SUPPORTING INFORMATION

Identification of 24 unknown substances (NIAS/IAS) from food contact polycarbonate by LC-Orbitrap Tribrid HRMS-DDMS^3. Safety assessment

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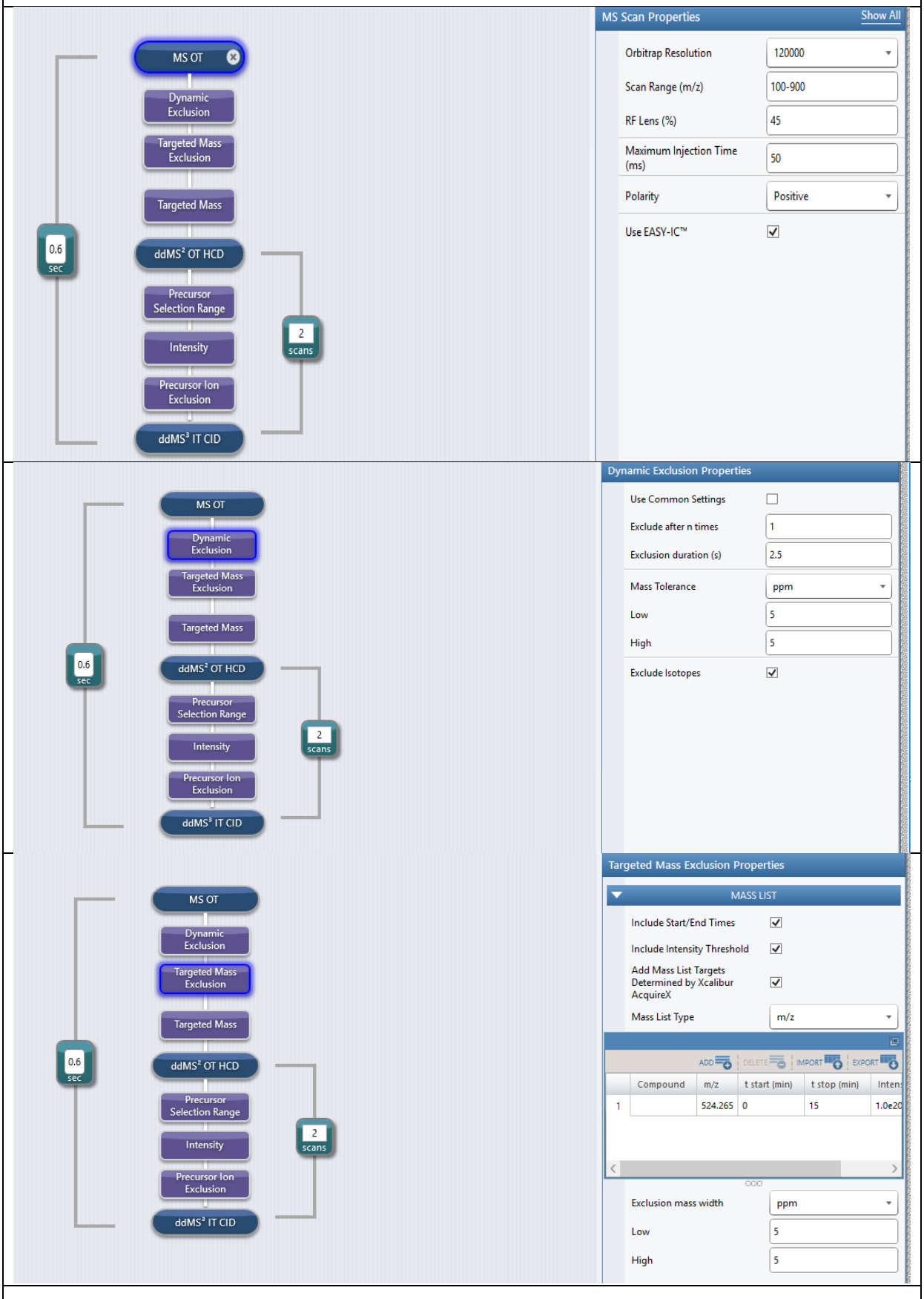
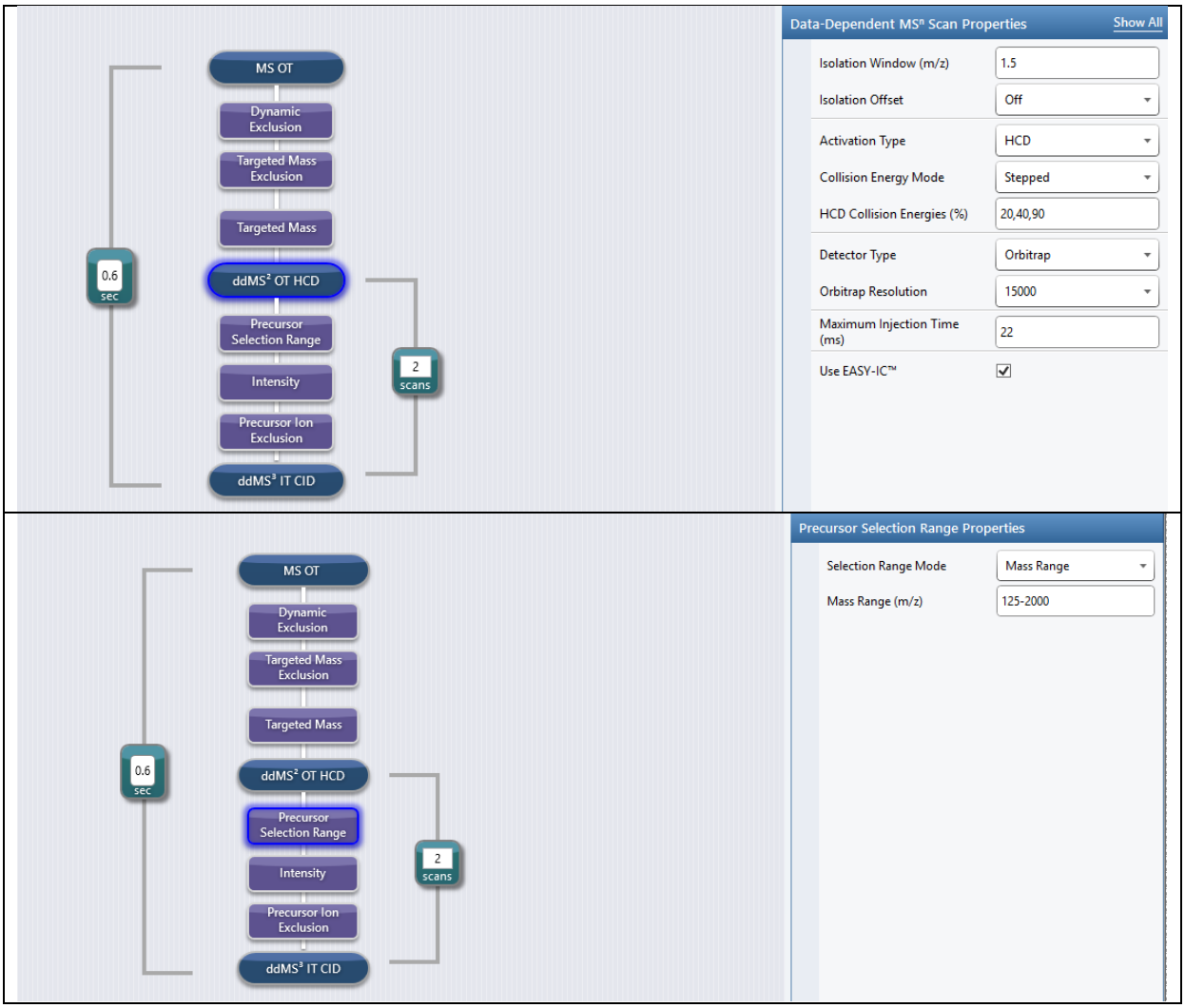
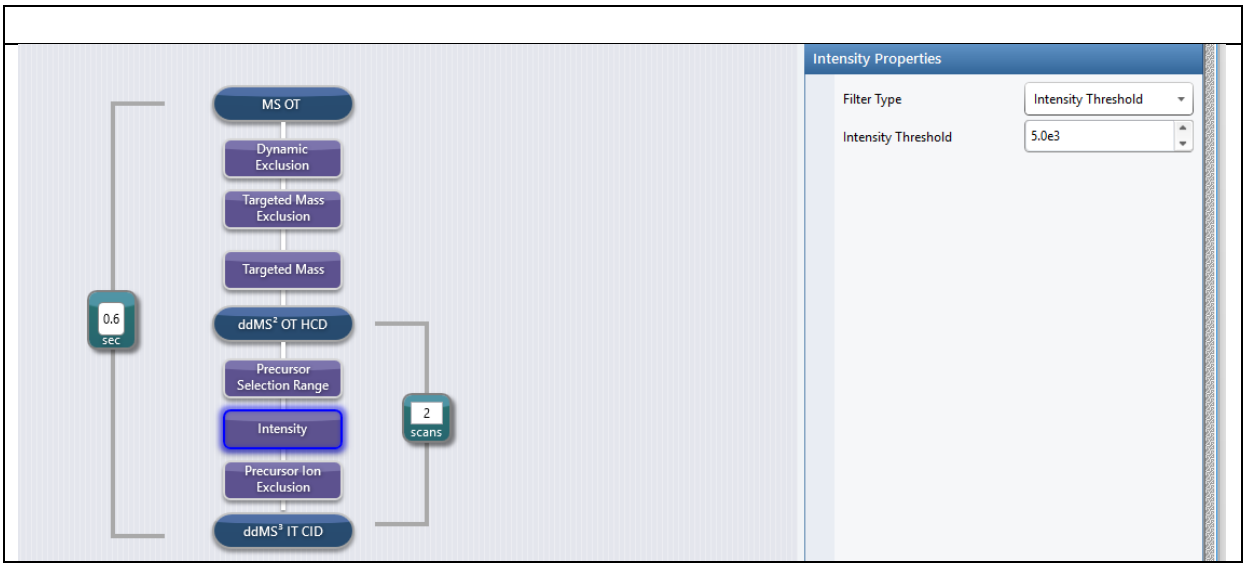
Figure SI-1: Workflow for the ddMS^3 used in AcquireX Deep Scan Mode




