LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR050720WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.510	43	53	73	rBV3	27716	92248	4.62%	0.513%
2	1.610	77	84	95	rVB	137529	162907	8.16%	0.906%
3	1.932	176	184	196	rVB	129175	163370	8.19%	0.908%
4	2.401	319	330	350	rVB	415355	623907	31.27%	3.469%
5	2.591	377	389	403	rBV	243999	394662	19.78%	2.194%
6	2.671	404	414	425	rVV2	13096	22810	1.14%	0.127%
7	3.218	574	584	595	rBV2	13140	28863	1.45%	0.160%
8	3.395	621	639	656	rVB3	29803	67802	3.40%	0.377%
9	3.735	732	745	765	rVB2	21673	47236	2.37%	0.263%
10	4.034	816	838	863	rBV	774737	1995489	100.00%	11.095%
11	4.571	986	1005	1022	rBV2	78638	191760	9.61%	1.066%
12	4.674	1022	1037	1067	rVV2	229690	632972	31.72%	3.519%
13	5.102	1153	1170	1191	rBV	221562	482017	24.16%	2.680%
14	5.420	1255	1269	1285	rBV2	22888	52435	2.63%	0.292%
15	5.761	1354	1375	1402	rBV2	443543	1207606	60.52%	6.714%
16	5.886	1402	1414	1428	rBV4	12733	32946	1.65%	0.183%
17	6.279	1520	1536	1561	rBV	372113	719433	36.05%	4.000%
18	6.719	1658	1673	1687	rBV	274837	547881	27.46%	3.046%
19	6.793	1689	1696	1707	rVB5	14316	26213	1.31%	0.146%
20	7.591	1928	1944	1958	rBV	145429	253443	12.70%	1.409%
21	7.738	1974	1990	2001	rBV4	12857	25627	1.28%	0.142%
22	7.922	2024	2047	2067	rBV	536630	1005040	50.37%	5.588%
23	8.201	2122	2134	2148	rBV	92657	157083	7.87%	0.873%
24	8.655	2262	2275	2309	rBV	807810	1456483	72.99%	8.098%
25	9.439	2504	2519	2521	rBV	558401	808250	40.50%	4.494%
26	9.465	2522	2527	2560	rVB	950981	1556222	77.99%	8.653%
27	10.124	2715	2732	2750	rVB4	18697	40408	2.02%	0.225%
28	10.500	2833	2849	2865	rBV	1047022	1673784	83.88%	9.306%
29	10.770	2922	2933	2956	rVB	225396	378938	18.99%	2.107%
30	10.906	2959	2975	2996	rBV4	94931	176203	8.83%	0.980%
31	11.002	2996	3005	3014	rBV3	12737	25291	1.27%	0.141%
32	11.304	3088	3099	3121	rVB2	34780	63671	3.19%	0.354%
33	11.433	3121	3139	3147	rBV2	47792	77865	3.90%	0.433%
34	11.651	3201	3207	3220	rVB5	16776	28342	1.42%	0.158%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR050720WMA.M
Title : TRACE VOA SOM01.0

35	11.825	3248	3261	3276	rVV2	595553	1063954	53.32%	5.916%
36	11.899	3276	3284	3297	rVB4	93177	144781	7.26%	0.805%
37	12.105	3336	3348	3361	rVB2	41569	68544	3.43%	0.381%
38	12.205	3364	3379	3400	rBV	605100	1049350	52.59%	5.834%
39	12.584	3486	3497	3507	rBV2	40881	60514	3.03%	0.336%
40	12.796	3554	3563	3568	rBV5	16858	28113	1.41%	0.156%
41	12.838	3568	3576	3585	rVV2	69825	114388	5.73%	0.636%
42	12.886	3585	3591	3603	rVB4	13721	23482	1.18%	0.131%
43	12.992	3615	3624	3632	rBV2	24178	36446	1.83%	0.203%
44	13.044	3632	3640	3649	rVB6	11995	20157	1.01%	0.112%
45	13.876	3888	3899	3912	rBV6	12527	23636	1.18%	0.131%
46	14.028	3937	3946	3965	rVB6	28713	52405	2.63%	0.291%
47	14.812	4178	4190	4198	rBV9	9246	21982	1.10%	0.122%
48	15.118	4273	4285	4294	rBV5	21891	37323	1.87%	0.208%
49	16.963	4853	4859	4871	rVB5	13471	21356	1.07%	0.119%

