38349300
C	2.01494300	-0.29854900	-1.51030000
C	2.07632800	-3.68373900	0.46202500
C	1.76190900	-4.50091100	-0.79585900
H	-2.55909800	1.04201100	-1.01481000
H	-2.95261400	-0.20732100	1.71224500
H	-5.07091000	0.79828200	0.70473800
H	-4.93932900	1.88441200	-0.67687300
H	-5.99092600	-0.40207800	-1.19101300
H	-4.63517600	0.02316600	-2.22417300
H	-2.63037700	-2.42688600	0.26346900
H	-4.61223800	-2.68351900	-2.55733500
H	-4.09617200	-3.64150800	-1.15706600
H	-5.73763700	-2.95945300	-1.22676100
H	-0.52205100	2.28585900	0.19466700
H	-1.51318300	3.26745700	-0.86848300
H	-1.10882000	3.86652800	0.75954800
H	1.43081000	-0.41391800	3.15847900
H	3.53805300	0.02129300	2.22124200
H	3.87954500	-0.13841100	0.49901200
H	-2.92501700	3.65819200	2.30731900
H	-4.14991400	2.27878100	2.18086500
H	4.81494100	-2.00263900	1.75186300
H	3.25624900	-2.40301900	2.46578500
H	3.52390600	-2.43507600	-0.56035300
H	4.22196600	-3.76485200	0.35207400
H	0.28768100	-0.43941900	-2.34077100
H	-0.61494700	-0.26265200	3.95202600
H	2.05883000	-4.33737900	1.34747900
H	1.28872000	-2.93941300	0.61153300
H	0.79934700	-5.01894000	-0.70980000
H	2.53664200	-5.25645100	-0.98460300
H	1.71139300	-3.84741400	-1.67427600

C	2.74702400	4.31188700	0.23449200
H	3.33590500	5.04365100	-0.33211600
H	3.26118000	4.11731600	1.18141700
H	1.76262700	4.74335300	0.44922800
C	2.60809700	3.02074600	-0.56643200
H	2.02836900	2.29884500	0.02877200
C	1.88583700	3.24370100	-1.89962200
H	1.80801200	2.30744000	-2.45999900
H	0.87168400	3.62676600	-1.73514100
H	2.44409700	3.96640700	-2.50737500
O	3.92736800	2.51261300	-0.77259600
H	3.83865900	1.60144900	-1.11900200

[THC – H]$^-$ ··· MeOH

O	-0.68478900	2.27996500	-0.37291300
O	-0.02682200	-2.47916900	-0.59261000
C	-2.63020100	0.98090500	0.16585200
C	-1.85966300	-0.34597200	0.07686100
C	-1.70951100	2.11977600	0.63486100
C	-3.92188500	0.75005400	0.95630800
C	-0.52002200	-0.14634800	-0.60468800
C	-4.83643800	-0.21014000	0.17532400
C	-2.75588800	-1.38500300	-0.56775700
C	-4.09097900	-1.33153400	-0.51885500
C	-0.01048400	1.13852100	-0.79255200
C	-2.42375700	3.47159600	0.64359100
C	-1.04861500	1.85482100	1.99445700
C	0.30452000	-1.28095700	-0.93796500
C	1.22525300	1.37635700	-1.40211800
C	1.99329500	0.28483600	-1.82514900
C	-4.96202100	-2.37764800	-1.16617500
C	1.53152600	-1.00810000	-1.61410800
C	3.38440400	0.52292800	-2.37700700
C	4.39884100	0.91053500	-1.27858800
C	4.56427700	-0.15910800	-0.19551100
C	5.50151800	0.25769400	0.94122700
C	5.62949900	-0.81661900	2.02639100
H	-2.91349300	1.25983300	-0.85910400
H	-1.66014500	-0.70758400	1.09819500
H	-4.45552000	1.68649400	1.14769000
H	-3.67509700	0.31420200	1.93101100
H	-5.40195500	0.35514800	-0.58230200
H	-5.59603200	-0.63525700	0.84648300
H	-2.24898300	-2.21545600	-1.04499500
H	-2.94199900	3.63526900	-0.30507600
H	-3.14874900	3.53067000	1.45872400
H	-1.68739700	4.26855600	0.77475100
H	-1.80626200	1.71226200	2.77044400
H	-0.42133200	0.96387800	1.96011400
H	-0.42052500	2.70653100	2.26948100
H	1.57295800	2.39819700	-1.50587600
H	-5.63872100	-1.92745400	-1.90594800
H	-5.59867100	-2.88013200	-0.42516400
H	-4.36317400	-3.13877300	-1.67144200
H	3.73689000	-0.38153600	-2.88654000
H	3.35966300	1.32210200	-3.12828200
H	4.06537400	1.84398500	-0.80919300
H	5.37442700	1.12079700	-1.73998100
H	3.58025600	-0.40297500	0.21629400

H	4.93498300	-1.08650400	-0.65342200
H	5.12599400	1.18597300	1.39022500
H	6.49491100	0.49428300	0.53621200
H	6.03187100	-1.74673900	1.61100400
H	6.29130700	-0.49818600	2.83870900
H	4.65164200	-1.04995100	2.45865000
H	2.14285900	-1.86539100	-1.88030000
C	1.33194600	-1.70626100	2.21230200
H	2.17940800	-2.32208600	1.87302900
H	1.48373800	-1.47230000	3.27236400
H	1.36262400	-0.76638700	1.64232900
O	0.09438100	-2.37315700	2.07990000
H	-0.04670700	-2.52458300	1.10669400

[CBD – H]$^-$ ··· MeOH

O	0.60023600	-2.10274000	-1.33951000
O	0.27534300	2.23908000	0.62431400
C	2.26638800	-1.12606800	1.09504600
C	1.96478800	-0.02769500	0.03980300
C	3.79334800	-1.20979000	1.30304300
C	4.49554300	-1.64453100	0.01172000
C	2.87446900	-0.17665400	-1.16157200
C	0.50284400	0.06433500	-0.35596700
C	4.00245900	-0.88923700	-1.20069600
C	1.53279500	-0.91980300	2.40680100
C	-0.14000100	-0.95969600	-1.04503500
C	-0.24039600	1.25901300	-0.02792100
C	4.83510200	-1.02165400	-2.44820800
C	1.64245400	0.42959900	3.06860300
C	-2.21049300	0.27268800	-1.15348000
C	-1.47634300	-0.88494300	-1.44991400
C	-1.60438200	1.30896000	-0.46245000
C	-3.67305800	0.35249200	-1.53599100
C	0.81958000	-1.91307600	2.94788100
C	-4.60944700	-0.20102900	-0.44694800
C	-6.08994600	-0.13790500	-0.83867200
C	-7.05148800	-0.73407900	0.20121600
C	-7.10925800	0.05426600	1.51595500
H	1.94057500	-2.08189000	0.67535900
H	2.20006400	0.93984400	0.49457200
H	4.02212200	-1.91021500	2.11366100
H	4.17330700	-0.22757600	1.60595000
H	4.34305700	-2.72254200	-0.15311600
H	5.58205500	-1.51117300	0.11149400
H	2.54745100	0.34959000	-2.05543700
H	5.85782000	-0.65458400	-2.28791800
H	4.40058500	-0.46663000	-3.28362800
H	4.92391500	-2.07429800	-2.75069400
H	1.21424300	0.41223100	4.07438100
H	2.68513300	0.75678500	3.14273100
H	1.11841000	1.18670500	2.47449700
H	-1.93349500	-1.71354900	-1.98726500
H	-2.15693100	2.21330700	-0.22442800
H	-3.94474300	1.39571800	-1.73696100
H	-3.84598400	-0.20119100	-2.46834200
H	0.30413300	-1.79200800	3.89631800
H	0.70439900	-2.86756400	2.44310400
H	-4.43088300	0.36084900	0.47548500

H	-4.32993600	-1.24018300	-0.23130100
H	-6.37136800	0.90723900	-1.02588400
H	-6.22598700	-0.66309000	-1.79319200
H	0.03822000	-2.69096000	-1.85177700
H	-6.75553100	-1.76997900	0.40907300
H	-8.05974300	-0.78368600	-0.22875600
H	-7.39605700	1.09487600	1.33135600
H	-7.84017600	-0.37731300	2.20690000
H	-6.14086100	0.06507900	2.02143100
C	2.97036600	3.51501400	-0.74952300
H	3.44328200	2.54542300	-0.96992200
H	3.70785900	4.30364600	-0.94550100
H	2.13646100	3.64615100	-1.45468500
O	2.55026500	3.61566900	0.59264300
H	1.70990000	3.09367900	0.67076100