MS OT
Dynamic Exclusion
Targeted Mass Exclusion
Targeted Mass
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Data-Dependent MSⁿ Scan Properties
Show All
Isolation Window (m/z)
1.5
Isolation Offset
Off
Activation Type
HCD
Collision Energy Mode
Stepped
HCD Collision Energies (%)
20,40,90
Detector Type
Orbitrap
Orbitrap Resolution
15000
Maximum Injection Time (ms)
22
Use EASY-IC™
MS OT
Dynamic Exclusion
Targeted Mass Exclusion
Targeted Mass
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Precursor Selection Range Properties
Selection Range Mode
Mass Range
Mass Range (m/z)
125-2000


MS OT
Dynamic Exclusion
Targeted Mass Exclusion
Targeted Mass
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Intensity Properties
Filter Type
Intensity Threshold
Intensity Threshold
5.0e3

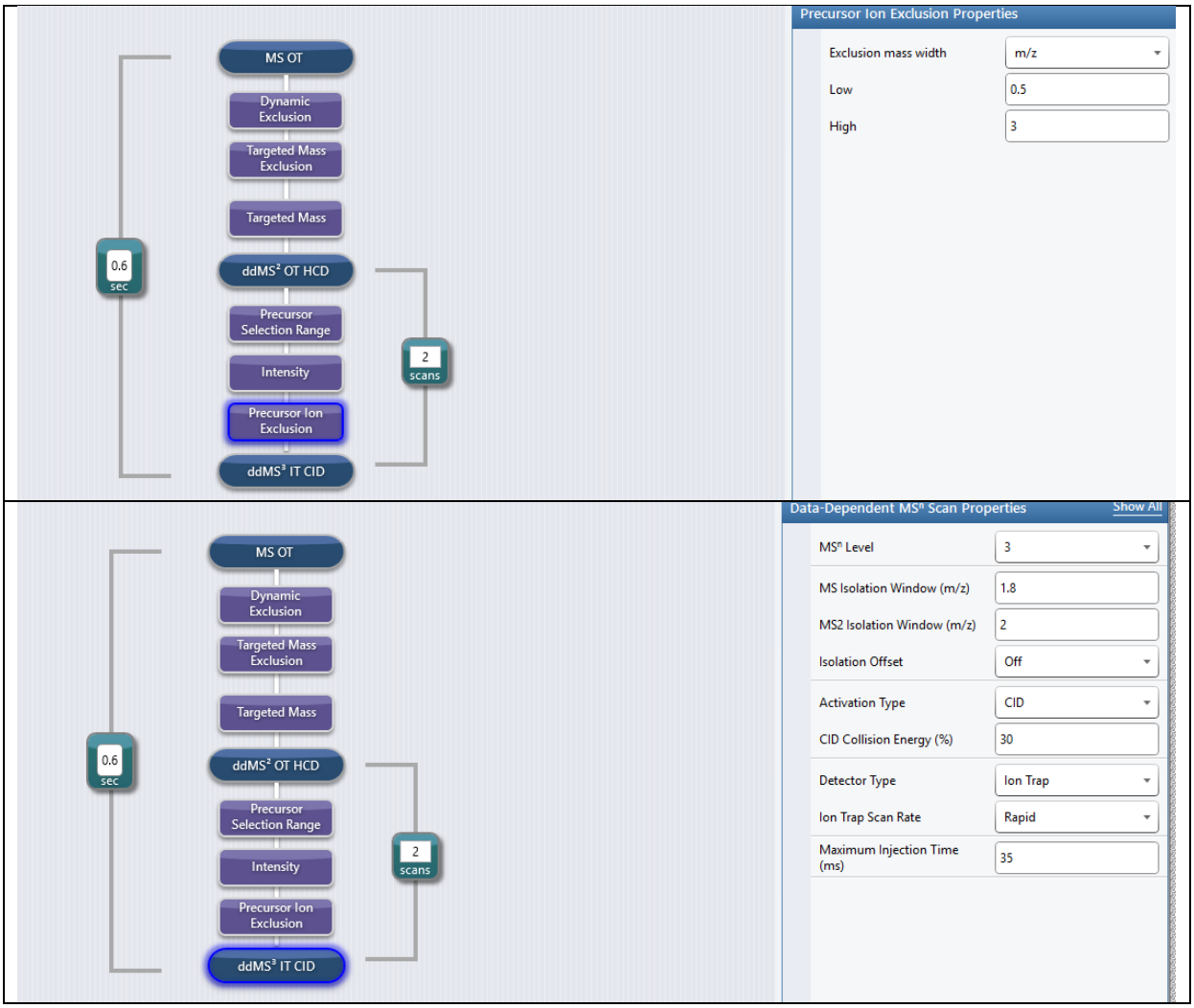
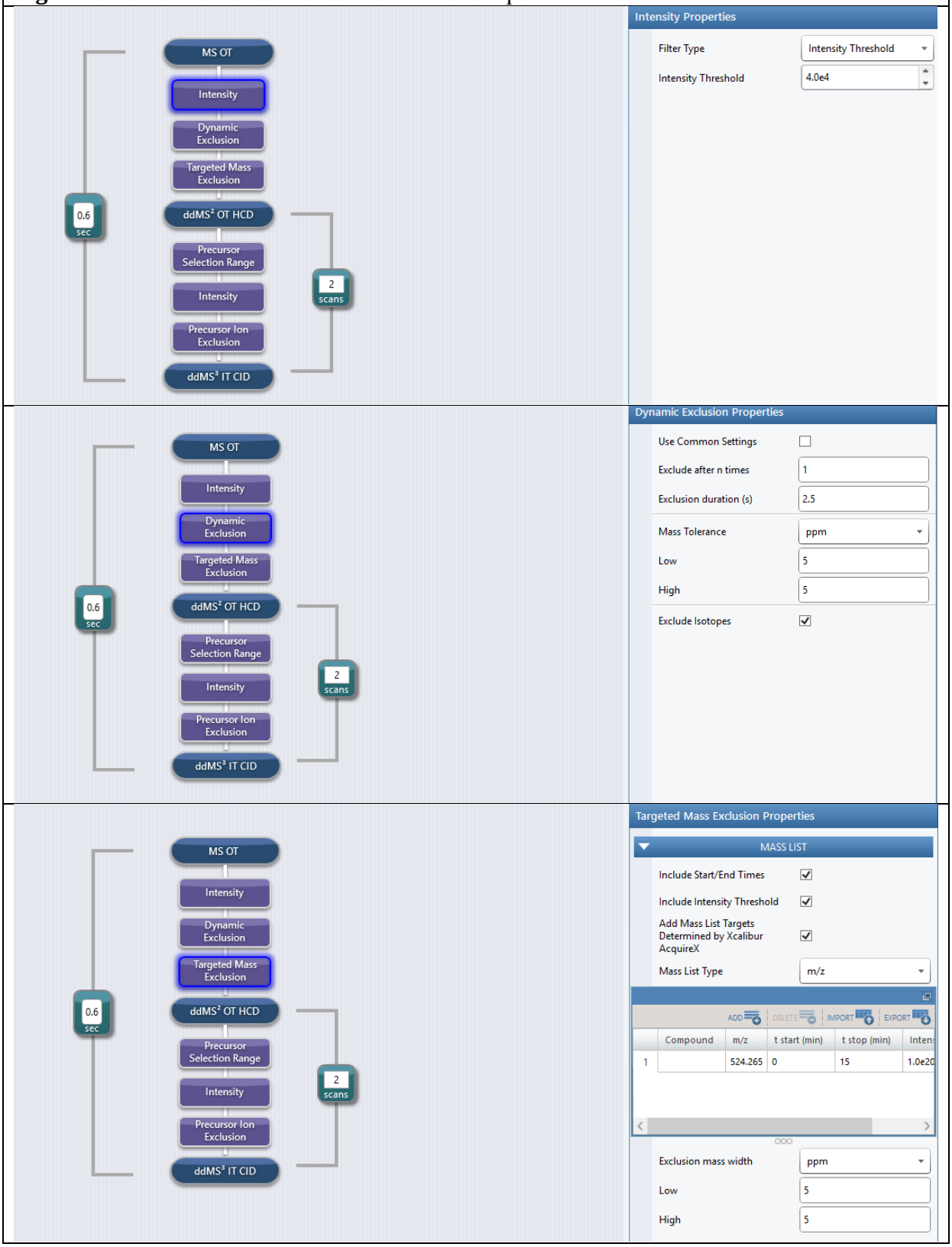
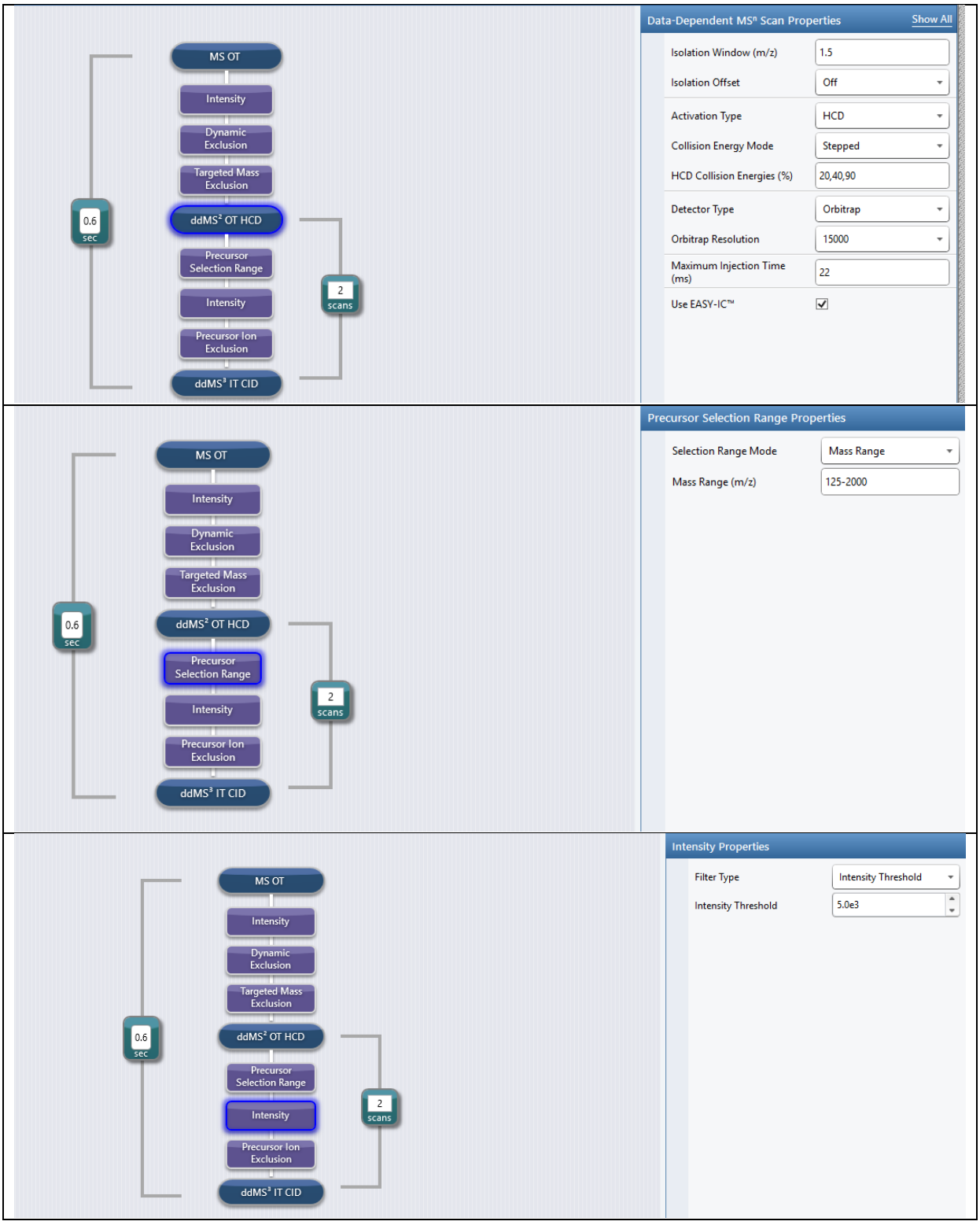

