LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-14

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_N\methods\82N090222W.M
Title : SW846 8260

Signal : TIC: VN074305.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	47	59	61	rBV5	12995	29839	1.99%	0.201%
2	2.404	83	88	94	rVV	103431	188017	12.56%	1.265%
3	2.557	110	114	118	rBV4	12518	16486	1.10%	0.111%
4	2.698	132	138	148	rVB3	76412	220386	14.73%	1.482%
5	3.087	196	204	231	rVB2	414083	1103785	73.75%	7.424%
6	3.457	260	267	276	rVB2	22294	57037	3.81%	0.384%
7	3.934	338	348	358	rBV4	16859	48033	3.21%	0.323%
8	4.998	515	529	535	rBV2	36451	130852	8.74%	0.880%
9	5.063	537	540	541	rVV2	31359	41464	2.77%	0.279%
10	5.092	541	545	568	rVV7	37413	147246	9.84%	0.990%
11	5.275	571	576	578	rVV2	11714	20140	1.35%	0.135%
12	5.298	578	580	590	rVB3	10113	17828	1.19%	0.120%
13	5.539	607	621	634	rBV3	175246	608636	40.67%	4.094%
14	6.416	756	770	783	rBV3	157555	530908	35.47%	3.571%
15	6.528	783	789	797	rVB7	9849	25134	1.68%	0.169%
16	6.816	829	838	843	rBV7	10256	27352	1.83%	0.184%
17	6.975	853	865	870	rBV3	12092	35760	2.39%	0.241%
18	7.075	870	882	889	rBV3	74577	215595	14.41%	1.450%
19	7.769	995	1000	1010	rVB7	10076	27000	1.80%	0.182%
20	7.951	1021	1031	1036	rBV2	210892	496399	33.17%	3.339%
21	8.016	1036	1042	1051	rVV2	408994	969319	64.77%	6.520%
22	8.104	1053	1057	1067	rVB6	26419	61872	4.13%	0.416%
23	8.286	1083	1088	1093	rVB5	7851	15890	1.06%	0.107%
24	8.375	1093	1103	1113	rBV2	260697	692182	46.25%	4.656%
25	8.469	1113	1119	1123	rBV4	23417	52024	3.48%	0.350%
26	8.551	1128	1133	1142	rVV4	40080	128247	8.57%	0.863%
27	8.645	1142	1149	1155	rVB6	17244	40603	2.71%	0.273%
28	8.904	1184	1193	1205	rBV	510429	1090132	72.84%	7.332%
29	9.133	1225	1232	1236	rBV5	6491	15429	1.03%	0.104%
30	9.357	1263	1270	1272	rBV4	25570	45492	3.04%	0.306%
31	9.392	1272	1276	1285	rVB4	42080	88984	5.95%	0.599%
32	9.822	1343	1349	1357	rVB4	25440	50685	3.39%	0.341%
33	9.910	1357	1364	1367	rBV4	31949	61644	4.12%	0.415%
34	9.951	1367	1371	1382	rVB3	50122	102471	6.85%	0.689%
35	10.139	1396	1403	1405	rBV4	28381	52051	3.48%	0.350%
36	10.169	1405	1408	1416	rVB4	46267	82574	5.52%	0.555%

LSC Area Percent Report

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Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-14

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_N\methods\82N090222W.M
Title : SW846 8260