[CBC – H]$^-$ ··· MeOH

O	-1.98318600	-0.67283000	-1.80645600
O	-1.66805600	2.90565500	1.36039400
C	-3.13618400	-1.27010700	-1.14990000
C	-2.63688300	-2.47752800	-0.31543100
C	-3.88417300	-0.24994100	-0.32006000
C	-1.25654200	0.29833000	-1.14071800
C	-4.00443600	-1.77697000	-2.30597800
C	-1.75894200	-2.11578300	0.89645200
C	-1.87345000	1.10651700	-0.17697200
C	0.83926200	1.43570700	-0.83943700
C	-3.25926200	0.85042600	0.13440000
C	2.32038000	1.52837100	-1.14102400
C	0.07690300	0.44398400	-1.49314800
C	3.12074600	0.37110400	-0.51862900
C	-1.12534000	2.14683300	0.48643900
C	0.25864500	2.25810500	0.11140400
C	4.61390600	0.40148900	-0.85414900
C	-1.13346500	-3.32430500	1.53003000
C	5.39242600	-0.77746100	-0.26042200
C	0.17135800	-3.62271600	1.59849900
C	6.87660600	-0.78010100	-0.63896400
C	0.65209500	-4.88456100	2.27529000
C	1.27580000	-2.76136100	1.03589700
H	-3.50836500	-3.05563400	0.02083400
H	-2.06499700	-3.12105800	-0.99454900
H	-4.92544700	-0.46006800	-0.09553400
H	-3.44273600	-2.48714200	-2.91962500
H	-4.90005300	-2.27421200	-1.92130200
H	-4.30904900	-0.93646100	-2.93260400
H	-2.37670500	-1.58800200	1.63117100
H	-0.99505200	-1.40636400	0.58738100
H	-3.76367000	1.57806300	0.76128900
H	2.48017000	1.52079500	-2.22764900
H	2.71647300	2.47996100	-0.76985200
H	0.50973700	-0.21050100	-2.24126000
H	2.69249600	-0.57812000	-0.85908400
H	2.98206300	0.39262300	0.56865300
H	0.84895900	3.01547300	0.61796000
H	4.73981300	0.40209200	-1.94564100
H	5.05319000	1.34286500	-0.49732700
H	-1.83394100	-4.03695500	1.96980700

H	4.92829300	-1.71419500	-0.59329100
H	5.29072800	-0.76095600	0.83143500
H	7.37146300	0.13464900	-0.29549400
H	7.40769000	-1.63078300	-0.19981700
H	7.00352900	-0.83428800	-1.72558900
H	1.34525000	-4.65036900	3.09377500
H	-0.17420100	-5.46964500	2.68741700
H	1.20556800	-5.52064000	1.57214500
H	1.92775700	-2.39629900	1.83943500
H	1.91273800	-3.34867500	0.36235200
H	0.91501400	-1.89477300	0.48367800
C	-0.42593900	5.82816800	0.84634100
H	-0.42249500	6.91585300	0.99555600
H	-1.26015900	5.57458100	0.17743600
H	0.50684100	5.55773100	0.32284700
O	-0.54334000	5.19253300	2.09791700
H	-0.92531100	4.28839000	1.92108000

[THCA – H]$^-$ ··· MeOH

O	-1.74891700	-2.20435500	0.79465700
O	-0.79816700	1.59313100	-1.91956700
O	1.42302800	2.55796000	-1.96746600
O	3.06541600	1.83787500	-0.66851600
C	-3.71553800	-1.10989600	-0.11917300
C	-2.85221800	-0.07910700	-0.88967000
C	-2.94839000	-2.44338100	0.02467100
C	-4.14927200	-0.52999500	1.23721700
C	-1.38622800	-0.17144000	-0.47618200
C	-5.00208100	0.72603900	1.05467900
C	-3.41819400	1.32244600	-0.76344300
C	-4.39156900	1.69295700	0.07172000
C	-0.93313800	-1.18247800	0.35310000
C	-3.71533100	-3.49510100	0.82799200
C	-2.56837000	-3.03354000	-1.34407200
C	-0.42379700	0.74593600	-1.01422000
C	0.39552100	-1.24561600	0.79594500
C	1.33198000	-0.31022300	0.37989000
C	-4.93643800	3.09739700	0.09768500
C	0.94494000	0.69840600	-0.54249800
C	2.74598100	-0.48854600	0.89944500
C	3.69777600	-1.11213800	-0.13509000
C	1.89485200	1.72427800	-1.05092800
C	5.13634200	-1.20671700	0.37805400
C	6.10421100	-1.82730000	-0.63410600
C	7.54500200	-1.90801600	-0.11923300
H	-4.61995100	-1.30818500	-0.70971300
H	-2.90198200	-0.31389500	-1.96281600
H	-3.25278100	-0.28443600	1.81427700
H	-4.71212000	-1.26671200	1.81532900
H	-5.14049600	1.22510800	2.02318200
H	-6.01451200	0.45188000	0.71800100
H	-2.96226900	2.04718000	-1.42611900
H	-3.84736800	-3.18021800	1.86286600
H	-4.69815000	-3.67384200	0.38216400
H	-3.15731500	-4.43453300	0.83317500
H	-3.46943900	-3.22937900	-1.93320900
H	-1.92335700	-2.36084300	-1.90869200
H	-2.03150900	-3.97441600	-1.20040100

H	0.67434800	-2.05660600	1.45859500
H	-4.77818400	3.56261500	1.07926400
H	-6.02027300	3.10348700	-0.08121400
H	-4.46207800	3.72761400	-0.65784100
H	3.16178000	0.46355000	1.22516600
H	2.70547400	-1.14374900	1.77794200
H	3.68043400	-0.50198800	-1.04070300
H	3.33092700	-2.11109200	-0.40598600
H	0.41902600	2.29072900	-2.11403200
H	5.48303000	-0.19961900	0.64054600
H	5.16080200	-1.79315500	1.30784600
H	6.07764500	-1.23819400	-1.55860100
H	5.75344400	-2.83235300	-0.90218200
H	8.21775400	-2.35173300	-0.86063800
H	7.92753400	-0.91184700	0.12603300
H	7.60329200	-2.51507200	0.79095000
C	2.28239400	3.15431900	2.16748600
H	2.28177900	3.54177800	3.19066400
H	1.74765500	2.19513600	2.15835200
H	1.72461100	3.85529300	1.53081500
O	3.63363900	3.02099800	1.75851900
H	3.61165000	2.66291800	0.85036100

[CBDA – H]$^{-}$ ⋯ MeOH

O	1.04501100	1.00639900	-0.98907500
O	0.10322000	-1.92711100	2.59966600
O	-2.40698200	3.11475400	-0.60589600
O	-0.43484400	2.80741000	-1.58663900
C	2.15945300	-1.82619000	-0.71422700
C	1.99473900	-1.08942700	0.64479700
C	3.62740300	-2.26801000	-0.86760000
C	4.55367600	-1.04801200	-0.91961300
C	3.10457600	-0.07524000	0.84450100
C	0.62558100	-0.45515700	0.80289500
C	4.25109100	-0.03924000	0.16374200
C	1.18099600	-2.97040800	-0.88548800
C	0.23044500	0.61768200	-0.05828300
C	-0.26777600	-0.87969700	1.76761100
C	5.27821500	1.04175000	0.36837900
C	-1.93649400	0.76718700	1.12106400
C	-1.05541000	1.25656800	0.12878600
C	1.24348700	-4.11086000	0.10159000
C	-1.53052200	-0.29271400	1.92543200
C	-3.34732600	1.28606500	1.32900500
C	0.28002500	-2.95386800	-1.87151300
C	-4.32996800	0.83215200	0.23015500
C	-4.47822500	-0.68742800	0.11451600
C	-1.38167800	2.45470000	-0.70298000
C	-5.44391900	-1.11715400	-0.99393100
C	-5.57792400	-2.63854600	-1.11569500
H	1.95261700	-1.08606200	-1.48997400
H	2.09879500	-1.83010600	1.44458000
H	3.91539200	-2.90149600	-0.01946000
H	3.74383800	-2.87180600	-1.77446600
H	5.60264900	-1.36723700	-0.84465800
H	4.46094000	-0.55091300	-1.89645900
H	2.90897000	0.68490200	1.59741600
H	5.42574300	1.61300300	-0.55730900
H	4.97552500	1.74438600	1.14840400
H	6.25552600	0.62153500	0.64084700