MS OT
Dynamic Exclusion
Targeted Mass Exclusion
Targeted Mass
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Precursor Ion Exclusion Properties
Exclusion mass width
m/z
Low
0.5
High
3
MS OT
Dynamic Exclusion
Targeted Mass Exclusion
Targeted Mass
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Data-Dependent MSⁿ Scan Properties
Show All
MSⁿ Level
3
MS Isolation Window (m/z)
1.8
MS2 Isolation Window (m/z)
2
Isolation Offset
Off
Activation Type
CID
CID Collision Energy (%)
30
Detector Type
Ion Trap
Ion Trap Scan Rate
Rapid
Maximum Injection Time (ms)
35

Figure SI-2: Workflow for the ddMS^3 used in AcquireX IPE Mode




MS OT
Intensity
Dynamic Exclusion
Targeted Mass Exclusion
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Data-Dependent MSⁿ Scan Properties
Show All
Isolation Window (m/z) 1.5
Isolation Offset Off
Activation Type HCD
Collision Energy Mode Stepped
HCD Collision Energies (%) 20,40,90
Detector Type Orbitrap
Orbitrap Resolution 15000
Maximum Injection Time (ms) 22
Use EASY-IC™
Precursor Selection Range Properties
Selection Range Mode Mass Range
Mass Range (m/z) 125-2000
Intensity Properties
Filter Type Intensity Threshold
Intensity Threshold 5.0e3

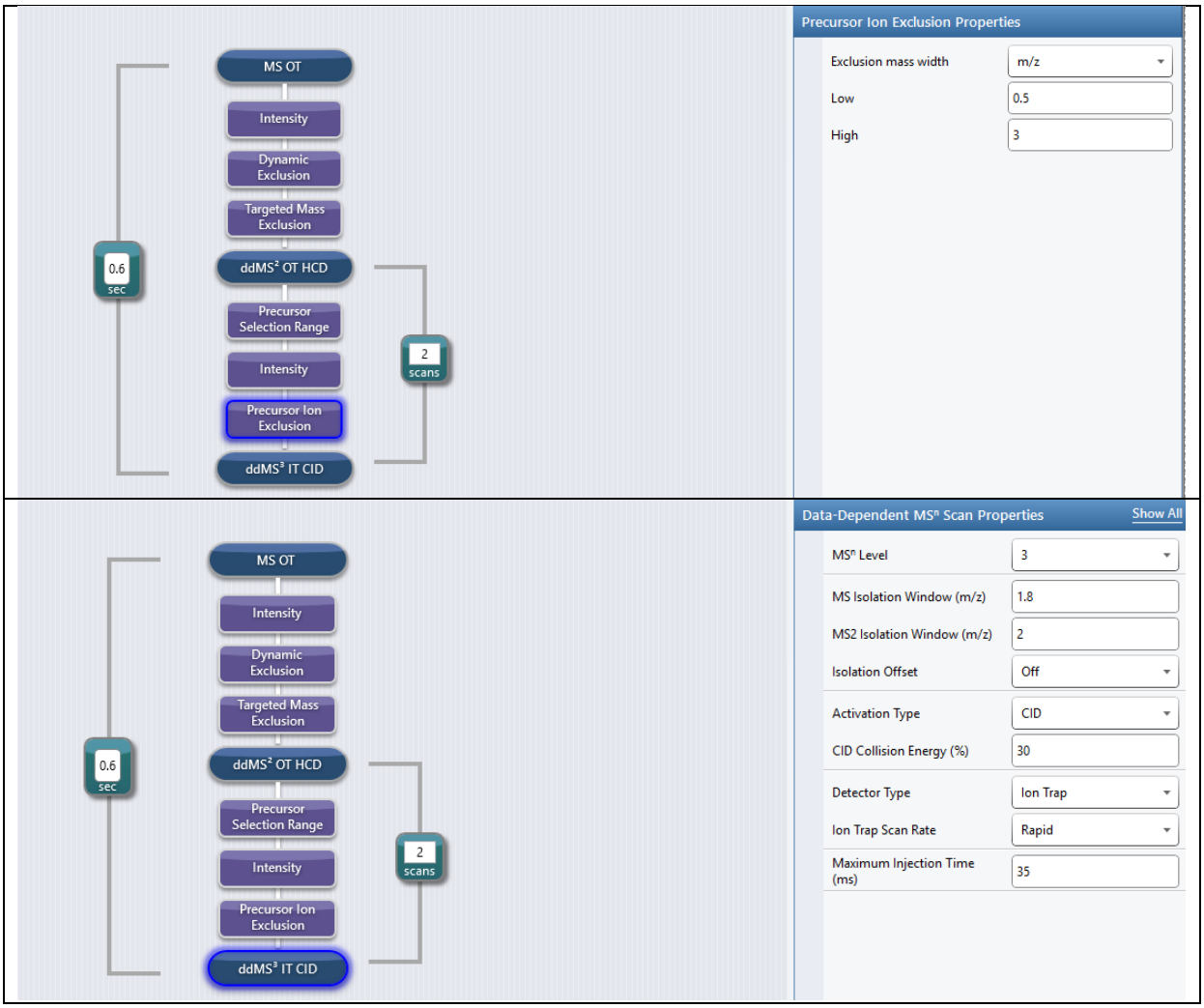

MS OT
Intensity
Dynamic Exclusion
Targeted Mass Exclusion
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Precursor Ion Exclusion Properties
Exclusion mass width
m/z
Low
0.5
High
3
MS OT
Intensity
Dynamic Exclusion
Targeted Mass Exclusion
ddMS² OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS³ IT CID
0.6 sec
2 scans
Data-Dependent MSⁿ Scan Properties
Show All
MSⁿ Level
3
MS Isolation Window (m/z)
1.8
MS2 Isolation Window (m/z)
2
Isolation Offset
Off
Activation Type
CID
CID Collision Energy (%)
30
Detector Type
Ion Trap
Ion Trap Scan Rate
Rapid
Maximum Injection Time (ms)
35