37	10.263	1419	1424	1429	rBV3	12303	21907	1.46%	0.147%
38	10.380	1436	1444	1451	rBV	778935	1430508	95.58%	9.622%
39	10.445	1451	1455	1459	rVV	58802	109535	7.32%	0.737%
40	10.492	1459	1463	1468	rVV2	46902	81938	5.47%	0.551%
41	10.580	1468	1478	1485	rVV2	92180	180354	12.05%	1.213%
42	10.651	1485	1490	1497	rVV2	95329	168447	11.26%	1.133%
43	10.798	1509	1515	1525	rVB4	22619	49307	3.29%	0.332%
44	11.151	1568	1575	1580	rBV6	9199	18946	1.27%	0.127%
45	11.551	1636	1643	1654	rVV2	34650	71663	4.79%	0.482%
46	11.680	1658	1665	1677	rVV	824262	1496611	100.00%	10.066%
47	11.786	1677	1683	1691	rVV3	80004	165512	11.06%	1.113%
48	11.898	1694	1702	1712	rVV3	91838	180567	12.07%	1.215%
49	12.216	1750	1756	1762	rVB7	12566	23886	1.60%	0.161%
50	12.292	1764	1769	1773	rBV2	8891	15176	1.01%	0.102%
51	12.515	1801	1807	1816	rVV4	39538	80011	5.35%	0.538%
52	12.668	1825	1833	1844	rVV	689119	1169595	78.15%	7.867%
53	12.774	1847	1851	1857	rVV4	22046	40461	2.70%	0.272%
54	12.857	1857	1865	1873	rVV	52445	98858	6.61%	0.665%
55	12.992	1884	1888	1896	rVB6	16461	34899	2.33%	0.235%
56	13.157	1910	1916	1921	rBV3	20983	33914	2.27%	0.228%
57	13.310	1936	1942	1948	rVB7	8959	19141	1.28%	0.129%
58	13.610	1985	1993	2005	rBV	841875	1479904	98.88%	9.954%
59	13.780	2017	2022	2023	rBV	17999	23553	1.57%	0.158%
60	13.815	2023	2028	2037	rVB	82888	136437	9.12%	0.918%
61	13.939	2043	2049	2054	rVB5	8389	17179	1.15%	0.116%
62	14.157	2082	2086	2091	rVB	17033	22698	1.52%	0.153%
63	14.262	2099	2104	2111	rBV2	45591	75021	5.01%	0.505%
64	14.474	2134	2140	2144	rBV5	14595	21469	1.43%	0.144%
65	14.745	2181	2186	2192	rBV6	11182	21362	1.43%	0.144%
66	14.868	2203	2207	2212	rVB4	16873	24082	1.61%	0.162%
67	15.433	2297	2303	2307	rVB5	8564	16905	1.13%	0.114%

Sum of corrected areas: 14867342

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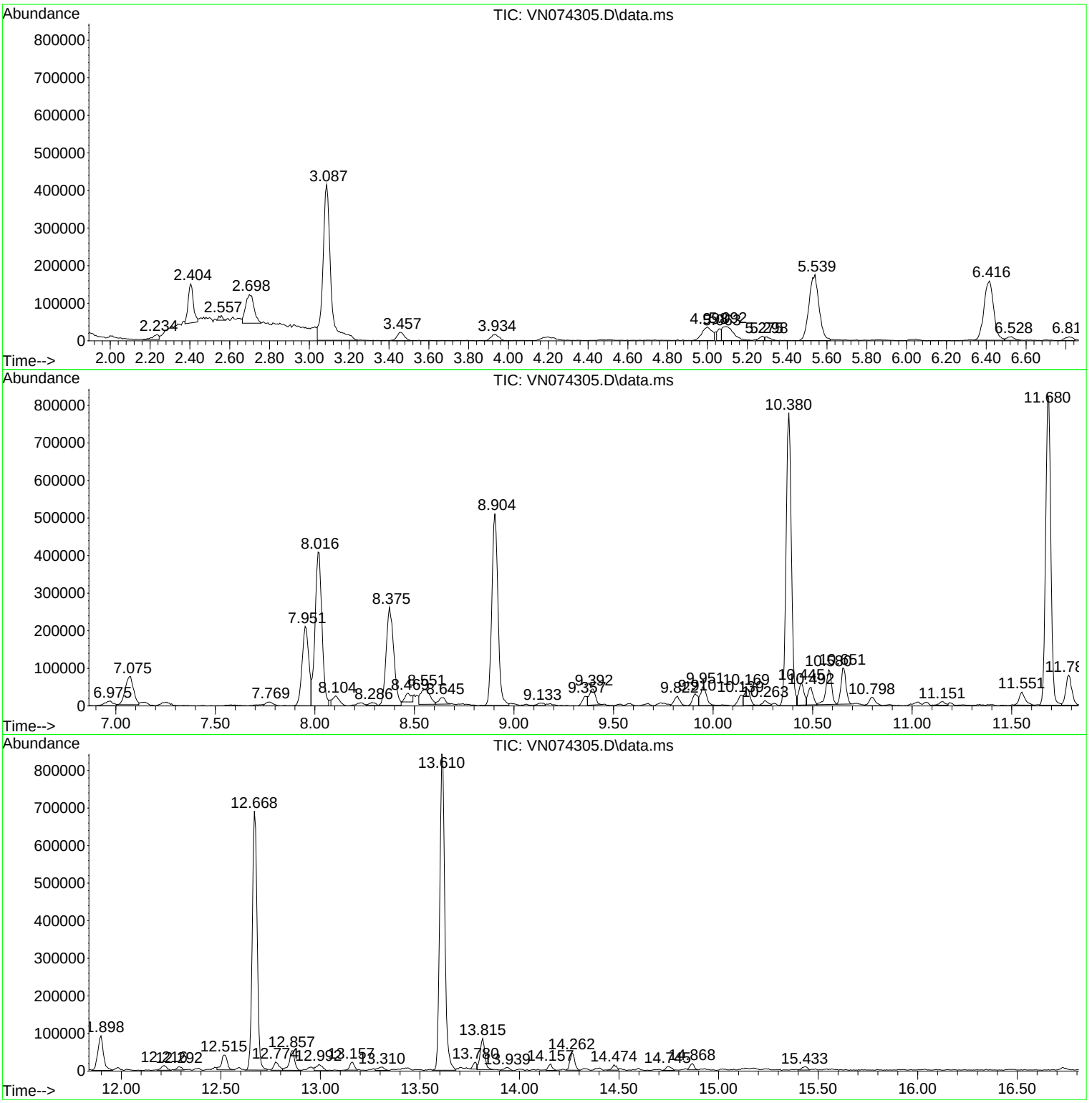
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
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Quant Title : SW846 8260