H	2.24809800	-4.54537300	0.14961800
H	0.99315600	-3.75919400	1.10704900
H	0.54198100	-4.90489900	-0.16691100
H	-2.20734900	-0.68378900	2.68117400
H	-3.34641600	2.37494200	1.35784600
H	-3.70800400	0.91894500	2.29832500
H	-0.43094700	-3.76398700	-2.00739600
H	0.20774800	-2.11355200	-2.55365900
H	-5.31212600	1.27851600	0.43660800
H	-3.99624000	1.24941000	-0.72267000
H	-3.49491100	-1.13372000	-0.07069600
H	-4.82241700	-1.10051300	1.07406300
H	0.32993400	2.07280400	-1.50138100
H	-0.61996800	-2.08816400	3.21299600
H	-6.43180700	-0.67438800	-0.81081400
H	-5.09710600	-0.70254400	-1.94810900
H	-5.95008400	-3.07570100	-0.18248200
H	-4.60780400	-3.09863600	-1.32931700
H	-6.26797200	-2.92348000	-1.91669800
C	1.89184300	3.94823600	0.41185100
H	2.22873400	2.99336200	-0.00692000
H	1.15077300	3.73075500	1.19434800
H	2.74239900	4.45631300	0.87569000
O	1.37094700	4.82106300	-0.58439200
H	0.65781000	4.34223700	-1.03888100

[THC – H]$^-$ ··· MeCN

O	-0.55530500	2.24382800	0.00414200
O	-0.39089000	-2.48475000	-0.89975700
C	-2.70153300	1.17098700	-0.08922700
C	-2.07760500	-0.22759500	-0.22626200
C	-1.79574400	2.10211600	0.73339000
C	-4.15455700	1.02089600	0.37243700
C	-0.60372800	-0.13227300	-0.57104200
C	-4.96982400	0.30690300	-0.71997500
C	-2.91388700	-1.03750100	-1.19905300
C	-4.21256300	-0.80511900	-1.41573500
C	0.06612300	1.08498800	-0.44900600
C	-2.34590000	3.52734600	0.79744600
C	-1.49665300	1.58267300	2.14562200
C	0.14168000	-1.31919800	-0.93746700
C	1.41898700	1.23646500	-0.77359100
C	2.13562600	0.11976000	-1.21973000
C	-5.02306500	-1.62405100	-2.38775000
C	1.51219500	-1.11911400	-1.30105200
C	3.61429800	0.25062100	-1.52159200
C	4.49894600	0.02906200	-0.28205100
C	5.99732500	0.15820900	-0.57016200
C	6.88092900	-0.06418400	0.66168300
C	8.37798400	0.06725400	0.36385300
H	-2.71444100	1.61530400	-1.09448600
H	-2.17140000	-0.73473200	0.74807100
H	-4.61269200	1.98991800	0.59366500
H	-4.18088400	0.43362600	1.29701500
H	-5.28925400	1.03855500	-1.47889100
H	-5.90006200	-0.09368100	-0.29345900
H	-2.40253900	-1.85767200	-1.68887800
H	-2.62030800	3.87646300	-0.20161900
H	-3.22271700	3.58330800	1.44667000
H	-1.57606200	4.19347300	1.19503400

H	-2.41908700	1.40259700	2.70340900
H	-0.93619600	0.64919200	2.10613500
H	-0.89427000	2.31618500	2.68822400
H	1.88264600	2.21029900	-0.66194800
H	-5.46610700	-0.98885700	-3.16742300
H	-5.85850700	-2.12833800	-1.88332500
H	-4.41074900	-2.38553700	-2.87605700
H	3.89917200	-0.47484500	-2.29340300
H	3.82418000	1.24669200	-1.93221100
H	4.28509500	-0.96498900	0.12813400
H	4.20801100	0.74858600	0.49262100
H	6.28075000	-0.56073300	-1.35120000
H	6.20370000	1.15403100	-0.98637900
H	6.67508800	-1.05871600	1.07613800
H	6.59737600	0.65358000	1.44132000
H	8.69289300	-0.66114700	-0.39104100
H	8.61474300	1.06410200	-0.02337400
H	8.98603600	-0.09609300	1.25936300
H	2.06709600	-1.99984100	-1.61374200
C	-1.30532500	-2.25176800	3.06534700
N	-2.17837200	-2.12570900	3.81142900
C	-0.20747300	-2.41341600	2.12783300
H	0.33828000	-1.47352800	2.01633000
H	0.48039300	-3.18225100	2.48752200
H	-0.55944100	-2.68597900	1.11920500

[CBD – H]$^-$ ··· MeCN

O	-1.46546500	-1.79595400	-1.57866700
O	-0.27615200	0.18412900	2.59297700
C	-2.31728800	1.04142000	-0.60283700
C	-2.23912800	-0.02743400	0.52274500
C	-3.72923900	1.66292800	-0.61128300
C	-4.78671200	0.60438400	-0.94194200
C	-3.46002100	-0.92144000	0.49903500
C	-0.94296200	-0.81499000	0.52714400
C	-4.60201000	-0.66673800	-0.14507100
C	-1.23688500	2.10096100	-0.50386900
C	-0.58697300	-1.67292400	-0.50385800
C	-0.04111500	-0.64774200	1.65325400
C	-5.76056800	-1.62885300	-0.15773800
C	-1.13263300	2.87866800	0.78309300
C	1.48873000	-2.27327400	0.57212400
C	0.61328600	-2.39748800	-0.51428300
C	1.15551600	-1.44127700	1.63015900
C	2.83380000	-2.97393000	0.54727000
C	-0.40995700	2.33036200	-1.52986200
C	4.01698700	-1.99349100	0.40986500
C	3.94957600	-1.12581600	-0.84982200
C	5.07138000	-0.08703300	-0.93891800
C	4.94068300	0.82786300	-2.16031200
H	-2.18583900	0.51898800	-1.55471900
H	-2.24112300	0.48973700	1.49011300
H	-3.77330000	2.48435300	-1.33513100
H	-3.94563900	2.08920300	0.37512300
H	-4.75273600	0.36320300	-2.01572700
H	-5.79288400	1.00895600	-0.76137400
H	-3.36202200	-1.84878900	1.05962800
H	-6.66803200	-1.16953300	0.25733500

H	-5.54155200	-2.53209900	0.41759000
H	-6.00612600	-1.93310400	-1.18468100
H	-0.37002000	3.65808700	0.71585900
H	-2.08676000	3.35537600	1.03493100
H	-0.88028300	2.20333300	1.60884300
H	0.86405100	-3.02949900	-1.36319800
H	1.82672300	-1.32921400	2.47733500
H	2.96763600	-3.55685200	1.46666500
H	2.86195200	-3.68814700	-0.28497400
H	0.35658200	3.09836100	-1.48296300
H	-0.46400300	1.74060200	-2.43975800
H	4.03355800	-1.34136500	1.29114300
H	4.96186100	-2.55455800	0.42160000
H	3.97700900	-1.77028200	-1.73942200
H	2.97964900	-0.61954800	-0.87849200
H	-1.08825300	-2.43261200	-2.19267500
H	6.04418900	-0.59618000	-0.95779800
H	5.06870500	0.52600500	-0.02924800
H	3.99773300	1.38188000	-2.13011800
H	5.75333300	1.55912000	-2.20723600
H	4.95459800	0.24714200	-3.08920900
C	2.61634200	2.98575700	0.82057400
N	3.01608100	4.05633300	0.65198200
C	2.12197400	1.63385100	1.01993300
H	2.95409300	0.93909400	1.13585500
H	1.47714000	1.55677700	1.90108500
H	1.52344000	1.31926200	0.16284800

[CBC – H]$^-$ ··· MeCN

O	-2.01665400	-0.79989900	-1.45987700
O	-2.79632200	2.29582900	2.04046300
C	-2.42223600	-1.89749700	-0.62255900
C	-1.16905200	-2.39453900	0.14464200
C	-3.46396500	-1.49286700	0.37028800
C	-1.83165500	0.40160500	-0.84358500
C	-2.93577100	-2.92056900	-1.64308900
C	0.08141900	-2.54859500	-0.72709500
C	-2.50850000	0.71043900	0.33889100
C	-0.73496800	2.52426200	-0.87773700
C	-3.45137600	-0.22985000	0.84847500
C	0.24540500	3.46398400	-1.53408000
C	-0.95736900	1.26922100	-1.48806900
C	1.64369300	3.28223800	-0.91617300
C	-2.27816300	1.99307200	0.96457700
C	-1.34793500	2.88305400	0.28969800
C	2.28044100	1.96088100	-1.36405100
C	1.29242800	-2.77182200	0.11808300
C	3.61818800	1.70367900	-0.65799200
C	2.54040700	-2.47696500	-0.27231900
C	3.41168200	1.13865900	0.74435700
C	3.70745600	-2.68016300	0.63845600
C	2.85931200	-1.92059900	-1.62040700
H	-0.96128500	-1.66316100	0.95216600
H	-1.41225700	-3.34325400	0.64679500
H	-4.16756300	-2.24237100	0.68141100
H	-3.21426800	-3.85514600	-1.15998400
H	-3.81797400	-2.52427000	-2.15896700
H	-2.17648000	-3.12477300	-2.40799200

