

Qualitative Summary Report

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Lab Name: Plant Sciences
Instrument: Thermo Scientific Instrument
User: ISQ140326
Batch: 26102018_processed

Method: 26102018_processed_GCMS_METABOLOMICS_GENESIS
 GCMS_METABOLOMICS_GENESIS
Call File: 26102018_processed.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
19	D3_14	D3_14	N/A		10/29/2018 9:55:59 PM	

Internal Standards

Internal Standard	ISTD#	RT	Response	Injected		Sample	
				Conc	Units	Conc	Units
phenyl_b_d_glucopyranoside hydrate 98%	1	27.81	24283898956	1500.000	ug mL	1500.000	ug mL

Qualitatively-identified Compounds

Compound	Uses ISTD#	RT	Response	Injected		Sample		Flag
				Conc	Units	Conc	Units	
Methoxyamine, 2TMS derivative	1	4.00	14764485861	911.992	ug mL	911.992	ug mL	
N-(tert-butyldimethylsilyl)-2,2,2-trifluoro-N-methylacetamide	1	4.42	3710764715	229.211	ug mL	229.211	ug mL	
4-Pyridinol, TMS derivative	1	4.95	495169566	30.586	ug mL	30.586	ug mL	
Decane, 2,4,6-trimethyl-	1	5.15	1040651294	64.280	ug mL	64.280	ug mL	
2-Undecanethiol, 2-methyl-	1	5.42	1004779377	62.065	ug mL	62.065	ug mL	
1-(3-Methylbutyl)-2,3,4,6-tetramethylbenzene	1	5.80	2212475794	136.663	ug mL	136.663	ug mL	
EIQTMS_N12C_NID1_1139.3_1267BK12_[NA]	1	6.27	2117673837	130.807	ug mL	130.807	ug mL	
EITTMS_N12C_ATHR_1436.4_1135EC44_	1	7.22	293605512	18.136	ug mL	18.136	ug mL	
Dodecane, 4,6-dimethyl-	1	7.65	145482121	8.986	ug mL	8.986	ug mL	
Dodecane, 1,2-dibromo-	1	7.77	190809706	11.786	ug mL	11.786	ug mL	
Ethanolamine, 3TMS derivative	1	8.13	111559512	6.891	ug mL	6.891	ug mL	
Glycerol, 3TMS derivative	1	8.26	3975550922	245.567	ug mL	245.567	ug mL	
2-Isopropyl-5-methyl-1-heptanol	1	8.67	819197903	50.601	ug mL	50.601	ug mL	
2-Isopropyl-5-methyl-1-heptanol	1	8.82	2167384342	133.878	ug mL	133.878	ug mL	
EIQTMS_N12C_LJALM_1340.8_2236BN40_Glyceric acid (3TMS)	1	9.25	847784003	52.367	ug mL	52.367	ug mL	
Tetradecane, 2,6,10-trimethyl-	1	9.47	61716632	3.812	ug mL	3.812	ug mL	
Cystathionine, 2TMS derivative	1	11.69	177047295	10.936	ug mL	10.936	ug mL	
Tetradecane, 2,6,10-trimethyl-	1	12.21	153912644	9.507	ug mL	9.507	ug mL	
tert-Hexadecanethiol	1	12.78	115161184	7.113	ug mL	7.113	ug mL	
Disulfide, di-tert-dodecyl	1	13.10	585903636	36.191	ug mL	36.191	ug mL	
EIQTMS_N12C_SD1_1744.0_3196BU08_Putrescine (4TMS)	1	17.40	249264238	15.397	ug mL	15.397	ug mL	
1-Hexadecanol, 2-methyl-	1	18.45	2438079714	150.599	ug mL	150.599	ug mL	
EIQTMS_N12C_LJARL_1875.9_2236BN14_Fructose methoxyamin	1	20.56	652794749	40.323	ug mL	40.323	ug mL	
D-(-)-Fructose, pentakis(trimethylsilyl) ether, methyloxime (syn)	1	20.76	822379147	50.798	ug mL	50.798	ug mL	
EITTMS_N12C_STUR_1888.1_1135EC29_Glucose methoxyamine	1	21.07	222041196	13.715	ug mL	13.715	ug mL	
EITTMS_N12C_SD1_1997.0_1288EC09_Gluconic acid (6TMS)	1	23.07	171587601	10.599	ug mL	10.599	ug mL	
Octatriacontyl pentafluoropropionate	1	26.11	3302797850	204.012	ug mL	204.012	ug mL	
EITTMS_N12C_SD1_3463.2_1288EC31_Melezitose (11TMS)); alp	1	30.14	1633738091	100.915	ug mL	100.915	ug mL	
EITTMS_N12C_SD1_2765.9_1344EC78_Maltose methoxyamine {B	1	30.94	817293703	50.484	ug mL	50.484	ug mL	

Manually integrated

 Flag legend: P = Library entry selected manually