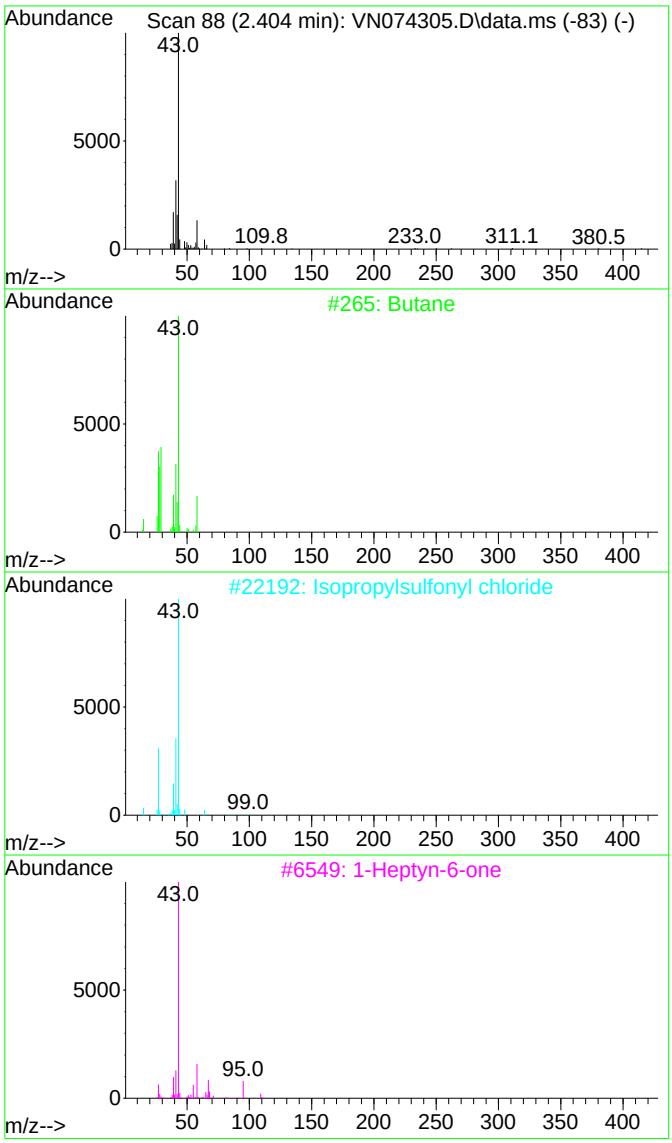
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