H	0.22035700	-1.63812700	-1.35412500
H	-0.04734400	-3.37929300	-1.44470600
H	-4.13998100	0.11698400	1.61862000
H	0.28224700	3.30051800	-2.62634200
H	-0.09261300	4.51002600	-1.40311500
H	-0.47738400	0.99774800	-2.40768300
H	1.56110300	3.30824500	0.18820100
H	2.28981600	4.13170600	-1.19590200
H	-1.18439000	3.84020600	0.75767400
H	1.57339500	1.12402300	-1.16370900
H	2.42225100	1.96265100	-2.45848400
H	1.09823500	-3.17730700	1.10950500
H	4.20939600	2.63522700	-0.61127300
H	4.22083300	0.99578000	-1.25608200
H	2.76073800	1.78744000	1.34757200
H	2.93295600	0.15121800	0.70993100
H	4.35408900	1.02493700	1.28371200
H	3.39684000	-2.79042300	1.68711400
H	4.27834700	-3.57225200	0.36480400
H	4.39018400	-1.82043700	0.61072700
H	3.92639700	-1.99060100	-1.86362600
H	2.30869900	-2.43287800	-2.41857300
H	2.58429400	-0.85249400	-1.66821100
C	1.08684700	-0.31641400	2.84044500
N	1.85133900	-0.99799400	3.39082500
C	0.14702800	0.52099200	2.16746900
H	0.24150800	0.48420800	1.05741300
H	-0.91667200	0.25033400	2.37286600
H	0.22109300	1.59083300	2.44043800

[THCA – H]$^-$ ··· MeCN

O	0.55926500	-2.18130800	0.75893800
O	1.14178400	2.23168100	-0.94064700
O	-0.79084400	3.58954400	-1.56356500
O	-2.85958600	2.78926900	-1.51121300
C	2.82542900	-1.60624400	0.20455000
C	2.45196500	-0.15164900	-0.13048600
C	1.90704900	-2.18204100	1.29466400
C	4.33516600	-1.68592400	0.44891900
C	0.94890000	-0.00934700	-0.26177700
C	5.08351700	-1.35520300	-0.85395900
C	3.25690400	0.28499000	-1.34094100
C	4.44074900	-0.24694000	-1.66162800
C	0.10543600	-1.01910000	0.16941300
C	2.18840700	-3.65943500	1.56512100
C	1.92421100	-1.38327200	2.60395500
C	0.36316900	1.21766800	-0.71180000
C	-1.28872500	-0.92927900	0.04642100
C	-1.88858800	0.20766600	-0.47909400
C	5.22093900	0.20309100	-2.87003500
C	-1.07208500	1.31153000	-0.85417300
C	-3.40356200	0.25314500	-0.60909100
C	-4.17230000	-1.00093700	-0.18185700
C	-1.66246400	2.59815900	-1.33619000
C	-5.68354200	-0.83620800	-0.38630100
C	-6.52641800	-2.01827000	0.11600700
C	-6.27875200	-3.33056700	-0.63821600
H	2.60264000	-2.20561800	-0.68929700

H	2.77446900	0.49467300	0.70261200
H	4.63729600	-2.67652700	0.80145000
H	4.61389500	-0.96868700	1.22939600
H	5.13998200	-2.25600400	-1.48438100
H	6.12641000	-1.09011700	-0.63288500
H	2.83768700	1.09355000	-1.92618300
H	2.23195500	-4.21854300	0.62674500
H	3.13166200	-3.78967300	2.09996800
H	1.38334000	-4.07495400	2.17584800
H	2.93603200	-1.34049300	3.01635200
H	1.57115200	-0.36329900	2.44767200
H	1.26828400	-1.86035400	3.33633300
H	-1.86526900	-1.77499500	0.39217000
H	5.40810100	-0.63636100	-3.55325700
H	6.20426700	0.59844800	-2.58293600
H	4.68983400	0.98051900	-3.42349400
H	-3.77842500	1.11526500	-0.04973000
H	-3.65352400	0.49315200	-1.64663600
H	-3.98211700	-1.22263200	0.87633200
H	-3.81510700	-1.86700700	-0.74937500
H	0.14821800	3.20485200	-1.36526600
H	-6.01161800	0.07625100	0.12647500
H	-5.88932200	-0.67283100	-1.45275200
H	-7.58897900	-1.75731600	0.03619500
H	-6.32875100	-2.17116000	1.18497500
H	-5.25133600	-3.68041800	-0.51032600
H	-6.94546100	-4.12434800	-0.28590400
H	-6.45119400	-3.20023500	-1.71226600
C	0.10026800	3.64909900	3.18440900
N	0.33238300	3.97887500	4.26632100
C	-0.18842900	3.23140600	1.82130800
H	0.72829200	3.10681100	1.23918300
H	-0.71870000	2.27708800	1.81432800
H	-0.80881200	3.97133200	1.31098800

[CBDA – H]$^-$ ⋯ MeCN

O	-1.16205100	-1.19766800	-1.32964800
O	-0.90817000	0.06409700	3.22483500
O	2.43616900	-3.10888200	-1.32323800
O	0.58438600	-2.51765100	-2.39254300
C	-2.51407000	1.28245200	-0.16192900
C	-2.45247800	0.09324500	0.83586900
C	-3.97780700	1.75513600	-0.27717200
C	-4.86155000	0.64879400	-0.86362200
C	-3.52571600	-0.92867300	0.51184700
C	-1.07706600	-0.54408500	0.92730200
C	-4.60867500	-0.70040400	-0.23313100
C	-1.58040900	2.42493400	0.18846100
C	-0.50288100	-1.19148600	-0.21697700
C	-0.35111100	-0.53496900	2.10349300
C	-5.61108600	-1.77611800	-0.55554500
C	1.52467900	-1.71672200	1.10342700
C	0.80527300	-1.81069100	-0.11136500
C	-1.64951700	2.99890100	1.58269600
C	0.93080600	-1.09366400	2.19584600
C	2.96396300	-2.16775600	1.27723800
C	-0.74273100	2.92274000	-0.72524300
C	3.97243200	-1.23121600	0.57780100
C	3.92333900	0.22353000	1.05350900

C	1.35424000	-2.53314200	-1.30244600
C	4.83704800	1.15410400	0.25003900
C	4.73948700	2.61781400	0.69018500
H	-2.21409200	0.88642800	-1.13450200
H	-2.68626900	0.48401800	1.83176900
H	-4.35519500	2.03191600	0.71514700
H	-4.02978600	2.65255900	-0.90267300
H	-5.92226600	0.91539500	-0.75391100
H	-4.68539500	0.56678400	-1.94649200
H	-3.36308600	-1.92154300	0.92448400
H	-5.67476400	-1.93317900	-1.64031500
H	-5.34335400	-2.72975100	-0.09357200
H	-6.61893900	-1.49968300	-0.21708400
H	-1.01226900	3.88173200	1.67736900
H	-2.67449400	3.28869200	1.84131900
H	-1.33225800	2.26071500	2.32389300
H	1.47995300	-1.00888600	3.13027600
H	3.09889400	-3.17234700	0.87898900
H	3.18816600	-2.19107900	2.35112200
H	-0.68547500	2.50437000	-1.72396500
H	-0.08133800	3.75617200	-0.50986300
H	4.98406800	-1.62964900	0.73104500
H	3.78908700	-1.27848100	-0.49793900
H	2.89409400	0.59320600	0.99270800
H	4.19307500	0.27679800	2.11837000
H	-0.27066000	-1.98088500	-2.13971800
H	-0.28043300	-0.02074500	3.94869900
H	5.87573800	0.80857600	0.33360500
H	4.57786900	1.08096200	-0.81276900
H	5.40355700	3.26050400	0.10436300
H	5.00524700	2.72947600	1.74753900
H	3.72035600	2.99465100	0.56038100
C	2.17516200	2.02425500	-2.47914200
N	2.57351500	3.03784900	-2.86196800
C	1.68548200	0.74672000	-1.98549800
H	0.71701600	0.49544800	-2.42196800
H	2.38921500	-0.05163100	-2.22779400
H	1.55557600	0.78315700	-0.90386300