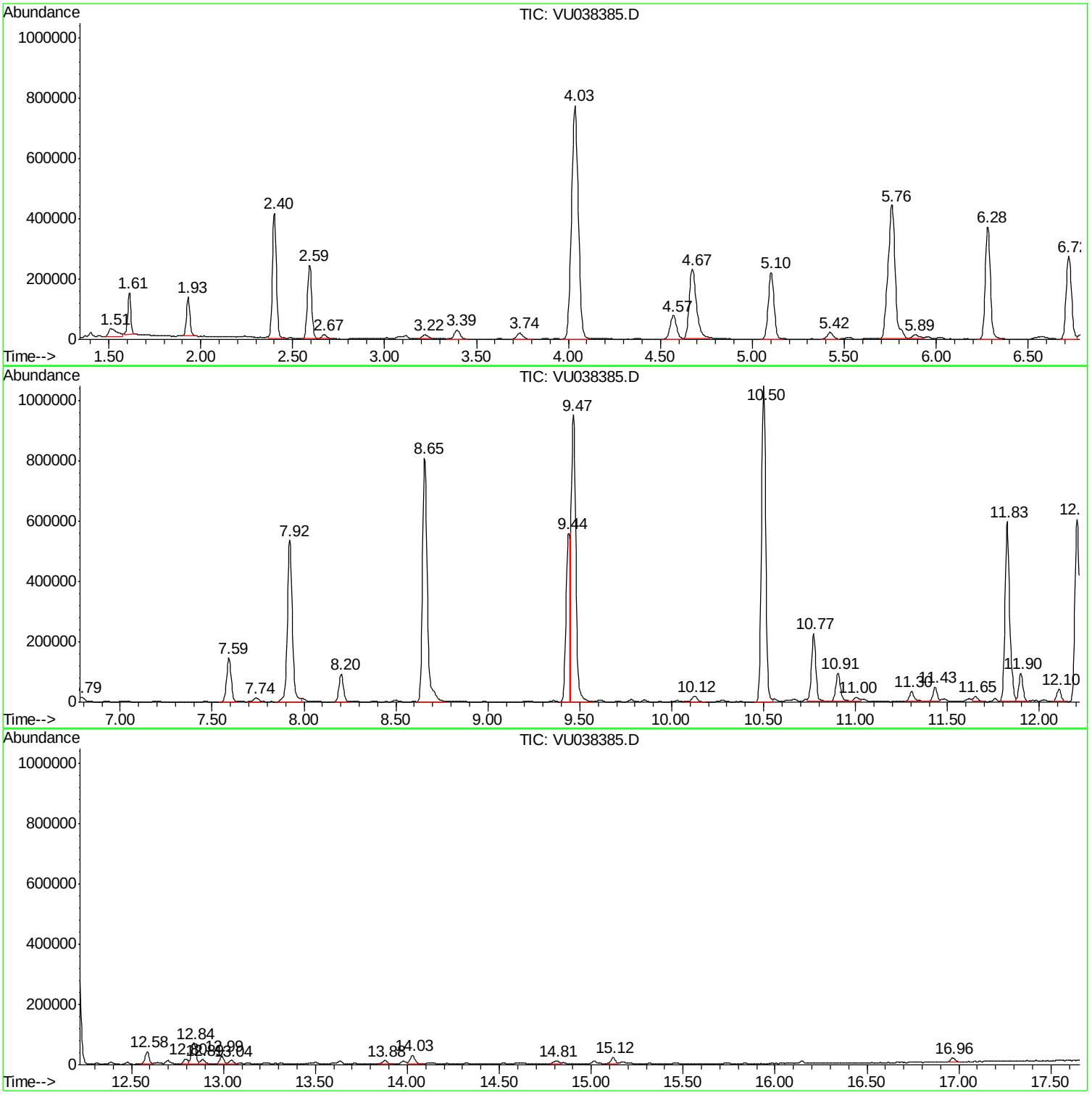
Sum of corrected areas: 17985638

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

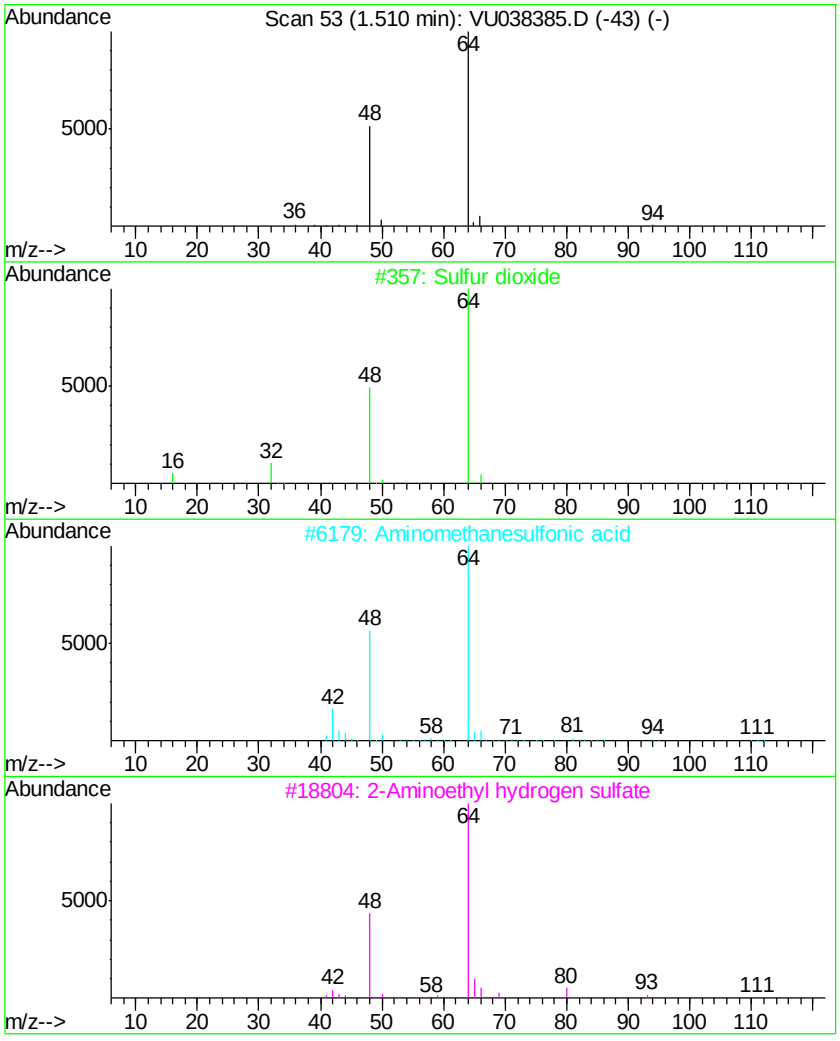
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