Figure SI-3. Compound Discover Workflow

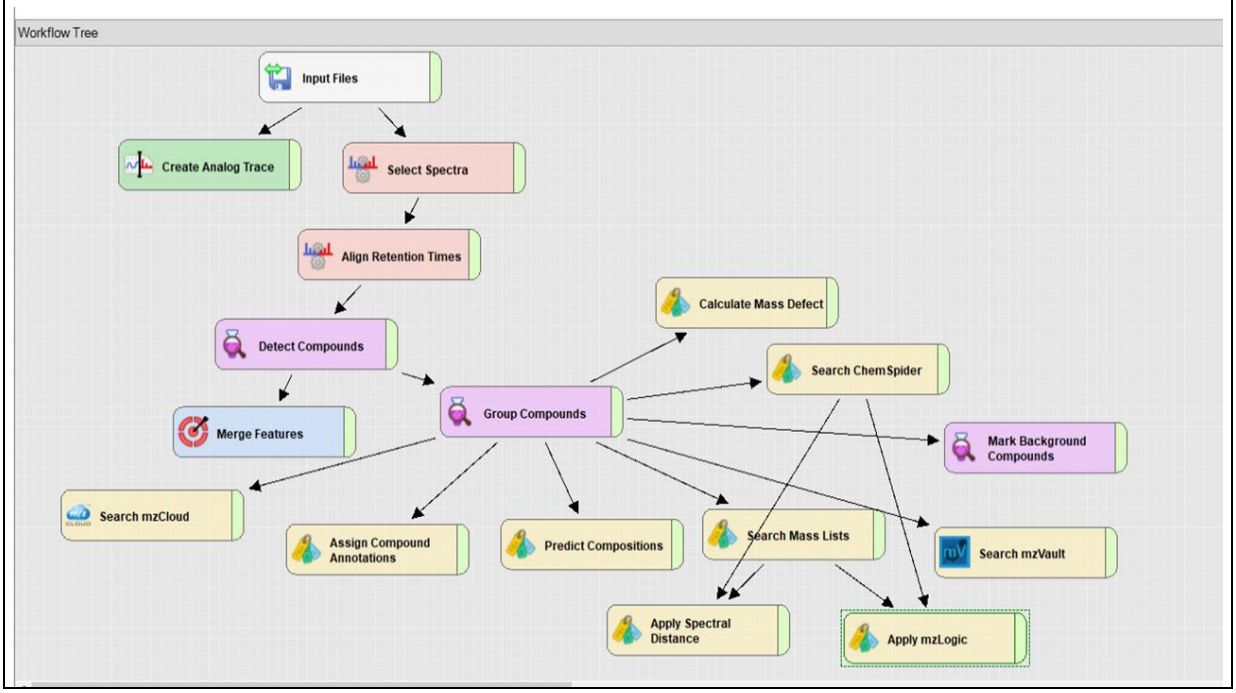
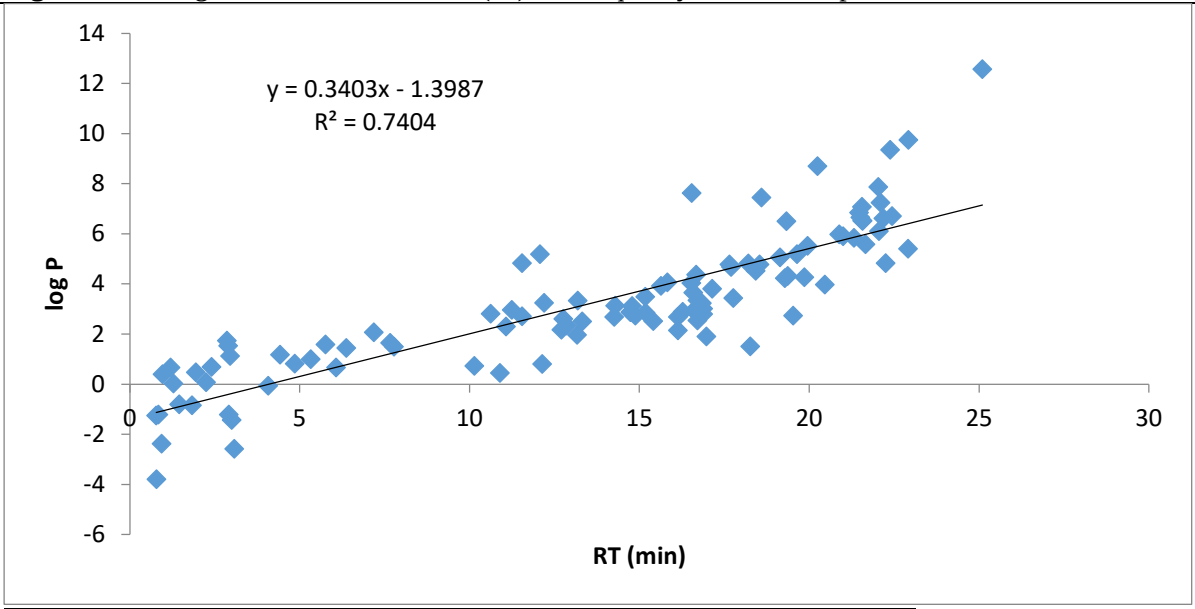


Figure SI-4. Log P and Retention Time (Rt) of the quality control compouds

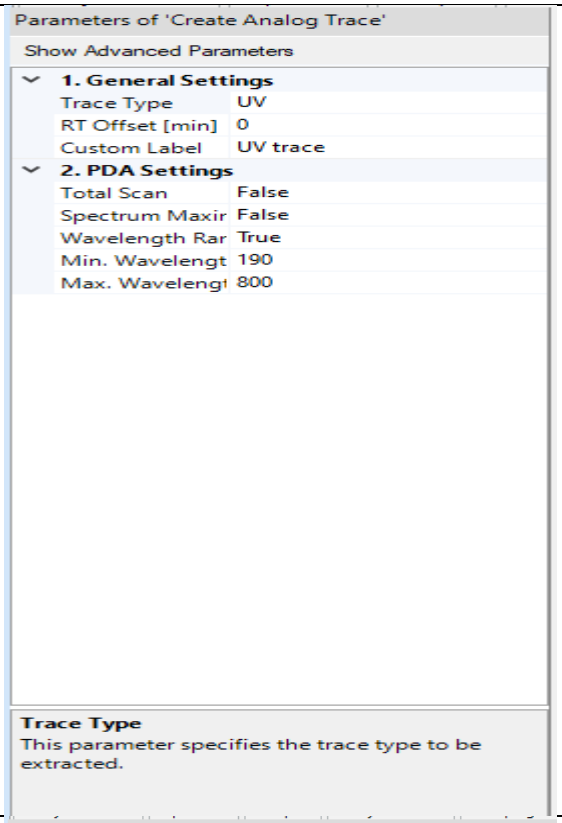
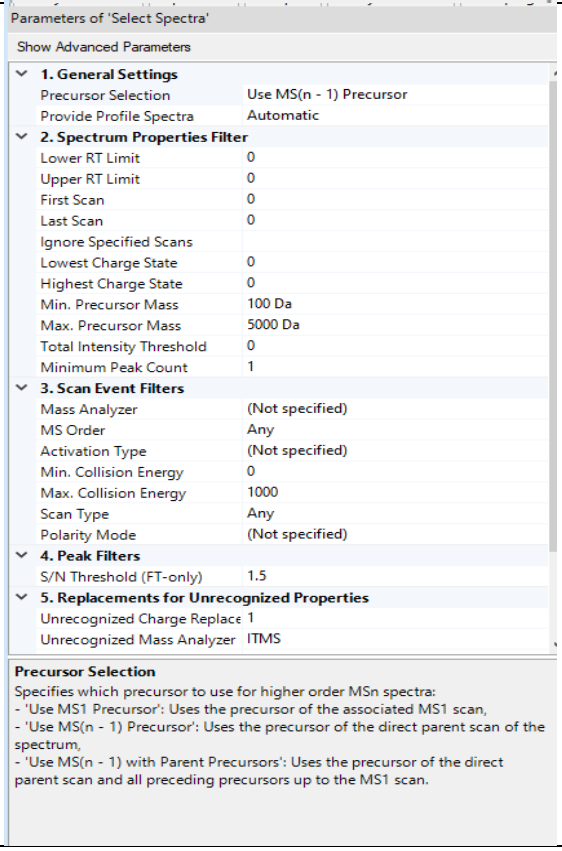


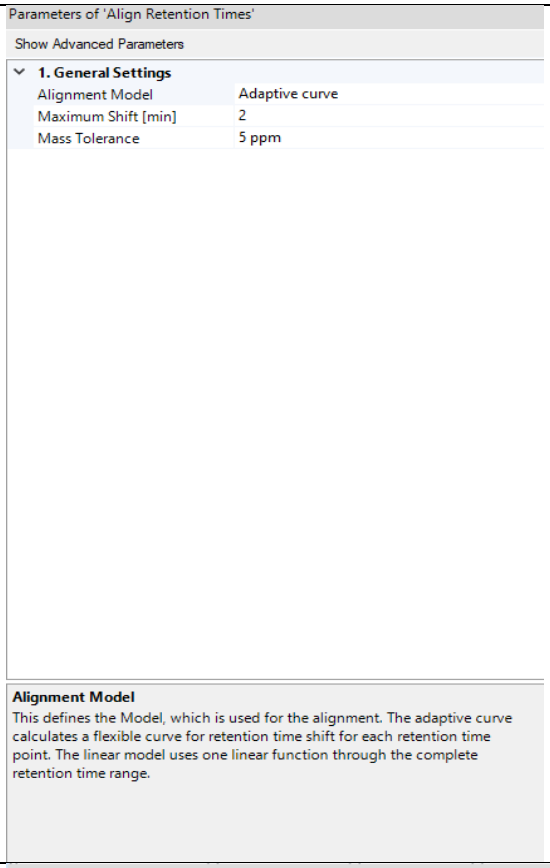
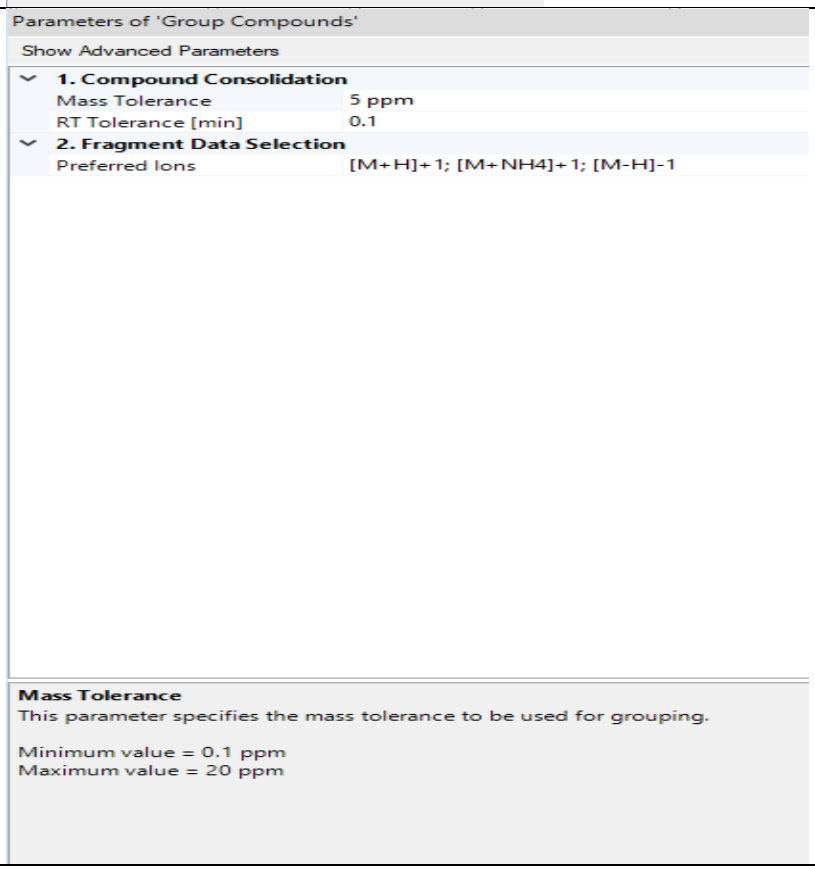
Analyte	Rt	log P
Sulfaguanidine	0,85	-1,22
Val-Tyr-Val	4,86	0,8
Reserpine	13,19	3,32
Caffeine	4,08	-0,07
Acetaminophen	1,95	0,46
Sulfadimethoxine	7,67	1,63
Terfenadine	16,55	7,62
2,4-D	12,77	2,59
2-diethylamino-6-methyl pyrimidin-4-ol/one	2,96	1,11
3,5,6-Trichloro-2-pyridinol	12,71	2,16
3-phenoxybenzoic acid	15,64	3,91
4-Fluoro-3-phenoxybenzoic acid	15,83	4,05
4-nitrophenol	5,77	1,57
5-hydroxy-thiabendazole	2,86	1,73
6-Chloronicotinic acid	5,33	0,98
Acetochlor	16,61	2,92
Acetochlor mercapturate	14,75	2,86
Alachlor mercapturate	14,75	2,86
Bentazone	10,63	2,8
Benzophenone-3 (Oxybenzone)	16,59	3,64
Carbendazim	2,9	1,52
Chlorfenvinphos	18,43	4,51
Chlormequat	0,79	-3,8
Desisopropylatrazine	4,43	1,16
Diethylthiophosphate	2,41	0,68
Dimethyldithiophosphate	1,2	0,65
Fenhexamid	16,54	4,02
Fenvalerate free acid	16,72	3,33