[THC – H]$^-$ ⋯ Acetic acid

O	1.62412200	-2.45355400	0.02007700
O	-0.06794900	1.96677500	-0.80469400
C	3.22468000	-0.69203300	0.33264300
C	2.17497700	0.40608000	0.09546600
C	2.58806400	-1.93954500	0.96805300
C	4.43225900	-0.07837400	1.04725500
C	0.91432000	-0.17800500	-0.51054300
C	5.10783400	0.94876900	0.12231400
C	2.81583000	1.52928900	-0.69775600
C	4.12907900	1.77962600	-0.68142800
C	0.70623900	-1.55904800	-0.51222600
C	3.59168900	-3.08198000	1.12257400
C	1.88393300	-1.66141700	2.30313100
C	-0.14190500	0.67322100	-0.96590400
C	-0.45072600	-2.14134900	-1.03665300
C	-1.44929800	-1.32057600	-1.56881000
C	4.74191400	2.90117900	-1.48022600
C	-1.28491000	0.06101100	-1.54330100
C	-2.73594100	-1.93797300	-2.07666200
C	-3.80561500	-2.11848000	-0.97609300
C	-4.42375900	-0.80748800	-0.48073300

C	-5.41981000	-0.99698200	0.66762100
C	-6.10475300	0.30897000	1.08479200
H	3.56232300	-1.02941700	-0.65730300
H	1.89916600	0.84119000	1.07100600
H	5.16104600	-0.84003300	1.34053200
H	4.09661400	0.41582200	1.96633800
H	5.77972000	0.42754700	-0.57715500
H	5.75798600	1.61317300	0.70810400
H	2.13716300	2.15954000	-1.25929300
H	4.13531400	-3.24189300	0.18776700
H	4.30939000	-2.87273700	1.91906400
H	3.05631500	-4.00177700	1.37027000
H	1.05279500	-0.96768900	2.17058800
H	1.48501700	-2.59413000	2.71011200
H	2.58312300	-1.23404000	3.02766400
H	-0.55511500	-3.22006100	-1.00369700
H	5.49903900	2.51994200	-2.17898000
H	5.25307500	3.62128000	-0.82735000
H	3.98733900	3.44057900	-2.05677900
H	-2.51621700	-2.91761000	-2.51657900
H	-3.15408800	-1.31787000	-2.87855500
H	-3.35085200	-2.65116200	-0.13165000
H	-4.60636300	-2.76629500	-1.35943400
H	-3.63272500	-0.12456000	-0.15988400
H	-4.92698400	-0.30818400	-1.31986100
H	-4.88987600	-1.42580000	1.52806800
H	-6.17673500	-1.73873700	0.37599900
H	-6.68920400	0.72113100	0.25473700
H	-6.78828100	0.15012200	1.92603100
H	-5.37536700	1.07011400	1.37490400
H	-2.06345400	0.71549500	-1.92018300
C	-1.77119200	1.59552100	1.74524200
H	-1.78719000	0.62536400	1.24031400
H	-2.13650600	1.48323800	2.76527500
H	-0.73313000	1.93287800	1.73199500
C	-2.67004400	2.57036900	0.99189900
O	-2.23643200	2.98436800	-0.17850900
H	-1.29945800	2.55805500	-0.47330100
O	-3.74362400	2.92638800	1.45653900

[CBD – H]$^-$ ··· Acetic Acid

O	-0.15878400	-2.66802500	-0.94230100
O	0.22799100	2.08912300	-0.61912300
C	1.34416200	-1.17283700	1.33568800
C	1.43770700	-0.50048100	-0.06331000
C	2.76805600	-1.33975500	1.89170300
C	3.59947500	-2.27237100	1.00121800
C	2.45521800	-1.20722700	-0.93237200
C	0.08876300	-0.31162700	-0.72710000
C	3.43258000	-1.99442200	-0.47613400
C	0.40834100	-0.40658500	2.26074700
C	-0.69266600	-1.39557800	-1.11845900
C	-0.43299000	1.01870700	-0.91113300
C	4.40928200	-2.68665500	-1.38963800
C	-0.94279200	-1.03674600	2.48633700
C	-2.51983800	0.02866700	-1.78681500
C	-1.98119900	-1.25650400	-1.64302400
C	-1.75322900	1.13060200	-1.44226500

C	-3.96092600	0.21124300	-2.21798200
C	0.73263900	0.77312400	2.79239900
C	-4.88092500	0.59214800	-1.03812900
C	-4.96045200	-0.49145200	0.04323000
C	-5.76817400	-0.08923800	1.28615500
C	-5.08856600	0.99126900	2.13696800
H	0.92716900	-2.17350000	1.18327900
H	1.81626900	0.50630900	0.11680300
H	2.73068000	-1.72597800	2.91596300
H	3.24994100	-0.35772200	1.94221200
H	3.32245900	-3.32097200	1.19267300
H	4.66244700	-2.19590500	1.26872000
H	2.35935700	-1.04102400	-2.00329200
H	5.44159100	-2.38465700	-1.16964800
H	4.20609900	-2.46633100	-2.44073600
H	4.36577000	-3.77624800	-1.25619400
H	-1.56445500	-0.43660300	3.15641100
H	-1.46683500	-1.14523700	1.53052700
H	-0.84194800	-2.04342400	2.91198400
H	-2.56298600	-2.13696000	-1.90574800
H	-2.14925100	2.13601800	-1.54787400
H	-4.02335200	0.99719500	-2.97941700
H	-4.33213600	-0.71050100	-2.68324200
H	0.02920400	1.31862100	3.41400700
H	1.67057200	1.27105100	2.57668300
H	-5.89199000	0.80323500	-1.41392800
H	-4.50410500	1.52320400	-0.60417100
H	-5.40007400	-1.39565400	-0.39873000
H	-3.94512700	-0.76500600	0.34885600
H	-0.81019400	-3.30585500	-1.24809000
H	-5.92708000	-0.97926400	1.90735300
H	-6.76669200	0.25332500	0.98206900
H	-4.97406200	1.92846400	1.58672900
H	-5.66577700	1.20647900	3.04192000
H	-4.08768800	0.67055500	2.44145300
C	3.19353400	2.48482200	-1.59304500
H	2.18698700	2.65124900	-1.97908800
H	3.36565800	1.40385200	-1.59226700
H	3.94960600	2.95937200	-2.21816200
C	3.33747300	2.98991000	-0.16414700
O	2.27731300	2.85386700	0.61608300
H	1.44458200	2.47804200	0.12212400
O	4.38254400	3.46250900	0.24727500

[CBC – H]$^-$ ··· Acetic Acid

O	0.82016400	-2.14628900	-1.73856200
O	-2.74490700	-1.10370500	1.27426700
C	1.19041500	-3.35979800	-1.02488200
C	2.45762700	-3.05079300	-0.18962000
C	0.04538700	-3.87611900	-0.18194000
C	-0.03425900	-1.24132500	-1.14189400
C	1.53940300	-4.35522300	-2.13539000
C	2.25540000	-2.03763100	0.95204100
C	-0.95779900	-1.66535600	-0.17786700
C	-0.81813500	1.02437300	-0.98035600
C	-0.94388500	-3.05789100	0.21083100
C	-0.64501800	2.48704300	-1.32845400
C	0.04809100	0.07912500	-1.56063600