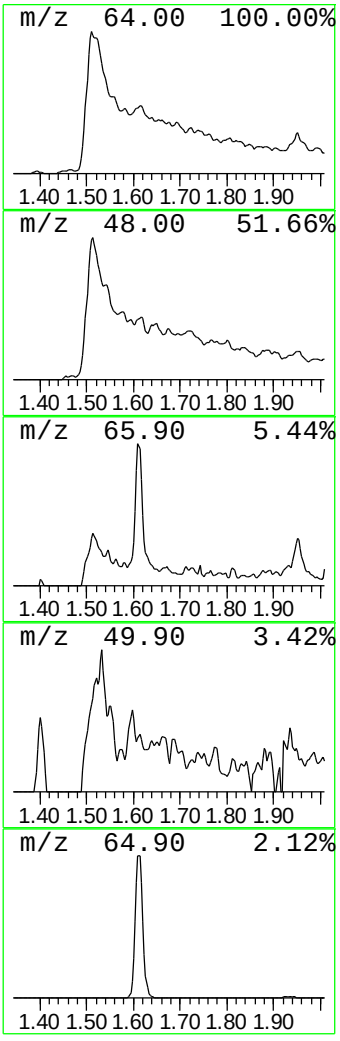
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	0.64 ug/L	92248	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

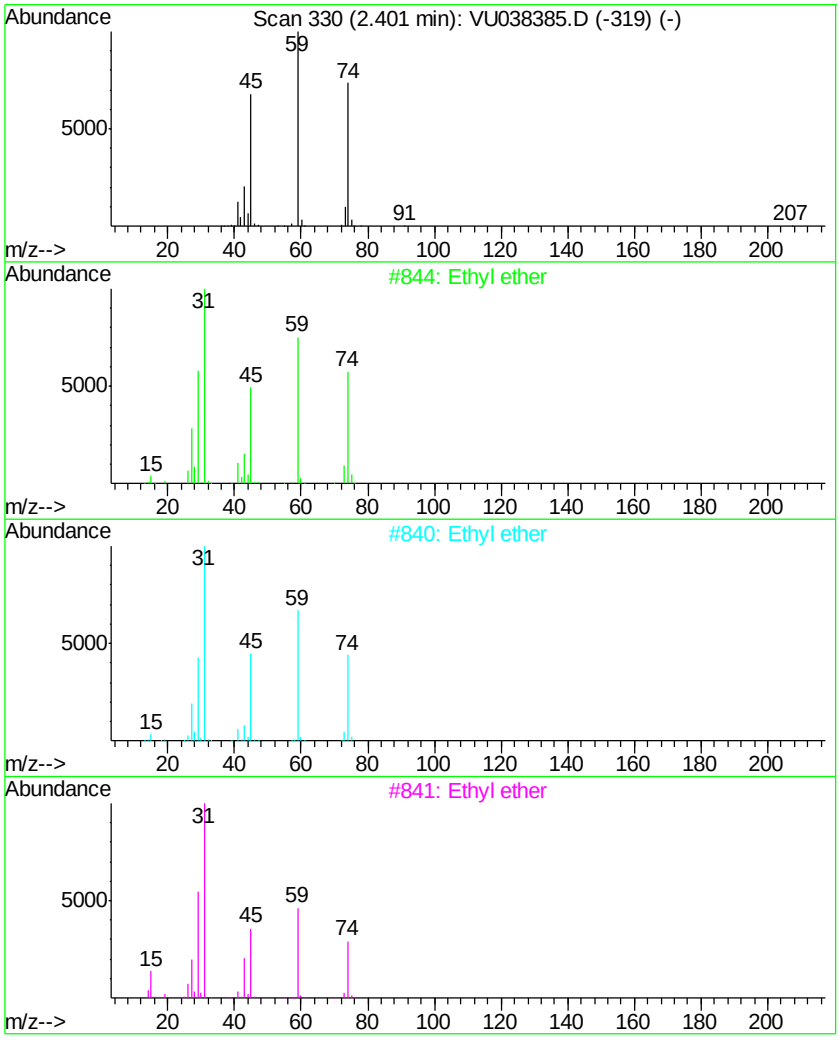
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