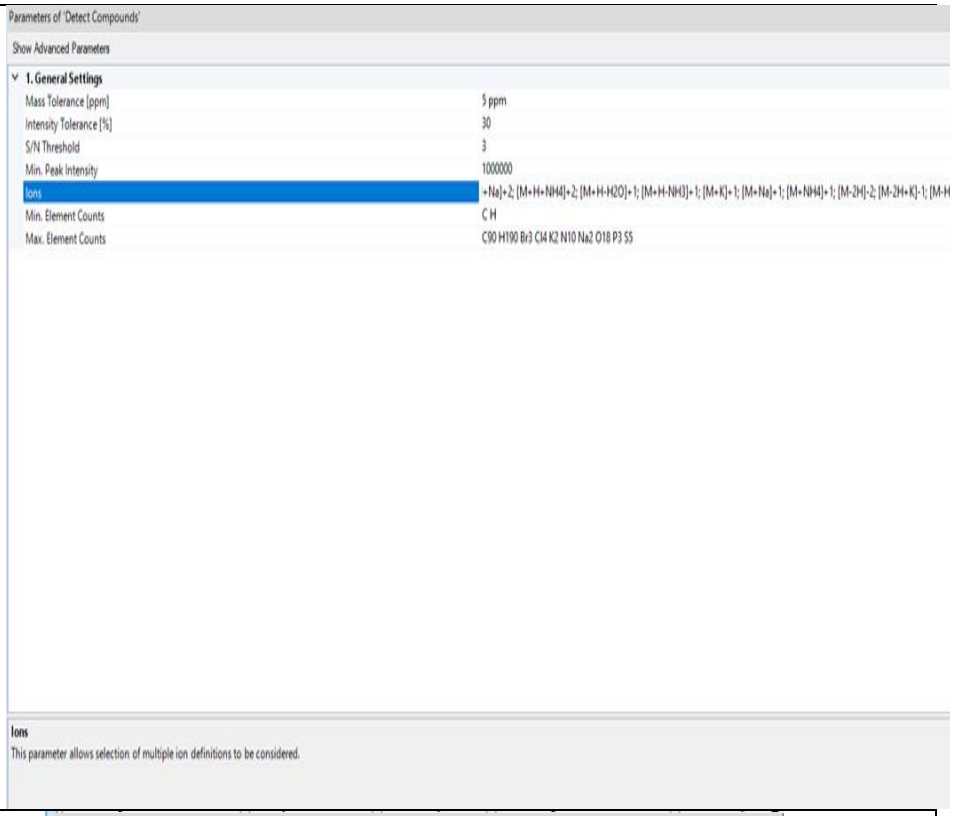
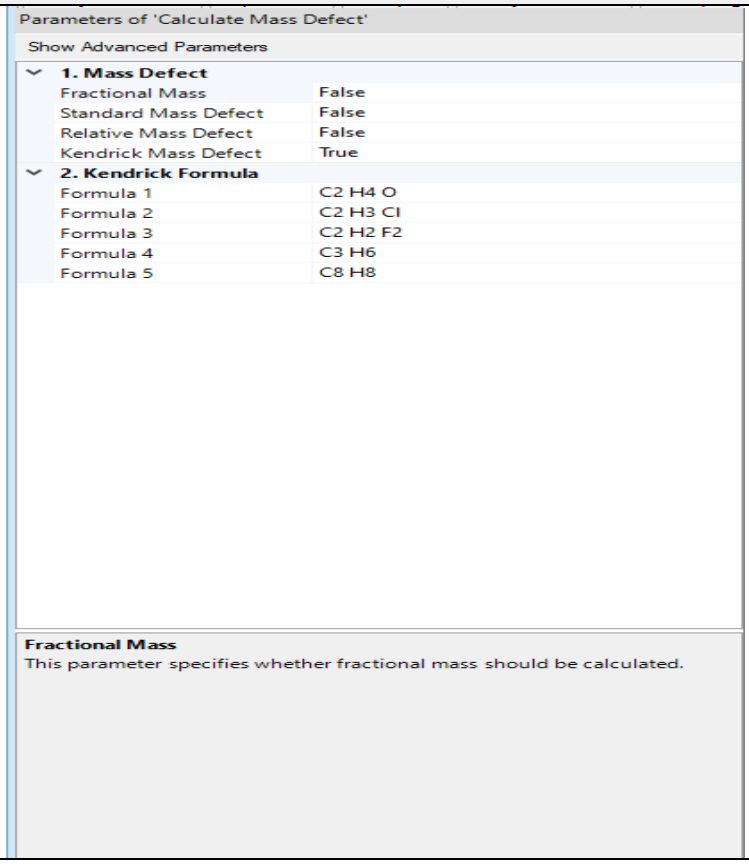
Fipronil	17,66	4,76	
Fipronil sulfone	18,6	7,44	
Fluopyram	16,68	4,36	
Hydroxy-tebuconazole	15,42	2,5	
Isoproturon	12,86	2,32	
Malathion dicarboxilic acid	7,78	1,48	
Mecoprop	15,19	2,84	
Metolachlor	16,89	3	
N,N-diethyl-m-toluamide ou DEET	13,17	1,96	
Omethoate	2,25	0,06	
Prochloraz	17,15	3,8	
p-Toluenesulfonamide	12,15	0,79	
Triclosan glucuronide	16,72	2,53	
Triclosan sulfate	17,71	4,66	
acetamiprid-N-desmethyl	6,08	0,65	
Acephate	1,84	-0,85	
Avermectin B1a (Abamectin)	21,57	6,51	
Benodanil	12,2	3,23	
benzoic acid	16,98	1,89	
Bromoxynil	11,25	2,95	
Butocarboxim	18,27	1,49	
Cefoperazone	6,38	1,43	
Dichlorvos	10,15	0,71	
Dinoterb	17,77	3,42	
Flamprop	15,18	3,47	
Inabenfide	14,27	2,67	
Ivermectin B1a	22,19	6,61	
MCPA	13,32	2,49	
Methamidophos	1,46	-0,82	
Nigericin	22,26	4,82	
Phenytoin	11,08	2,29	
Rifaximin	16,85	3,22	
Salicylic acid	7,19	2,06	
salinomycin	22,06	6,1	
Simazine 2-Hydroxy	2,92	-1,22	
Spinosad A (Spinosyn A)	18,21	4,8	
TCMTB	14,29	3,12	
Tepraloxydim	16,28	2,88	
Trichlorfon (Dylox)	10,9	0,43	
triclosan	19,65	5,17	
Valproic acid	14,89	2,72	
Vancomycin	3	-1,44	
1-Stearoylglycerol	22,11	7,23	
4-tert-Butylcyclohexyl acetate	20,47	3,96	
Bis(2-ethylhexyl)adipate	22,04	7,85	

