LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX120418\
Data File : VX006272.D
Acq On : 04 Dec 2018 12:29
Operator : JC/MD
Sample : J5762-07
Misc : 6.14g/5mL/100ul/5.00ml/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BU-02-112918

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_X\METHOD\82X112918W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.666	63	84	88	rBV4	116602	624793	19.13%	3.167%
2	5.501	699	713	725	rBV	398831	1162151	35.58%	5.890%
3	5.659	727	739	756	rVB	708225	1989580	60.91%	10.083%
4	6.068	794	806	819	rBV	391548	1023722	31.34%	5.188%
5	6.854	925	935	951	rBV	997148	2384979	73.02%	12.087%
6	8.714	1233	1240	1248	rBV	2118645	3266288	100.00%	16.554%
7	9.335	1336	1342	1347	rBV2	22299	42711	1.31%	0.216%
8	9.445	1350	1360	1366	rBV2	13874	44186	1.35%	0.224%
9	10.116	1464	1470	1479	rBV	2075368	2845765	87.13%	14.423%
10	11.140	1632	1638	1648	rBV	1923528	2432322	74.47%	12.327%
11	11.384	1671	1678	1684	rBV	31166	68450	2.10%	0.347%
12	12.079	1786	1792	1801	rBV	2594700	3143113	96.23%	15.930%
13	12.914	1925	1929	1935	rVV3	18798	33462	1.02%	0.170%
14	13.347	1997	2000	2006	rVB7	22258	35310	1.08%	0.179%
15	13.475	2016	2021	2028	rBV8	19072	46627	1.43%	0.236%
16	14.280	2148	2153	2156	rBV6	19225	35906	1.10%	0.182%
17	14.481	2183	2186	2192	rVV	38913	55276	1.69%	0.280%
18	14.542	2193	2196	2204	rVB9	19883	36763	1.13%	0.186%
19	14.841	2243	2245	2249	rVB3	30547	33041	1.01%	0.167%
20	15.249	2307	2312	2318	rBV6	23696	48045	1.47%	0.243%
21	15.487	2348	2351	2356	rVB4	26457	39006	1.19%	0.198%
22	15.554	2358	2362	2368	rBV3	23990	41214	1.26%	0.209%
23	15.688	2380	2384	2387	rBV2	32945	45856	1.40%	0.232%
24	15.822	2401	2406	2412	rVB6	29183	60922	1.87%	0.309%
25	16.035	2437	2441	2445	rBV2	65270	93594	2.87%	0.474%
26	16.170	2459	2463	2469	rBV9	16759	35357	1.08%	0.179%
27	16.413	2500	2503	2512	rVB2	29537	62615	1.92%	0.317%

Sum of corrected areas: 19731054

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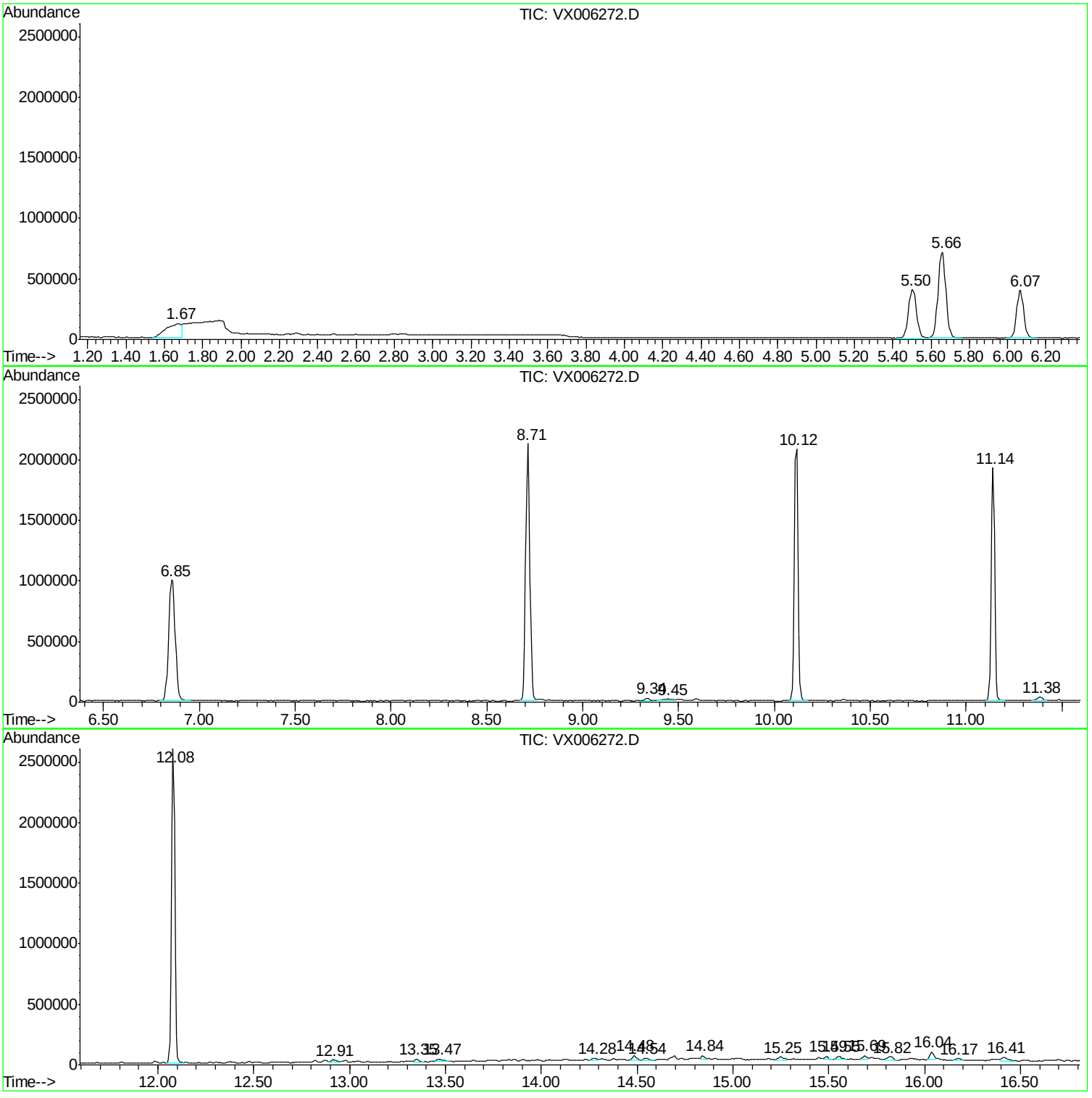
BU-02-112918