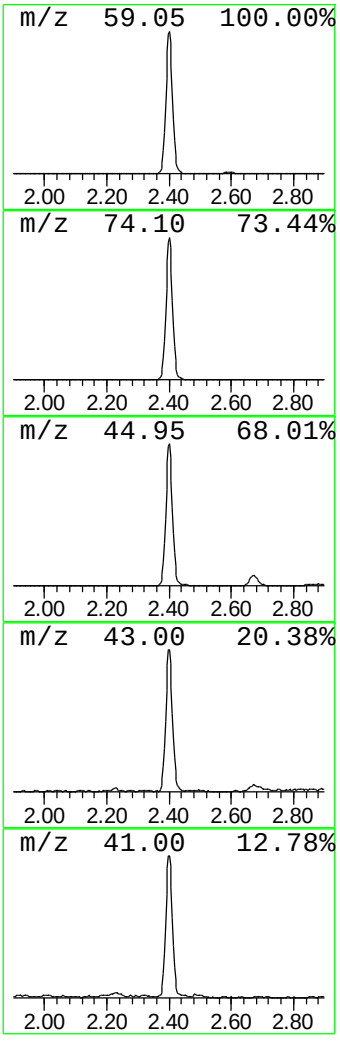
****

Peak Number 2 Ethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	4.34 ug/L	623907	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl ether	74	C4H10O	000060-29-7	90
2	Ethyl ether	74	C4H10O	000060-29-7	90
3	Ethyl ether	74	C4H10O	000060-29-7	83
4	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	72
5	Ethyl ether	74	C4H10O	000060-29-7	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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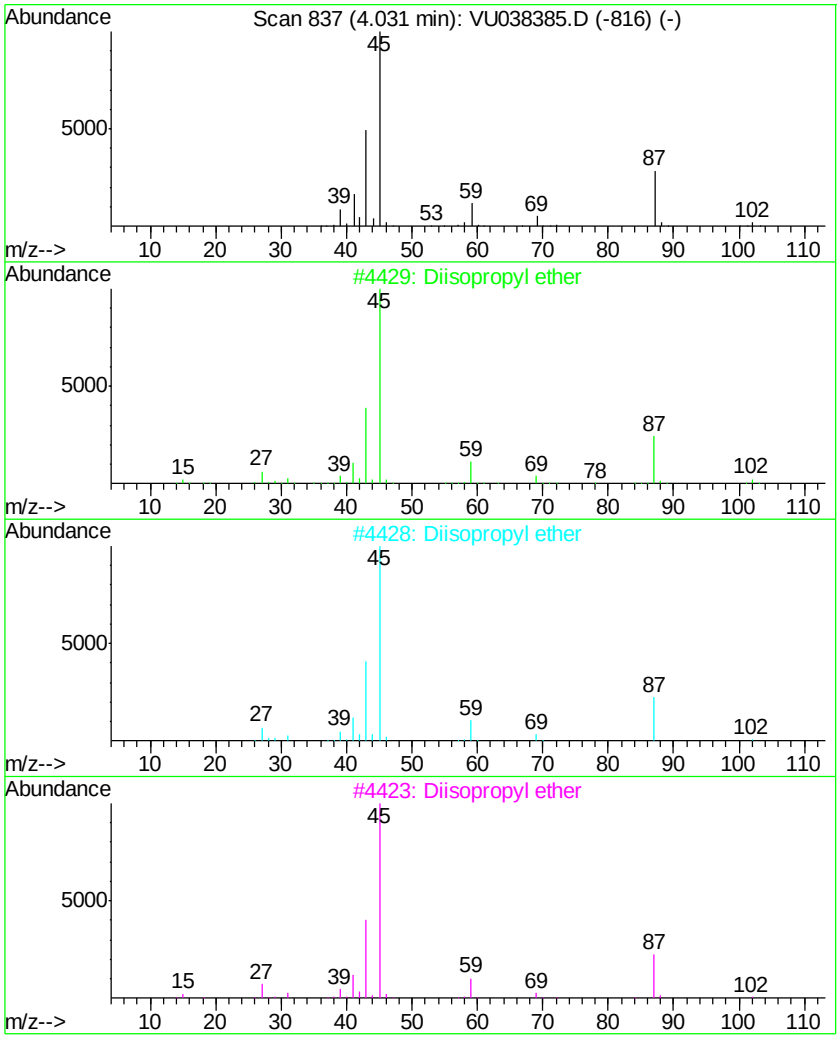
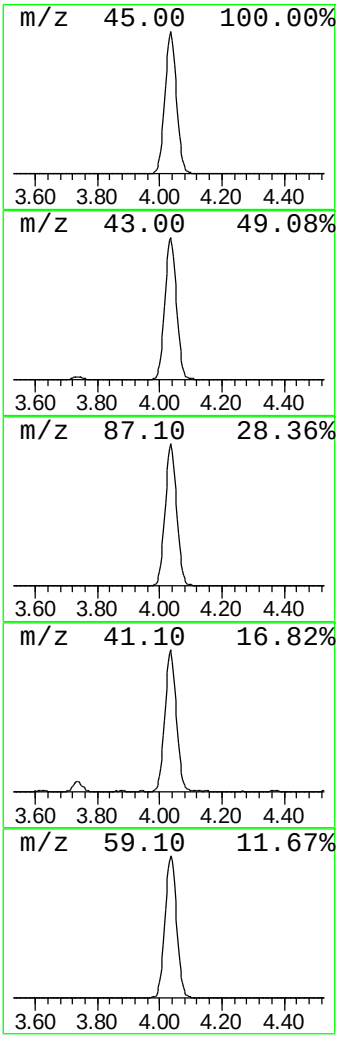
Peak Number 3 Diisopropyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	13.87 ug/L	1995490	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	91
2	Diisopropyl ether	102	C6H14O	000108-20-3	83
3	Diisopropyl ether	102	C6H14O	000108-20-3	83
4	Acetoin	88	C4H8O2	000513-86-0	59
5	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