C	0.53426400	3.12236500	-0.56937800
C	-1.87115400	-0.72412500	0.40180300
C	-1.75340200	0.63249300	-0.03300600
C	0.76251500	4.59778000	-0.90565000
C	3.55778300	-1.62323800	1.57265200
C	1.94411700	5.21342100	-0.14788400
C	4.12402900	-0.40925500	1.54137400
C	2.18558300	6.68520700	-0.49620600
C	5.46418400	-0.15365100	2.18892700
C	3.51907200	0.80176400	0.87383200
H	2.84752300	-3.99335000	0.21740900
H	3.21259200	-2.66216700	-0.88323900
H	0.07668500	-4.92309500	0.10327900
H	2.33792100	-3.95400600	-2.76548400
H	1.87144600	-5.30485600	-1.70593400
H	0.66071900	-4.53695400	-2.75653700
H	1.60378800	-2.48581000	1.70944100
H	1.72047500	-1.17174500	0.57023200
H	-1.75569600	-3.40257500	0.84174000
H	-0.47348900	2.59735400	-2.40705000
H	-1.56270100	3.03765800	-1.09454000
H	0.78634400	0.36109400	-2.30265300
H	1.44471100	2.55322700	-0.78942300
H	0.35881200	3.01030200	0.50710800
H	-2.41197300	1.36594900	0.42140000
H	0.93198300	4.70332300	-1.98638000
H	-0.14839000	5.17007900	-0.68339500
H	4.10600600	-2.41875100	2.08025400
H	2.84958700	4.63154300	-0.36164400
H	1.76861500	5.11495800	0.93052000
H	1.30391200	7.29285400	-0.26534200
H	3.03198500	7.09963000	0.06098400
H	2.39737500	6.80582200	-1.56429000
H	5.38693100	0.62699000	2.95689400
H	5.87100200	-1.05352000	2.65727700
H	6.19272100	0.20670400	1.45047400
H	4.16075700	1.14455000	0.05287500
H	2.52446700	0.62560900	0.46753000
H	3.44966900	1.63571600	1.58233700
C	-5.27437700	-0.41951700	-0.35415700
H	-6.14791200	-0.43998300	-1.00373600
H	-4.96534400	-1.43041000	-0.08060500
H	-4.42791000	0.02638200	-0.88443700
C	-5.58433400	0.40555200	0.88921500
O	-4.66376500	0.39325300	1.83538100
H	-3.83586900	-0.21843100	1.60203100
O	-6.61646400	1.04857700	0.99176300

[THCA – H]$^-$ ⋯ Acetic Acid

O	1.19558100	-2.19954300	-0.57129900
O	0.59803700	2.30299800	0.90289900
O	-1.56221700	3.41709700	0.66005000
O	-3.30689800	2.42286100	-0.28337000
C	3.22740000	-1.02246300	-0.06925200
C	2.47205100	0.21135200	0.45543100
C	2.42959600	-2.31311500	0.17718700
C	4.66787600	-0.98002900	0.44939400
C	1.00919300	0.14412000	0.06292300

C	5.39398500	0.23450500	-0.15428900
C	3.21400800	1.45488500	-0.00006900
C	4.52436500	1.46946500	-0.26547900
C	0.46929000	-1.03041000	-0.43629300
C	3.11200300	-3.53815100	-0.43090600
C	2.09889700	-2.56165900	1.65477500
C	0.13244600	1.25573600	0.30111800
C	-0.86923800	-1.11693400	-0.83971400
C	-1.72334800	-0.02824900	-0.71228500
C	5.23664600	2.71760000	-0.71997800
C	-1.24795100	1.17396600	-0.13046500
C	-3.15838800	-0.23567500	-1.15817100
C	-4.11406800	-0.51882800	0.01299700
C	-2.13134800	2.36578200	0.06388300
C	-5.57232800	-0.64275700	-0.43365800
C	-6.53971700	-0.93789600	0.71688800
C	-8.00007700	-1.04543200	0.26584600
H	3.26716700	-0.92884000	-1.16352500
H	2.52110600	0.21184200	1.55712900
H	5.21637200	-1.89354400	0.20062800
H	4.65677300	-0.89978800	1.54254300
H	5.76493800	-0.02133900	-1.15889100
H	6.29132300	0.46894900	0.43494900
H	2.62568200	2.36134400	-0.06543000
H	3.40041200	-3.34019100	-1.46651000
H	4.00159600	-3.81823000	0.13779400
H	2.41568500	-4.38020200	-0.42332400
H	3.01443500	-2.61723900	2.25076000
H	1.47108800	-1.76416800	2.05385900
H	1.55640500	-3.50497900	1.75728500
H	-1.22412500	-2.05956000	-1.24033600
H	5.71623600	2.56470600	-1.69638800
H	6.03507000	2.99738100	-0.01965700
H	4.54907000	3.56160300	-0.80721000
H	-3.51785600	0.64420000	-1.69141300
H	-3.18493100	-1.08771500	-1.84905200
H	-4.02870500	0.29661700	0.73471300
H	-3.79952100	-1.44109500	0.51943700
H	-0.58506800	3.14178900	0.86873900
H	-5.86920000	0.29291500	-0.92382600
H	-5.66269400	-1.43345700	-1.19279800
H	-6.44597600	-0.14755800	1.47111300
H	-6.23937400	-1.87014200	1.21243900
H	-8.33267400	-0.11364900	-0.20356000
H	-8.12574700	-1.84705100	-0.47046100
H	-8.67127600	-1.25478800	1.10543700
C	-1.65116904	5.21647743	-1.74078340
H	-1.46911334	5.69990425	-2.69784472
H	-1.53159878	4.13481995	-1.85315476
H	-0.91330574	5.56602990	-1.01256925
C	-3.05455224	5.54762157	-1.27256623
O	-3.41470870	5.00044958	-0.07448252
H	-2.69481406	4.47414091	0.29301125
O	-3.83228481	6.23398486	-1.87063666

[CBDA – H]$^-$ ⋯ Acetic Acid

O	-1.09463700	1.26840000	-0.44776100
O	-1.77730500	-3.37701100	0.11565100

O	2.97557300	1.03251100	0.00197200
O	1.12655300	2.25925500	-0.29414200
C	-3.59115500	0.02384100	0.81782100
C	-2.96432200	-0.83520800	-0.32344600
C	-5.06369400	0.30512400	0.47164900
C	-5.17751400	1.13189900	-0.81528400
C	-3.32416700	-0.27653500	-1.68746700
C	-1.46411400	-1.03276000	-0.16789600
C	-4.30674800	0.59733900	-1.93154300
C	-3.39115300	-0.62201800	2.18267300
C	-0.56203800	0.05589200	-0.22714300
C	-0.92035900	-2.29494300	0.07035100
C	-4.57730100	1.15247900	-3.30611200
C	1.34555200	-1.40196100	0.20948200
C	0.84713400	-0.10056900	-0.04453000
C	-2.24431800	-0.08141600	3.00031400
C	0.45248700	-2.47625700	0.26206200
C	2.81293800	-1.73630200	0.39662900
C	-4.16743100	-1.62300100	2.63122100
C	3.56574500	-1.85078500	-0.94543400
C	5.04772500	-2.26082400	-0.79750000
C	1.74226500	1.12312400	-0.11328900
C	5.33429100	-3.76821500	-0.97374200
C	4.61803400	-4.67616300	0.02662500
H	-3.05689300	0.97990600	0.81604100
H	-3.41631400	-1.83080400	-0.24523700
H	-5.59888000	-0.64471800	0.34187600
H	-5.55349700	0.82341800	1.30618400
H	-6.22561800	1.16571100	-1.14899000
H	-4.89159200	2.17772200	-0.61825400
H	-2.70294100	-0.62523500	-2.50992900
H	-4.46651900	2.24501200	-3.31006600
H	-3.89053300	0.74358200	-4.05329500
H	-5.60632500	0.93846000	-3.62876200
H	-2.37605900	0.99275200	3.18655700
H	-2.15091700	-0.59434300	3.96315200
H	-1.30188200	-0.18855600	2.45457600
H	0.83543200	-3.47839600	0.45422500
H	2.88176000	-2.68315100	0.94320600
H	3.30490300	-0.96323500	0.99285200
H	-4.98253900	-2.02924900	2.04368500
H	-3.98948900	-2.08331900	3.60048500
H	3.04496800	-2.56825200	-1.59543400
H	3.50388000	-0.87240600	-1.42816000
H	5.64578600	-1.72052200	-1.54119400
H	5.41867000	-1.93271600	0.18163200
H	-0.28704100	1.90819400	-0.43071900
H	-1.26573400	-4.16540900	0.33383100
H	5.04472000	-4.06215600	-1.99189500
H	6.41749600	-3.93140700	-0.90039700
H	4.91724400	-5.72558800	-0.10285500
H	3.53329400	-4.62928000	-0.08369100
H	4.85662000	-4.39308700	1.06224400
C	3.18848900	3.93826300	1.56102600
H	3.84914300	4.34472400	2.32964800
H	3.53040700	2.95402900	1.22425700
H	2.18172800	3.79455600	1.96780000
C	3.13686000	4.89919000	0.38578000
O	2.38290800	4.51593800	-0.64682000
H	1.95369400	3.61050500	-0.50165200
O	3.73938200	5.96366900	0.37045000