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Instrument : MSVOA_X
ClientSampleId : BU-02-112918

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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

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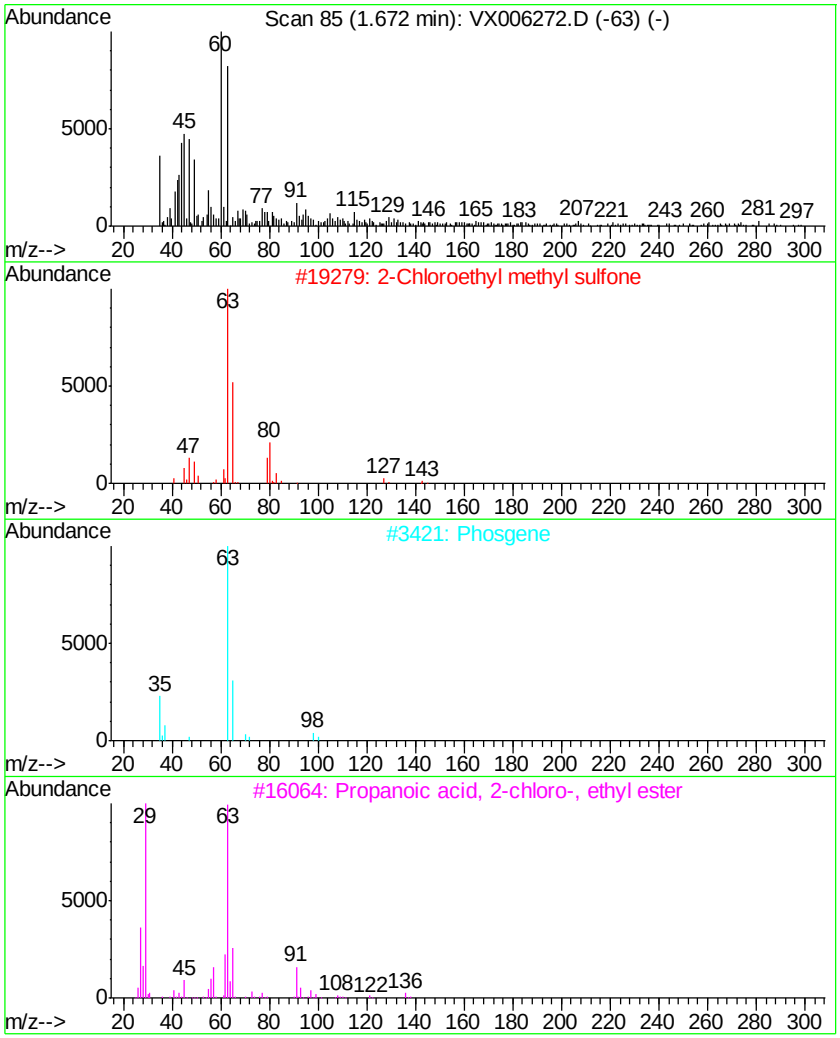
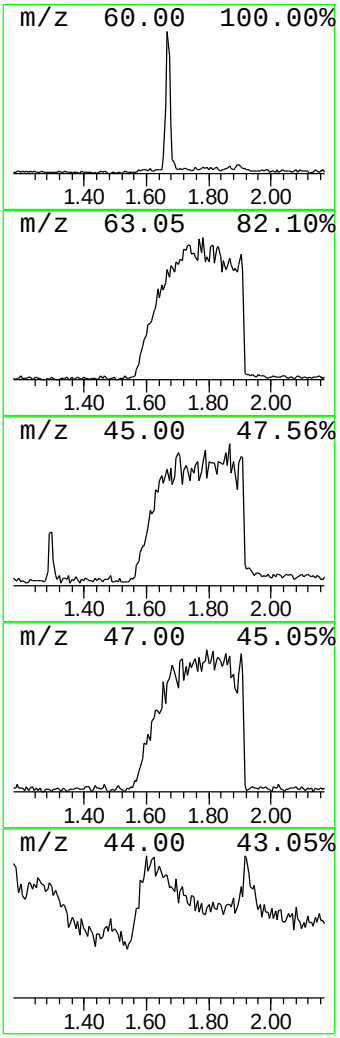
Peak Number 1 2-Chloroethyl methyl sulfone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	15.70 ug/l	624793	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfone	142	C3H7ClO2S	050890-51-2	53
2	Phosgene	98	CCl2O	000075-44-5	35
3	Propanoic acid, 2-chloro-, ethyl...	136	C5H9ClO2	000535-13-7	25
4	Trichloroacetic acid, 2-chloroet...	224	C4H4Cl4O2	1000330-88-7	25
5	Benzene, 1-chloro-2-[2-(2-chloro...	234	C10H12Cl2O2	007501-11-3	23





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Chloroethyl met...	1.67	15.7	ug/l	624793	1	5.66	1989580	50.0