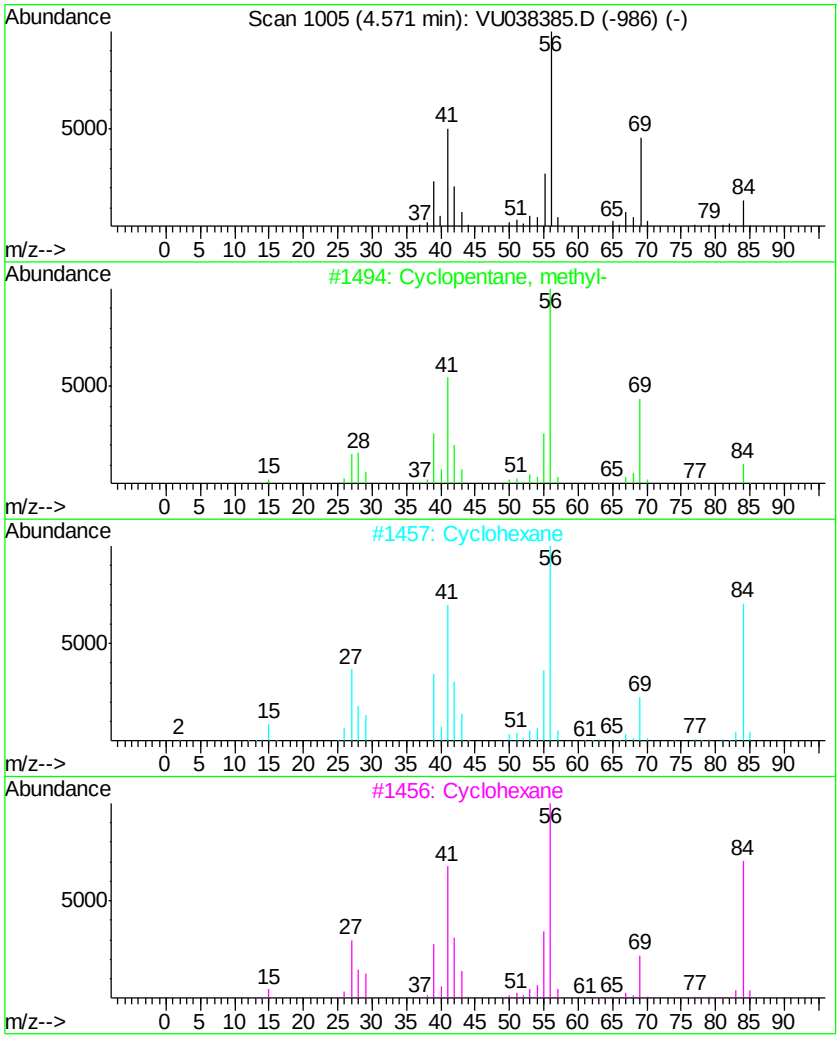
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

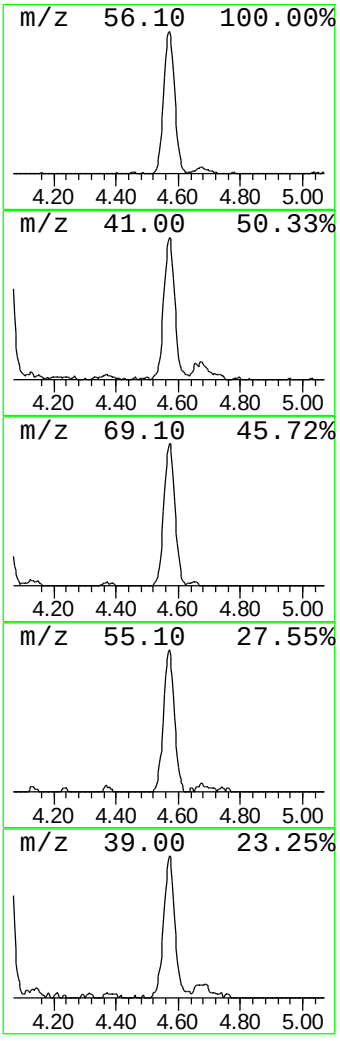
****

Peak Number 4 (DEL) Alkane: Cyclic4.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	1.33 ug/L	191760	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	86
3	Cyclohexane	84	C6H12	000110-82-7	86
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
5	Cyclohexane	84	C6H12	000110-82-7	78