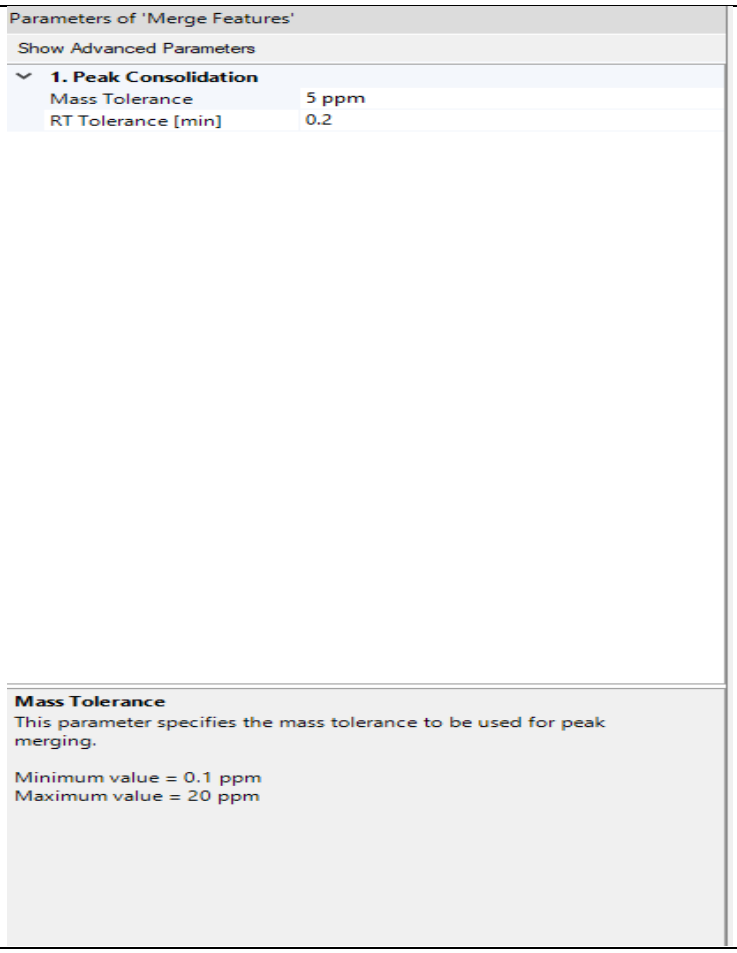
Citroflex A-4	19,34	6,49	
Dibutyl phthalate	11,55	4,82	
Dibutyl sebacate	20,89	5,97	
Diethyl phthalate	11,55	2,7	
Dimethyl sebacate	16,89	2,79	
Dipentyl phthalate	21	5,89	
Erucamide	22,93	9,74	
Ethyl Oleate	20,25	8,69	
Galaxolidone	19,96	5,5	
Hexadecanamide	21,48	6,84	
Hexadecanedioic acid	19,15	5,05	
L-Histidine	0,78	-1,26	
Monobutyl phthalate	19,53	2,72	
N,N'-Dicyclohexylurea	14,79	3,1	
Octyl decyl phthalate	22,39	9,336	
Oleamide	21,56	7,07	
Palmitoleic acid	21,51	6,64	
Palmitoyl ethanolamide	21,32	5,82	
PEG n5	3,08	-2,59	
Pyrene	12,08	5,17	
L-Pyroglutamic acid	0,94	-2,39	
Tributyl phosphate	19,86	4,26	
Triethyleneglycol bis(2-ethylhexanoate)	21,66	5,57	
L-Tyrosine	0,97	0,38	
Urocanic acid	1,29	0,01	
Dibutyl hexanodioate	19,291	4,22	
Benzyl octyl adipate	21,58	6,5	
D,L-Camphor	16,139	2,13	
Irgafos 168	25,103	12,56	
Benazol P	19,378	4,3	
3,5-ditert-butyl-4-hydroxybenzaldehyde	18,544	4,77	
Methyl dihydrojasmonate	16,142	2,67	
Stearamide	22,447	6,7	
Dodecyl sulfate	22,916	5,39	

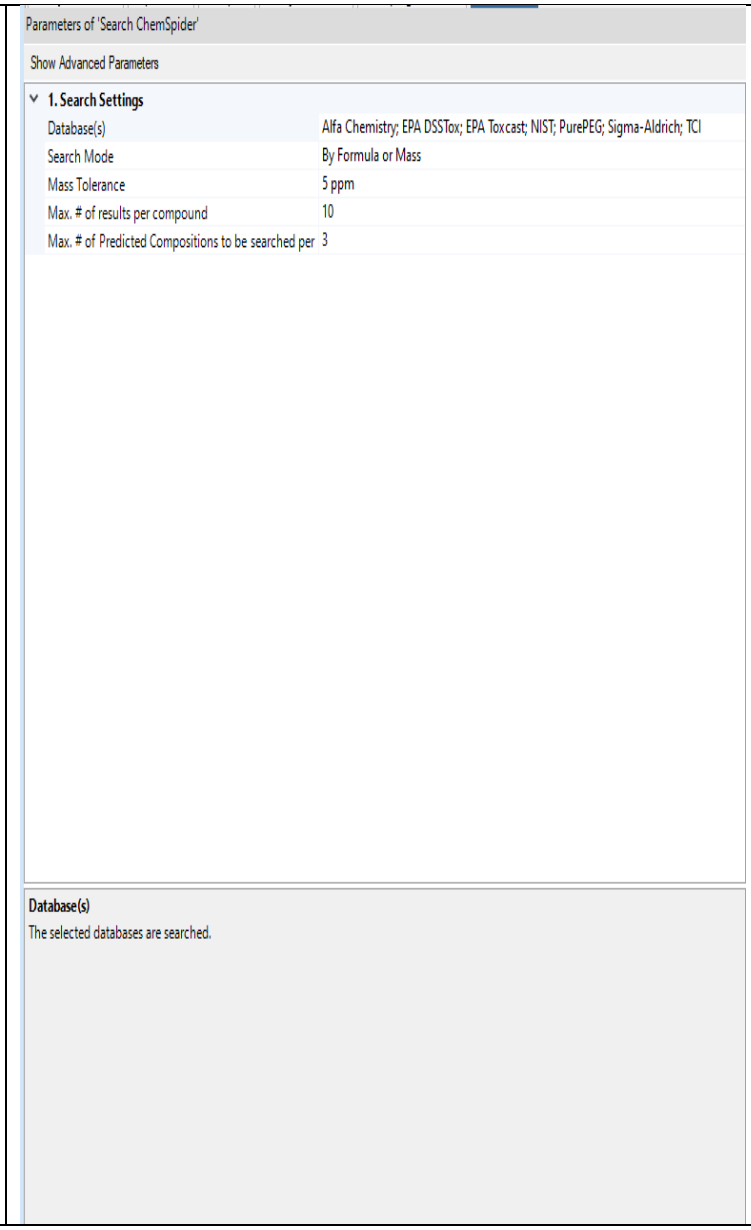
Table SI-1. Description of the different nodes of the CD workflow

