

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051421\
 Data File : VD069184.D
 Acq On : 14 May 2021 18:44
 Operator : VA/SY
 Sample : M2372-03
 Misc : 5.48G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 CHRT-27051

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051221S.M
 Title : SW846 8260

Signal : TIC: VD069184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.315	59	67	71	rBV4	11674	22574	1.85%	0.297%
2	4.961	505	517	518	rBV3	12596	22526	1.85%	0.297%
3	7.914	1007	1019	1025	rBV	186642	459211	37.67%	6.044%
4	7.979	1025	1030	1042	rVB	264036	572454	46.96%	7.535%
5	8.332	1079	1090	1102	rBV2	161522	370259	30.37%	4.874%
6	8.867	1171	1181	1190	rBV	418577	845356	69.34%	11.127%
7	10.338	1423	1431	1441	rBV	695284	1219138	100.00%	16.047%
8	11.643	1645	1653	1663	rBV	589640	1000742	82.09%	13.172%
9	12.485	1790	1796	1801	rBV6	10653	16906	1.39%	0.223%
10	12.632	1812	1821	1829	rBV	653232	1096438	89.94%	14.432%
11	12.732	1833	1838	1843	rVB4	7611	12323	1.01%	0.162%
12	13.573	1972	1981	1989	rBV	496556	831001	68.16%	10.938%
13	13.896	2031	2036	2041	rBV7	9915	23082	1.89%	0.304%
14	14.090	2065	2069	2074	rBV5	18450	31032	2.55%	0.408%
15	14.273	2094	2100	2106	rBV8	33947	69184	5.67%	0.911%
16	14.349	2108	2113	2117	rVV8	8795	15428	1.27%	0.203%
17	14.432	2117	2127	2134	rVV3	66398	155661	12.77%	2.049%
18	14.537	2140	2145	2152	rBV2	42712	85612	7.02%	1.127%
19	14.608	2153	2157	2165	rVB7	27999	66701	5.47%	0.878%
20	14.873	2200	2202	2208	rVB6	25630	34393	2.82%	0.453%
21	15.026	2217	2228	2234	rBV3	96531	225070	18.46%	2.963%
22	15.090	2234	2239	2244	rBV4	59538	121855	10.00%	1.604%
23	15.155	2245	2250	2253	rBV	53858	99494	8.16%	1.310%
24	15.237	2262	2264	2268	rBV4	23219	35276	2.89%	0.464%
25	15.437	2292	2298	2301	rBV5	79296	165537	13.58%	2.179%