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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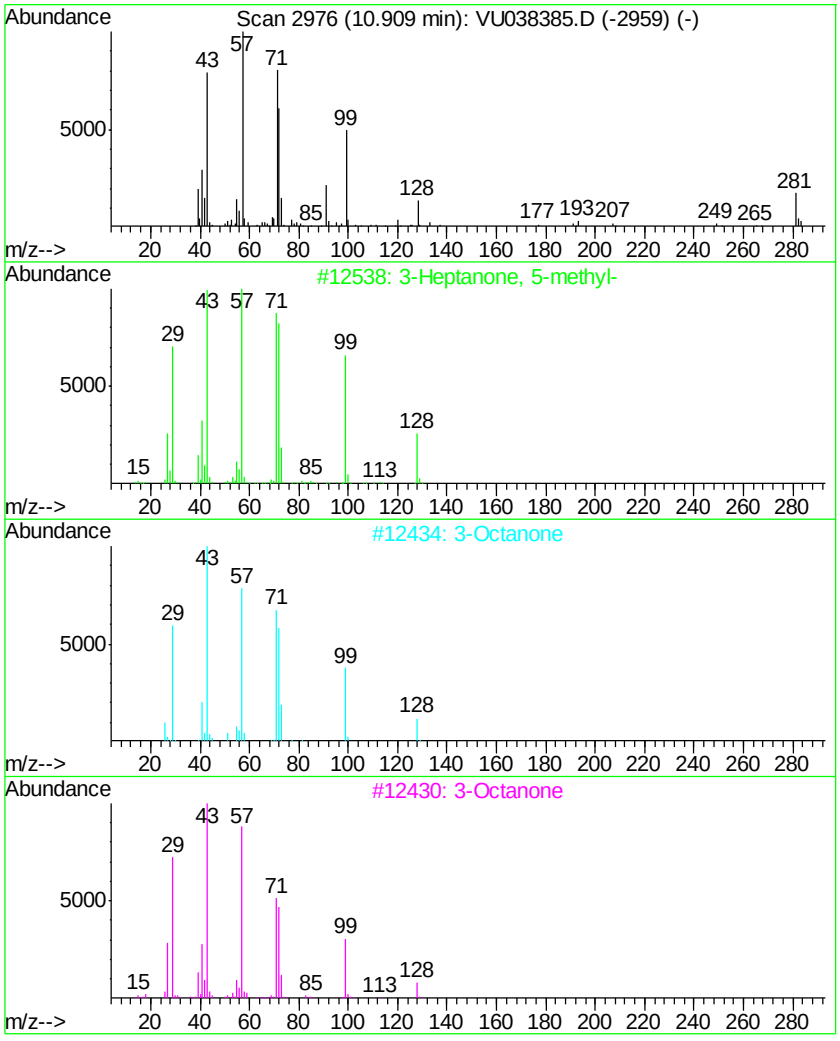
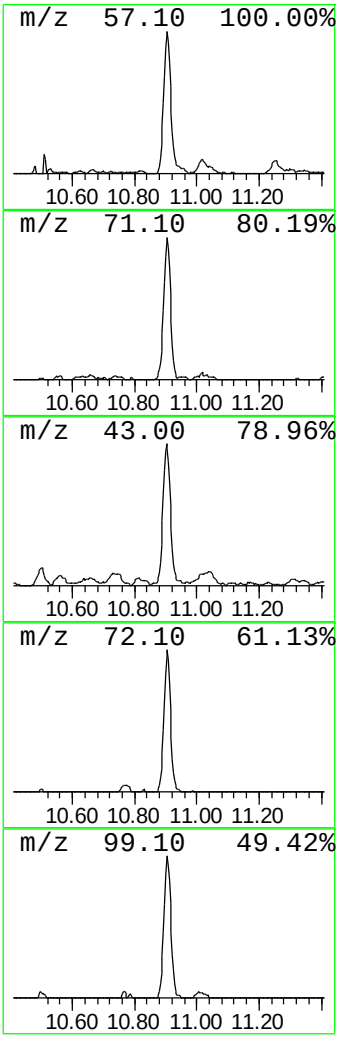
Peak Number 6 3-Heptanone, 5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	0.83 ug/L	176203	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	87
2	3-Octanone	128	C8H16O	000106-68-3	87
3	3-Octanone	128	C8H16O	000106-68-3	87
4	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	87
5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	83