[THC – H]$^-$ ⋯ ACE

O	-1.78116700	-1.96066500	1.04390700
O	-0.32590800	0.39208000	-2.89961600
C	-3.22596900	-0.12607700	0.38999400
C	-2.39679800	0.14785800	-0.88853000
C	-3.15072900	-1.62654200	0.75406100
C	-2.74359300	0.77935500	1.53566100
C	-1.09347900	-0.64816200	-0.89087300
C	-2.91796000	2.25970700	1.19077700
C	-2.18596600	1.63380900	-1.10071800
C	-2.43396200	2.58816700	-0.19973600
C	-0.84440900	-1.62001700	0.07221200
C	-3.91149900	-1.96958000	2.03706300
C	-3.67072400	-2.51556800	-0.38978400
C	-0.12006500	-0.43117500	-1.94861100
C	0.36439700	-2.32543900	0.15039900
C	1.34344700	-2.09157900	-0.82067100
C	-2.22419600	4.05005700	-0.49956300
C	1.09483600	-1.18748100	-1.84632400
C	2.67475800	-2.81872600	-0.75616900
C	3.88233200	-1.88428000	-0.54504600
C	3.85219800	-1.13027300	0.78693800
C	4.99069000	-0.11714500	0.94112200
C	4.94192300	0.64475600	2.26894600
H	-4.27666000	0.11722600	0.17994200
H	-2.98128600	-0.18215700	-1.76108800
H	-1.68736800	0.56678100	1.72252700
H	-3.28194300	0.56085000	2.46125400
H	-2.37720400	2.87610700	1.92225400
H	-3.97610100	2.55101700	1.28699000
H	-1.78136500	1.88490500	-2.07369800
H	-3.46107000	-1.48334300	2.90229000
H	-4.95724000	-1.65745000	1.95734800
H	-3.87988600	-3.04881900	2.20671900
H	-4.71166300	-2.26759100	-0.62034900
H	-3.07355800	-2.39322200	-1.29296800
H	-3.61767700	-3.56521400	-0.08927700
H	0.50048700	-3.05186200	0.94290100
H	-1.46426400	4.48284000	0.16464700
H	-3.14612700	4.62499700	-0.33667500
H	-1.90162600	4.20594300	-1.53153600
H	2.64890500	-3.55822300	0.05346800
H	2.82772000	-3.37891700	-1.68726400
H	3.91554000	-1.15943800	-1.36669500
H	4.81092900	-2.46854600	-0.61100600
H	2.89160000	-0.61708100	0.88484300
H	3.89069000	-1.85324500	1.61377700
H	4.94392100	0.60262900	0.11532600
H	5.95426300	-0.63599100	0.84403300
H	4.96760600	-0.04628700	3.11935900
H	5.78775900	1.33255500	2.36702400
H	4.02933100	1.24207800	2.33775000
H	1.82725600	-1.02615700	-2.63233400
C	2.14744900	2.31030700	0.09621700
C	1.03910300	1.58888500	0.82194700
H	1.16471900	1.68458300	1.90085400
H	0.98465800	0.53955200	0.52201500
H	0.08118100	2.02188100	0.51604800

C	2.25193200	2.05221000	-1.38570900
H	2.67491000	1.05104800	-1.52250000
H	1.27390200	2.00339400	-1.87500800
H	2.90241800	2.79288800	-1.85239500
O	2.92144500	3.05281800	0.67943700

[CBD – H]$^-$ ··· ACE

O	1.41021700	-0.55666700	-2.38886600
O	0.20908700	-0.49115600	2.22254600
C	3.43485900	-0.48285200	0.02223500
C	2.10875600	0.29569200	0.24094400
C	4.62189700	0.47333500	0.26132100
C	4.61549700	1.61489400	-0.76158600
C	2.14624600	1.62138500	-0.48865100
C	0.87073800	-0.52138900	-0.07171100
C	3.24598400	2.22838500	-0.94254700
C	3.54190400	-1.73910100	0.86529900
C	0.54409900	-0.91904200	-1.35967300
C	-0.00664000	-0.88553600	1.02574500
C	3.20106800	3.53120900	-1.69667600
C	3.33825700	-1.60653900	2.35269800
C	-1.46507700	-2.03315800	-0.61705800
C	-0.61392500	-1.65008400	-1.66104100
C	-1.15137500	-1.68045600	0.68727800
C	-2.75179400	-2.77804900	-0.92232700
C	3.80885500	-2.91822600	0.29483100
C	-4.01986100	-2.01869900	-0.48240000
C	-4.14189900	-0.61959800	-1.09224900
C	-5.36869400	0.15653800	-0.60362700
C	-5.43190300	1.58453500	-1.15450500
H	3.46274700	-0.78285700	-1.02979100
H	2.01635900	0.52179900	1.31071200
H	5.56618700	-0.07972300	0.20770600
H	4.55107200	0.89439800	1.27097200
H	4.97229000	1.24602900	-1.73586500
H	5.33111600	2.39363500	-0.46122900
H	1.17994800	2.09276700	-0.64903600
H	3.78757000	4.30874600	-1.18876600
H	2.17734300	3.89654900	-1.81095900
H	3.63432700	3.41817700	-2.70014700
H	3.54740200	-2.54980900	2.86451900
H	3.99291300	-0.83554500	2.77569400
H	2.30605500	-1.30691500	2.57006100
H	-0.84291700	-1.91182000	-2.69158000
H	-1.79489600	-1.97609200	1.50973800
H	-2.80986600	-2.97538200	-1.99978800
H	-2.74104800	-3.75670800	-0.42606700
H	3.90779200	-3.01600000	-0.78180800
H	3.90250900	-3.82669700	0.88282400
H	-4.01991700	-1.93050400	0.61007300
H	-4.90714000	-2.61254700	-0.74241100
H	-3.23490200	-0.05350100	-0.85758300
H	-4.17034600	-0.69851500	-2.18779700
H	1.04196400	-0.89031800	-3.21214900
H	-5.35550500	0.19635100	0.49212500
H	-6.28039200	-0.39055900	-0.87933000
H	-5.43458100	1.58287500	-2.25034100
H	-6.33229700	2.10645700	-0.81594200

H	-4.57110000	2.16924300	-0.81890400
C	-2.58207500	2.12508200	1.60054100
C	-1.35750300	2.14134400	0.71993600
H	-1.27484800	3.09376200	0.19600800
H	-0.46899300	1.94155700	1.32684800
H	-1.39469500	1.31175000	0.00661400
C	-2.80724500	0.85583700	2.38483100
H	-3.56052200	1.01745600	3.15702400
H	-3.15692600	0.08743100	1.68775600
H	-1.86536500	0.46762200	2.78851500
O	-3.34959900	3.07205300	1.66290200

[CBC – H]$^-$ ··· ACE

O	1.27450500	-0.90889900	-1.42736200
O	-0.72547700	-0.95514000	2.92945500
C	2.22489000	-1.96773300	-1.12624900
C	3.61835900	-1.31946700	-0.93580300
C	1.79930200	-2.77714500	0.07823200
C	0.56821500	-0.30056800	-0.40556300
C	2.23570900	-2.83591300	-2.38924000
C	3.72337100	-0.34676200	0.25046700
C	0.38189800	-0.94777200	0.81920900
C	-0.76024300	1.57295000	0.31106200
C	0.95049600	-2.26148900	0.98452200
C	-1.40442900	2.91754400	0.02193700
C	0.00398900	0.93927800	-0.68997200
C	-2.94568200	2.87865200	0.02392300
C	-0.44569500	-0.34847700	1.85270200
C	-0.95581500	0.96277500	1.53979900
C	-3.54039700	1.94074000	-1.02983400
C	5.09518400	0.25252500	0.36042200
C	-5.06792000	1.84463900	-0.96982800
C	5.44893400	1.53691200	0.22139000
C	-5.65021800	0.88010800	-2.00770600
C	6.88916700	1.97170900	0.35417800
C	4.48765000	2.66303900	-0.06823300
H	4.35766900	-2.12355900	-0.81904700
H	3.86649900	-0.78403600	-1.86034100
H	2.22812000	-3.76913400	0.18195900
H	1.24435700	-3.26403300	-2.54921700
H	2.50294200	-2.23283500	-3.26152700
H	2.95976000	-3.64996300	-2.28729700
H	3.48455100	-0.89128300	1.17057600
H	2.96041200	0.42361500	0.14965500
H	0.65714000	-2.81071000	1.87348800
H	-1.07358100	3.64879500	0.76988700
H	-1.05819200	3.28636600	-0.95091400
H	0.15793900	1.39004800	-1.66312200
H	-3.33371600	3.89485600	-0.13214600
H	-3.29078700	2.56747300	1.01670000
H	-1.54751600	1.44863300	2.31012100
H	-3.23325800	2.27610000	-2.03003600
H	-3.10780100	0.94368400	-0.90532000
H	5.89291600	-0.46449800	0.56262900
H	-5.50037300	2.84522900	-1.10628100
H	-5.36672200	1.51518400	0.03254900
H	-6.74381700	0.85927500	-1.96534500
H	-5.35784300	1.17292400	-3.02245900
H	-5.29813000	-0.13941100	-1.83077300
H	7.55304300	1.12907700	0.56326200
H	7.23780300	2.46215800	-0.56405800