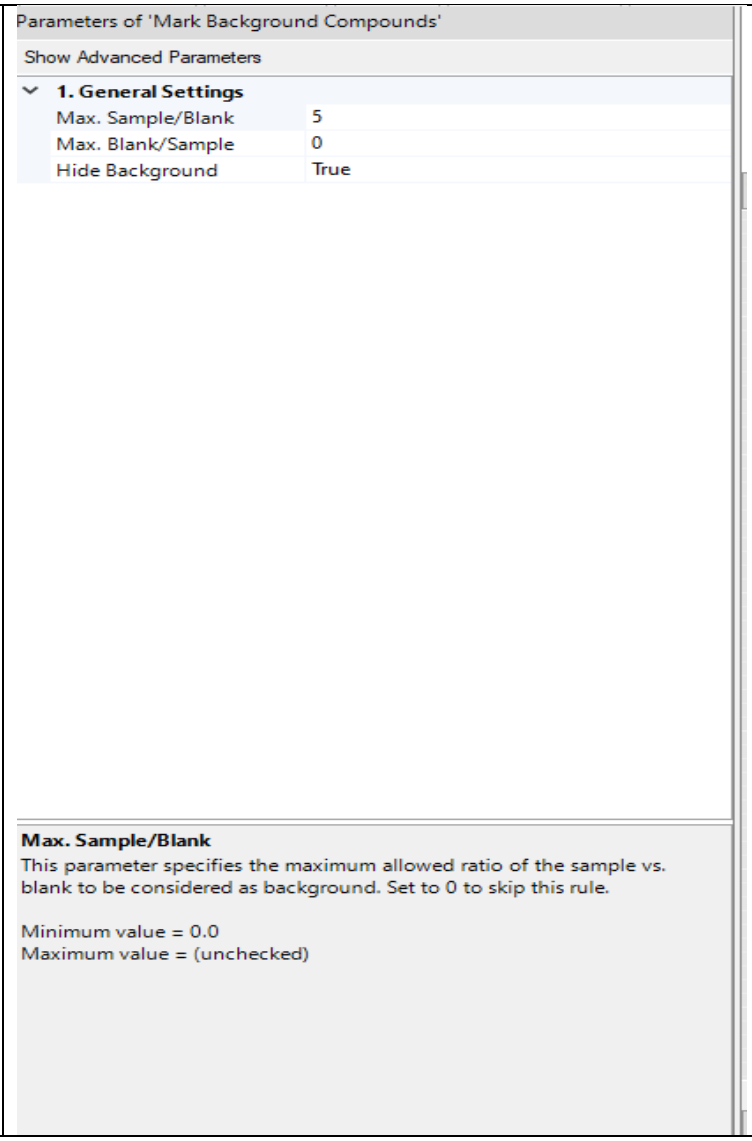
NODE	
CREATE AMONG TRACE	
SELECT SPECTRA	

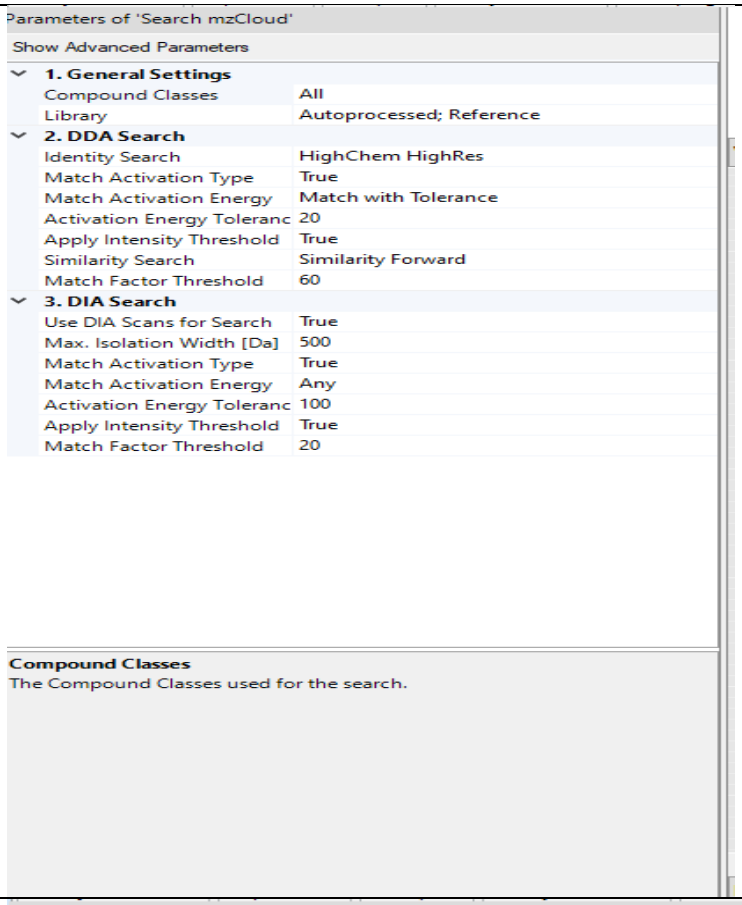
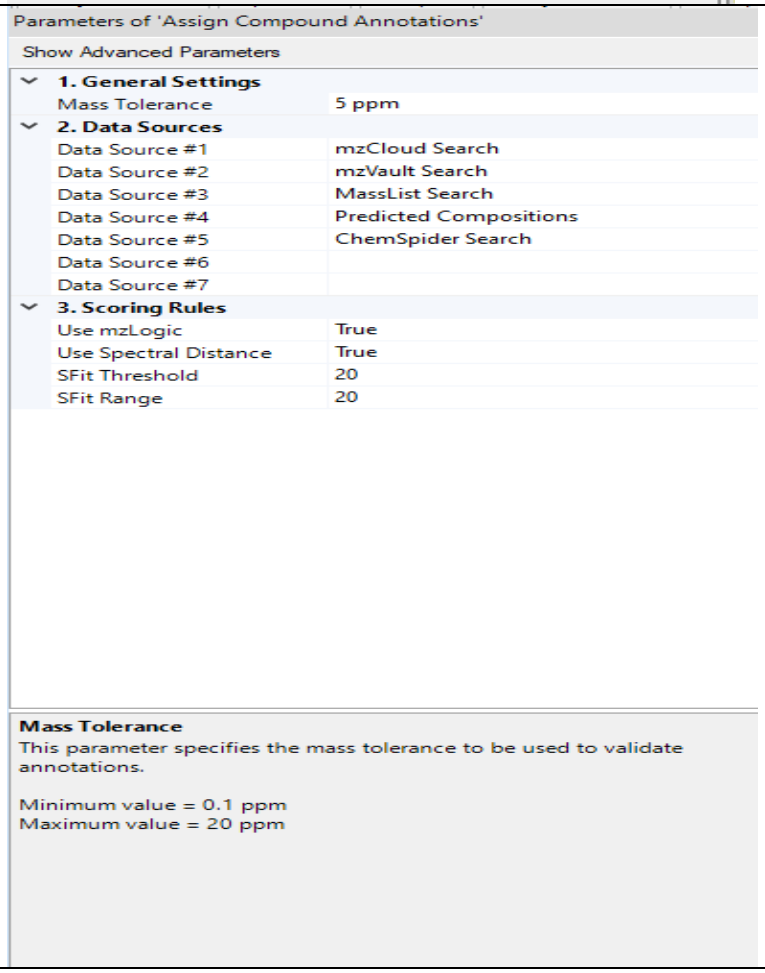
ALIGN RETENTION TIME	
GROUP COMPOUNDS	