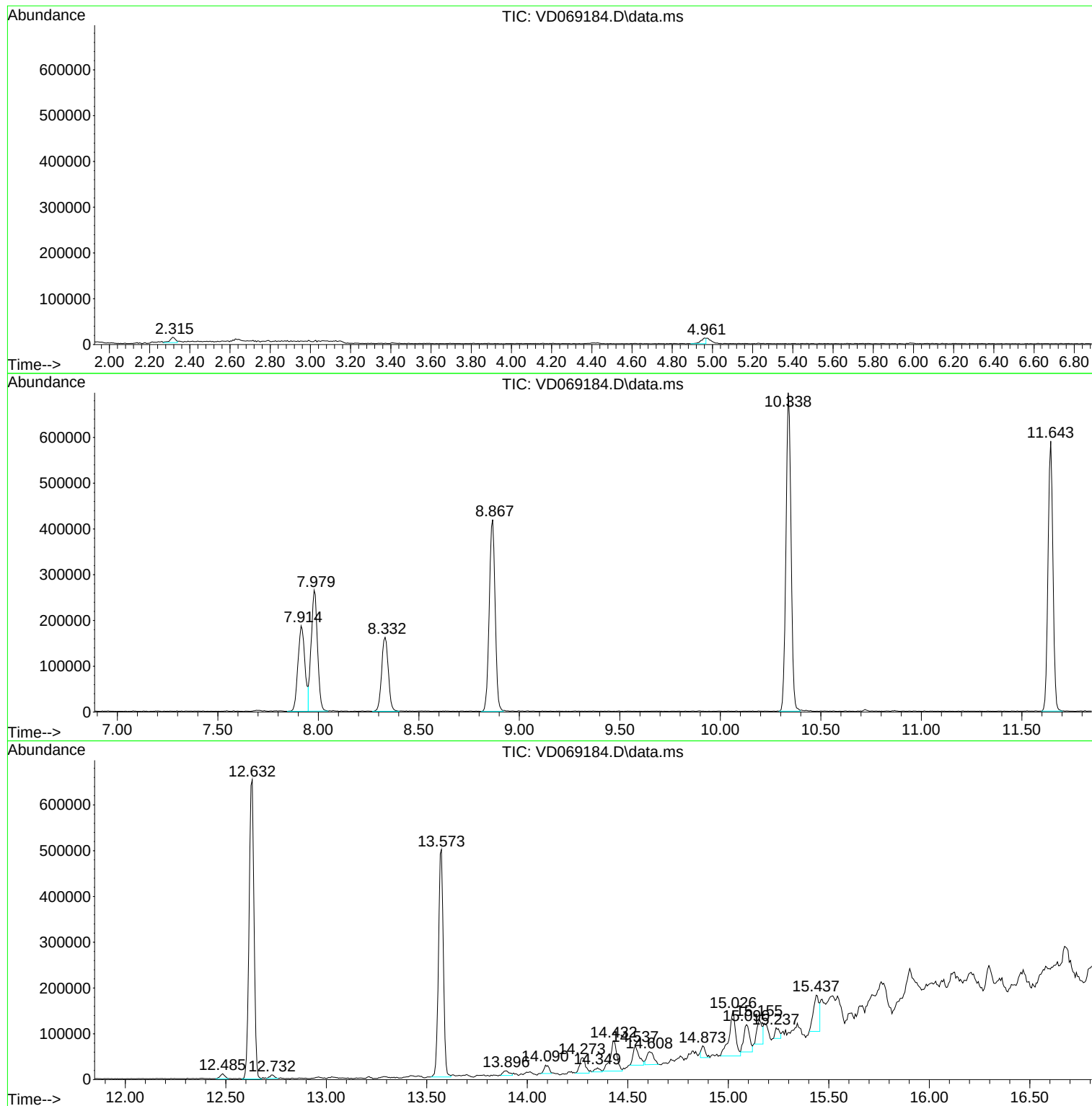
Sum of corrected areas: 7597253

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Peak Number 1 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.432	9.37 ug/l	155661	1,4-Dichlorobenzene-d4		13.573	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, 1-ada...		312	C14H17F5O2	1000283-03-8	64
2	N-Adamantan-1-ylmethyl-2-chloro-...		348	C18H21ClN2O3	227327-87-9	64
3	Benzenesulfonamide, N-adamantan-...		384	C17H21ClN2O4S	1000303-35-0	64
4	1-Adamantaneethanol		180	C12H20O	006240-11-5	64
5	2-Adamantan-1-yl-5-(4-nitro-1H-p...		315	C14H17N7O2	1000301-14-4	64

Peak Number 2 4-Amino-2-methyl-5,6-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.537	5.15 ug/l	85612	1,4-Dichlorobenzene-d4			13.573
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Amino-2-methyl-5,6-trimethylen...		149	C8H11N3	076881-49-7	62
2	Pyridine, pentamethyl-		149	C10H15N	003748-83-2	53
3	1,4-Dimethyladamantane		164	C12H20	024145-89-9	50
4	o-Toluic acid, 1-adamantylmethyl...		284	C19H24O2	1000292-22-6	50
5	Adamantane, 1,3-dimethyl-		164	C12H20	000702-79-4	49

Peak Number 3 2-Methyladamantane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.026	13.54 ug/l	225070	1,4-Dichlorobenzene-d4	13.573	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyladamantane	150	C11H18	000700-56-1	87
2	Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	80
3	3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	74
4	2H-Inden-2-one, 1,4,5,6,7,7a-hex...	150	C10H14O	054725-16-5	72
5	Cyclohexanone, 2-(2-butyryl)-	150	C10H14O	054166-48-2	72

Peak Number 4 1-Methyl-3-ethyladamantane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.090	7.33 ug/l	121855	1,4-Dichlorobenzene-d4	13.573

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Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	64	
2	1H-5-Triazolo[1,5-a]pyridin-4-yl...	149	C7H7N3O	013980-64-8	50	
3	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	50	
4	Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	50	
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47	

Peak Number 5 1,4-Dimethyladamantane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.155	5.99 ug/l	99494	1,4-Dichlorobenzene-d4	13.573

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane	164	C12H20	024145-88-8	81	
2	1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	50	
3	Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	46	
4	Benzene, 1-(1,1-dimethylethyl)-4...	164	C11H16O	005396-38-3	43	
5	Benzene, 1-butyl-4-methoxy-	164	C11H16O	018272-84-9	43	

Peak Number 6 Tricyclo[4.3.1.1(3,8)]undec... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.437	9.96 ug/l	165537	1,4-Dichlorobenzene-d4	13.573

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane	164	C12H20	024145-89-9	80	
2	1,4-Dimethyladamantane	164	C12H20	024145-88-8	72	
3	Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	59	
4	4-(2-Methyl-cyclohex-1-enyl)-but...	164	C11H16O	041437-92-7	58	
5	3-Methyl-1-adamantaneacetic acid	208	C13H20O2	014202-13-2	58	

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentafluoroprop...	14.432	9.4	ug/l	155661	4	13.573	831001	50.0
4-Amino-2-methy...	14.537	5.2	ug/l	85612	4	13.573	831001	50.0
2-Methyladamantane	15.026	13.5	ug/l	225070	4	13.573	831001	50.0
1-Methyl-3-ethy...	15.090	7.3	ug/l	121855	4	13.573	831001	50.0
1,4-Dimethylada...	15.155	6.0	ug/l	99494	4	13.573	831001	50.0
Tricyclo[4.3.1....	15.437	10.0	ug/l	165537	4	13.573	831001	50.0