H	7.00477100	2.70569300	1.16214900
H	3.45649500	2.33138700	-0.18369600
H	4.51397500	3.40627000	0.73855000
H	4.78048200	3.18798400	-0.98643800
C	-4.04718800	-1.62190000	0.57745300
C	-2.76048500	-1.96658600	-0.13240800
H	-2.96934100	-2.49131600	-1.06470600
H	-2.17069700	-1.06559300	-0.32276400
H	-2.13223500	-2.58116500	0.51923500
C	-3.91491500	-0.81192900	1.84371300
H	-3.65676400	0.21390800	1.56073900
H	-4.85864500	-0.81349400	2.39047200
H	-3.07846000	-1.15094800	2.46434200
O	-5.13478600	-1.96189300	0.13967400

[THCA – H]$^-$ ··· ACE

O	2.24934300	-2.35007600	-0.65958400
O	0.25746400	1.07928200	1.98716000
O	-2.09020200	1.00204700	2.56068300
O	-3.48095600	-0.49489800	1.70759900
C	3.58806300	-0.37263900	-0.39914000
C	2.59055400	0.26651700	0.58275000
C	3.57829500	-1.90549400	-0.28696600
C	4.94061600	0.33223100	-0.26117000
C	1.27041700	-0.47779300	0.54838100
C	4.80179600	1.79622900	-0.71327000
C	2.50486100	1.75094600	0.27749600
C	3.49566900	2.43989000	-0.29739900
C	1.17199600	-1.70841000	-0.08468500
C	4.48536400	-2.56650400	-1.32388000
C	3.90188200	-2.42499900	1.11950800
C	0.12856400	0.01523500	1.25367300
C	-0.04464300	-2.39242800	-0.17869600
C	-1.20692500	-1.87561500	0.38232100
C	3.37826800	3.91205000	-0.59694500
C	-1.14273200	-0.66937000	1.12641300
C	-2.47442000	-2.67652200	0.11243500
C	-3.00146800	-2.45915300	-1.32627800
C	-2.33177900	-0.07643400	1.81201700
C	-3.54938500	-1.04119900	-1.61116500
C	-5.08241900	-0.95460300	-1.68959700
C	-5.80577400	-1.36701200	-0.40247000
H	3.21198900	-0.16874700	-1.41140500
H	2.99641100	0.18227000	1.60410700
H	5.71740300	-0.16027400	-0.85356800
H	5.26325200	0.29577100	0.78575800
H	4.88274900	1.85160900	-1.80965200
H	5.64192400	2.39118000	-0.32987700
H	1.59591200	2.25071300	0.58457600
H	4.29551700	-2.15281000	-2.31755400
H	5.53905200	-2.42258700	-1.07510100
H	4.27919800	-3.63909300	-1.35309900
H	4.88656300	-2.07470600	1.44190700
H	3.15835500	-2.08685200	1.84222700
H	3.90239000	-3.51792500	1.11793300
H	-0.05740800	-3.34007600	-0.70520000
H	3.51901400	4.10784300	-1.66822400
H	4.15013800	4.48746500	-0.06898200
H	2.40156600	4.30441700	-0.30635300

H	-2.22771100	-3.73935200	0.22352900
H	-3.24988400	-2.43046200	0.83136300
H	-3.78533300	-3.20124700	-1.52766200
H	-2.18613400	-2.68337000	-2.02180800
H	-1.06413300	1.19820700	2.47082700
H	-3.19605700	-0.36316500	-0.83209300
H	-3.13679900	-0.67063600	-2.55628500
H	-5.43188600	-1.57791800	-2.52497200
H	-5.36220100	0.07596300	-1.94308800
H	-6.88985600	-1.25027800	-0.50917400
H	-5.60892300	-2.41486100	-0.15548700
H	-5.46321000	-0.77126700	0.44503300
C	-2.66017000	3.22709300	-0.73782900
C	-1.35938600	2.45991500	-0.72307500
H	-1.52619400	1.40160200	-0.94309100
H	-0.65659400	2.88754600	-1.43795100
H	-0.92444300	2.48169500	0.28171200
C	-3.77990500	2.66402300	0.10764600
H	-4.09566200	1.69740500	-0.29697200
H	-3.43473100	2.45439900	1.12423900
H	-4.62587500	3.35171200	0.11444200
O	-2.79845200	4.24740700	-1.39092200

[CBDA – H]$^{-}$ ··· ACE

O	-0.61387500	-0.58468500	-1.60215300
O	-0.87782600	-0.63428400	3.13009200
O	3.18696600	0.83794600	-1.72404000
O	1.42799700	-0.03328200	-2.76587100
C	-3.18124900	-0.05728500	-0.05766800
C	-2.24567800	-1.05988500	0.67252900
C	-4.58224900	-0.69431300	-0.18790000
C	-4.53054500	-1.95365000	-1.06313000
C	-2.36383000	-2.44357900	0.05691800
C	-0.79497500	-0.61003700	0.74621100
C	-3.37658300	-2.86543000	-0.71087400
C	-3.24783400	1.30992200	0.59856800
C	-0.03228300	-0.41088100	-0.45196500
C	-0.15091100	-0.43581700	1.96344300
C	-3.40740300	-4.24028500	-1.32787400
C	1.96973400	0.13018100	0.90188800
C	1.36358300	-0.00975400	-0.36938100
C	-3.51661900	1.37532600	2.08411200
C	1.20048300	-0.07510900	2.04866200
C	3.44009700	0.44876500	1.14301000
C	-3.09748900	2.42430400	-0.13090800
C	4.23538700	-0.77007000	1.67000300
C	4.31140500	-1.96400000	0.70278000
C	2.07980700	0.29359400	-1.65354000
C	5.10254400	-1.71994800	-0.59452800
C	6.58779400	-1.40610800	-0.36890400
H	-2.77720600	0.07034800	-1.06625500
H	-2.59996400	-1.14970900	1.70683600
H	-4.96092000	-0.96104700	0.80914300
H	-5.28260300	0.03455900	-0.61367500
H	-5.47884000	-2.50774900	-0.98518400
H	-4.43868600	-1.66599700	-2.12309700
H	-1.53604100	-3.12054700	0.26533600
H	-3.43670600	-4.17271300	-2.42517900
H	-2.52680800	-4.82921400	-1.05163300
H	-4.30509200	-4.79782100	-1.02240600

H	-3.66434300	2.40840500	2.41441800
H	-4.41098500	0.79810400	2.35344400
H	-2.68305200	0.94624800	2.65090100
H	1.65948800	0.04023800	3.03000700
H	3.49653900	1.24001400	1.90408800
H	3.89604000	0.83603700	0.23502300
H	-3.15762900	3.41642400	0.30889300
H	-2.87580900	2.37705400	-1.19350900
H	5.24931300	-0.43575300	1.93025700
H	3.77856300	-1.11568100	2.60743100
H	4.76119700	-2.81537600	1.23737500
H	3.28873200	-2.26507900	0.44224600
H	0.46402600	-0.34631400	-2.46063300
H	-0.29104700	-0.48001300	3.88066800
H	5.02015900	-2.61989100	-1.21969900
H	4.63998300	-0.90765900	-1.16344500
H	6.72322600	-0.45629000	0.16051400
H	7.12130900	-1.32398700	-1.32312200
H	7.07770100	-2.19048500	0.22491700
C	-0.14720000	3.84452300	-0.62468200
C	0.04341700	3.02613000	-1.88078700
H	1.11089300	2.84219300	-2.05029500
H	-0.41943400	2.03927100	-1.77413300
H	-0.38130200	3.55050900	-2.73914600
C	0.31293600	3.20780200	0.66771000
H	1.36277300	2.90629500	0.59107000
H	0.17191000	3.90122700	1.49948800
H	-0.25360000	2.28699700	0.84405300
O	-0.64523800	4.96443200	-0.64888500