DETECT COMPOUND	
CALCULATE MASS DEFECT	

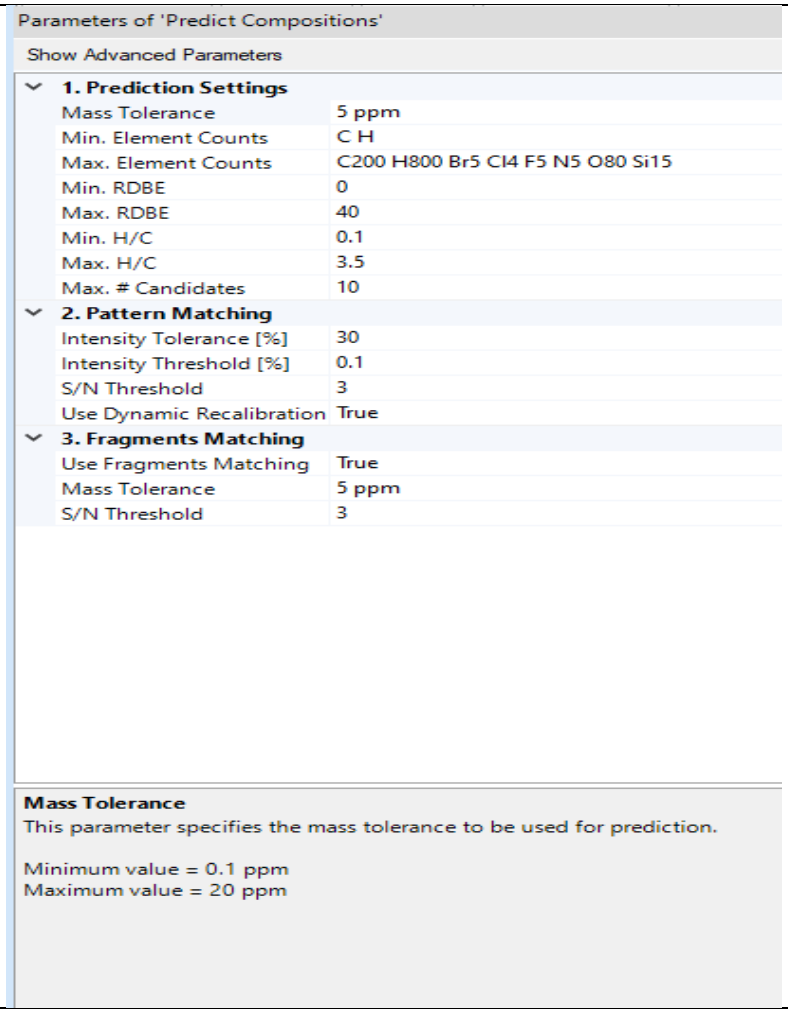
MERGE FEATURES		

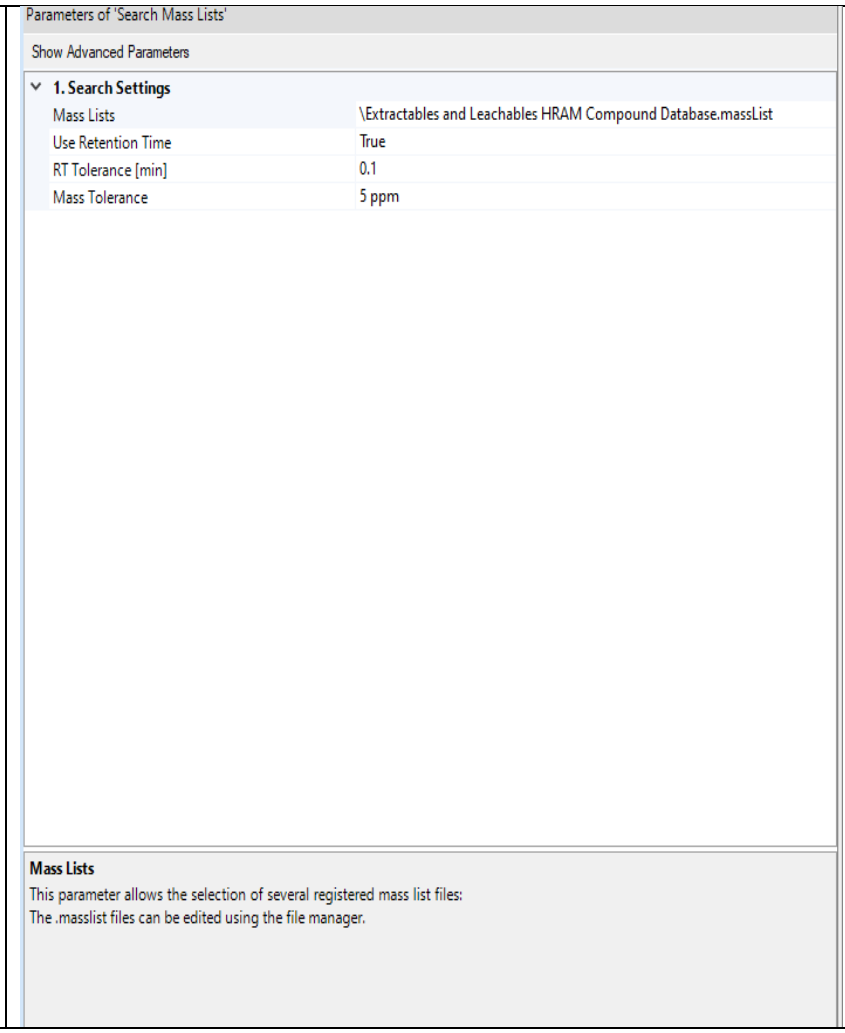
SEARCH CHEMSPIDER	

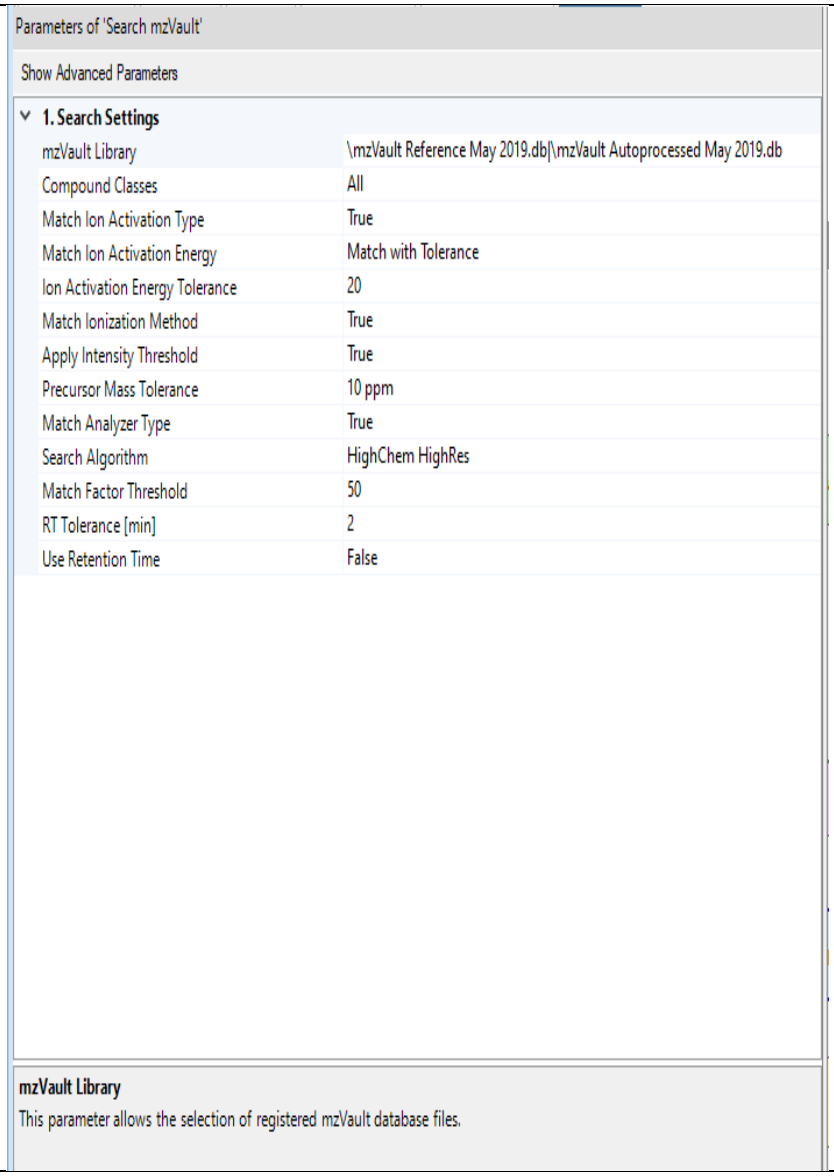
MARK BACGROUND COMPOUNDS		

SEARCH mzCLOUD	
ASSIGN COMPOUND ANNOTATIONS	

PREDICT COMPOSITION



SEARCH MASS LIST		

SEARCH mz VAULT	

Parameters of 'Search mzVault'

Show Advanced Parameters

1. Search Settings

mzVault Library	\mzVault Reference May 2019.db|\mzVault Autoprocessed May 2019.db
Compound Classes	All
Match Ion Activation Type	True
Match Ion Activation Energy	Match with Tolerance
Ion Activation Energy Tolerance	20
Match Ionization Method	True
Apply Intensity Threshold	True
Precursor Mass Tolerance	10 ppm
Match Analyzer Type	True
Search Algorithm	HighChem HighRes
Match Factor Threshold	50
RT Tolerance [min]	2
Use Retention Time	False

mzVault Library

This parameter allows the selection of registered mzVault database files.

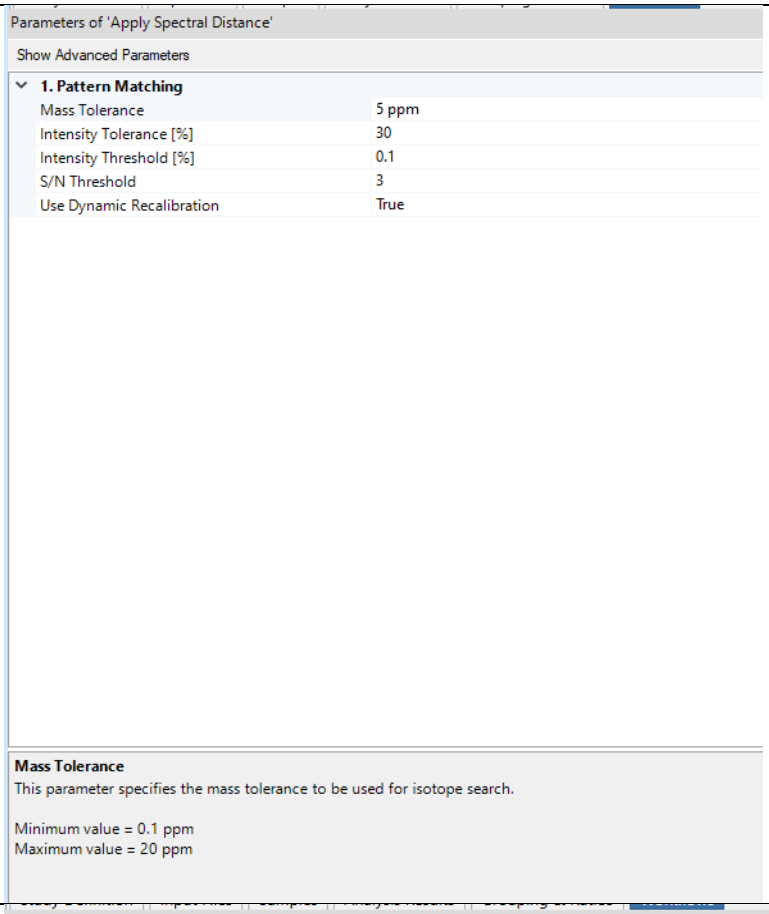
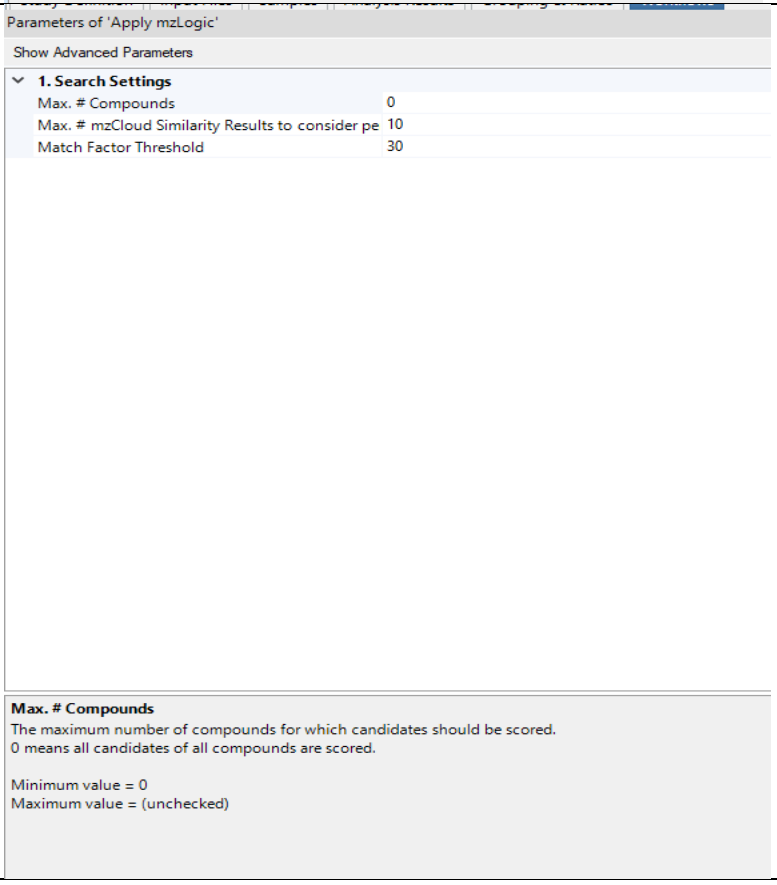
APPLY SPECTRAL DISTANCE	
APPLY mzLOGIC	

Table SI-2. Calculation of the average response factor			
Analytes	**Area**	**Concentration ($ng \cdot mL^{-1}$)**	**Response factor**
Sulfaguanidine	826910	10	82691
Val-Try-Val	3709775	10	370978
Reserpine	3548764	10	354876
Caffeine	2631124	10	263112
Acetominophen	4351886	10	435189
Sulfadimethoxine	5639812	10	563981
Terfenadine	19167123	10	1916712
AVERAGE			569648

Table SI-3. Experimental MS^3 transitions	
Substance	[1]Acquired MS^3 (m/z MS^2 precursor > m/zMS^3 fragment)
3,5-ditert-butyl-4-hydroxybenzaldehyde	179.1063 > 123.05
4-tert-butylcyclohexyl acetate	135.1166 > 107.08
Benazol P	183.0679 > 155.06
Benzyl octyl adipate	129.0544 > 100.93
Bis(2-ethylhexyl)adipate	129.0545 > 111.06
Citroflex A-4	129.0180 > 111.00
D,L-Camphor	-
DEET	173.449 > 131.02
Dibutyl hexanodioate	129.0536 > 111.08
Dibutyl phthalate	149.0231 > 121.04
Dibutyl sebacate	185.1172 > 139.03
Diethyl phthalate	177.0546 > 149.05
Dipentyl phthalate	149.0229 > 121.08
Dodecyl sulfate	247.0226 > 219.03
Erucamide	321.3157 > 163.23
Galaxolidone	255.17455 > 227.24
Hexadecanamide	130.1224 > 88.02
Irgafos 168	147.1167 > 132.09
Methyl dihydrojasmonate	153.1271 > 97.06
N,N'-Dicyclohexylurea	143.1181 > 60.92
Octyl decyl phthalate	149.0231 > 121.04
Oleamide	135.1166 > 107.08
Palmitoyl ethanolamide	283.2638 > 109.12
Stearamide	130.1222 > 88.02
[1]The fragmentation of the MS^2 precursor in the Linear Ion Trap was performed at 40 eV	