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

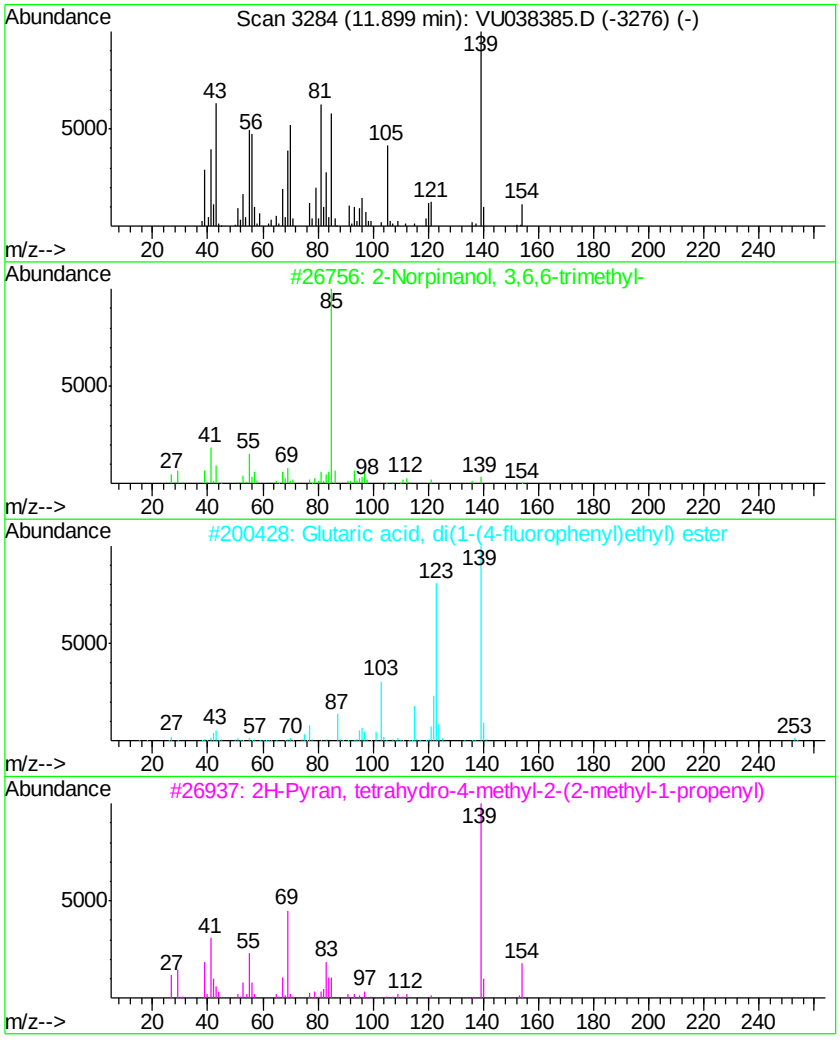
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

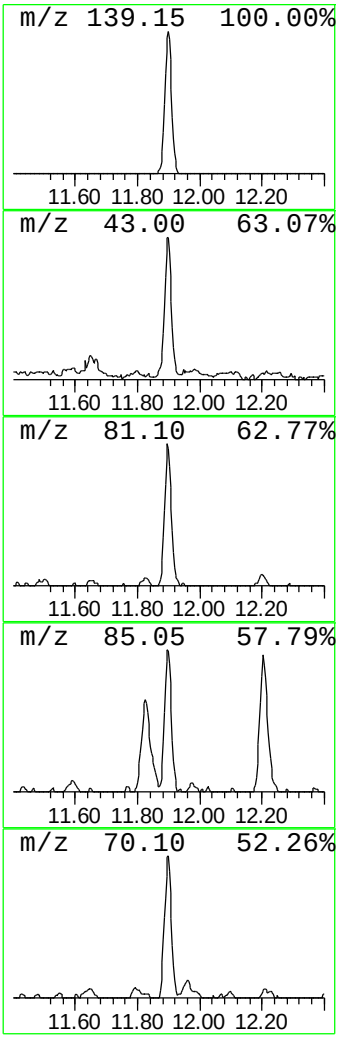
****

Peak Number 7 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	0.68 ug/L	144781	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Norpinanol, 3,6,6-trimethyl-	154	C10H18O	029548-09-2	38
2	Glutaric acid, di(1-(4-fluorophe...	376	C21H22F2O4	1000377-11-0	35
3	2H-Pyran, tetrahydro-4-methyl-2-...	154	C10H18O	016409-43-1	27
4	Silane, (cyclopentylidenemethyl)...	154	C9H18Si	094012-70-1	27
5	3-Pyridinecarboxylic acid, 1,6-d...	139	C6H5NO3	005006-66-6	27





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

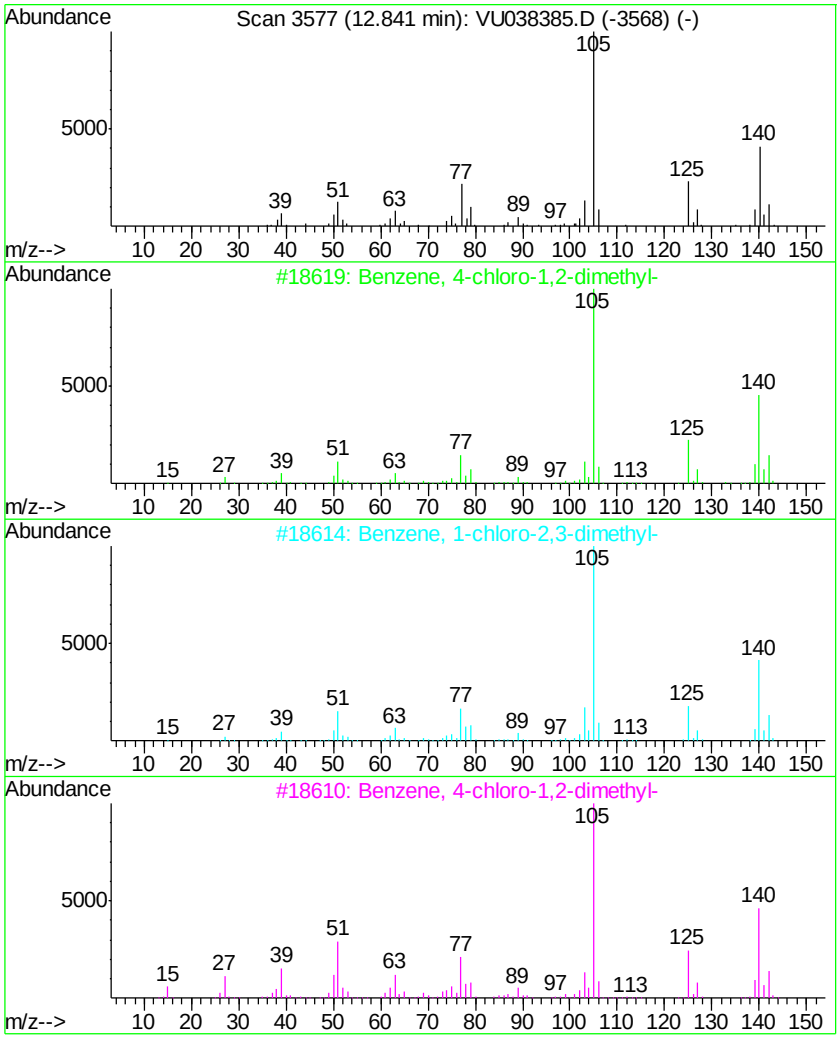
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

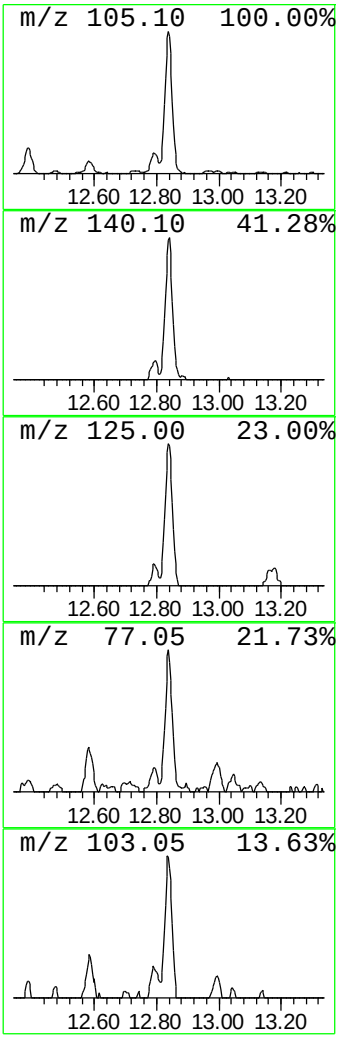
****

Peak Number 8 Benzene, 4-chloro-1,2-dimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	0.54 ug/L	114388	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-chloro-1,2-dimethyl-	140	C8H9Cl	000615-60-1	95
2	Benzene, 1-chloro-2,3-dimethyl-	140	C8H9Cl	000608-23-1	94
3	Benzene, 4-chloro-1,2-dimethyl-	140	C8H9Cl	000615-60-1	94
4	Benzene, 2-chloro-1,4-dimethyl-	140	C8H9Cl	000095-72-7	93
5	Benzene, 4-chloro-1,2-dimethyl-	140	C8H9Cl	000615-60-1	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038385.D
Acq On : 29 May 2020 18:52
Operator : JC/MD
Sample : L2749-09DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X4DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.51	0.6	ug/L	92248	1	6.28	719433	5.0
Ethyl ether	2.40	4.3	ug/L	623907	1	6.28	719433	5.0
Diisopropyl ether	4.03	13.9	ug/L	1995490	1	6.28	719433	5.0
(DEL) Alkane: Cyc...	4.57	1.3	ug/L	191760	1	6.28	719433	5.0
3-Heptanone, 5-me...	10.91	0.8	ug/L	176203	3	11.83	1063950	5.0
unknown-01	11.90	0.7	ug/L	144781	3	11.83	1063950	5.0
Benzene, 4-chloro...	12.84	0.5	ug/L	114388	3	11.83	1063950	5.0