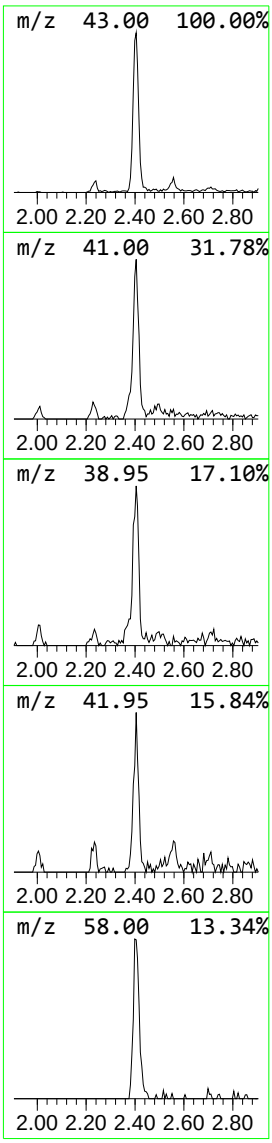
****

Peak Number 1 unknown2.404 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.404	9.70 ug/l	188017	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	47
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	37
3	1-Heptyn-6-one	110	C7H10O	000928-39-2	25
4	Methyl glyoxal	72	C3H4O2	000078-98-8	9
5	Isobutane	58	C4H10	000075-28-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

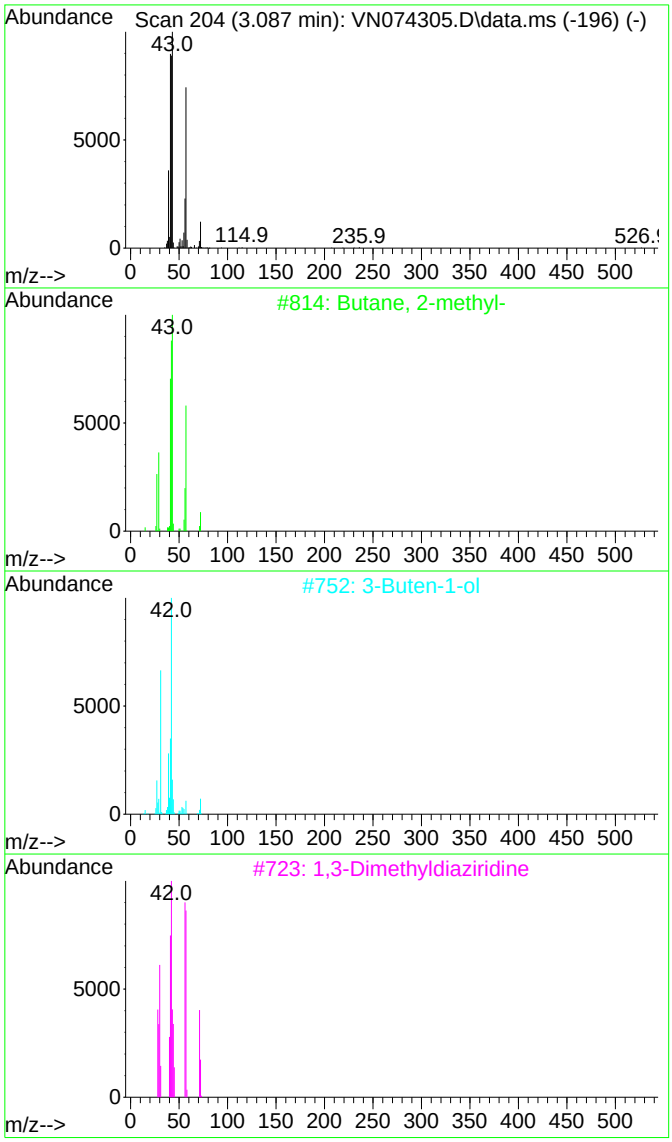
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

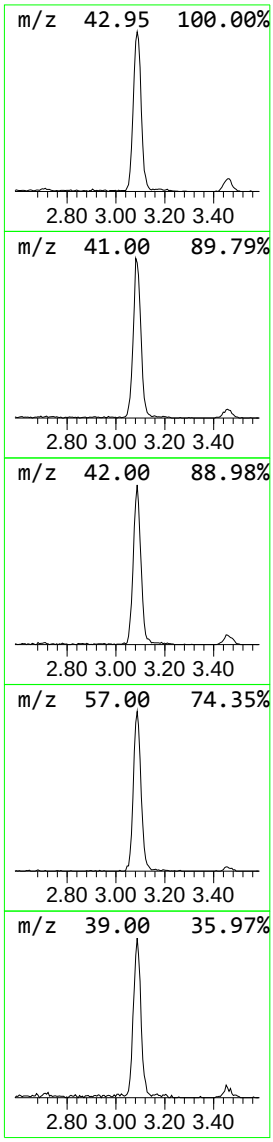
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	56.94 ug/l	1103790	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	37
3	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36
4	Pentane	72	C5H12	000109-66-0	33
5	Ethenamine, N-methyl-N-nitroso-	86	C3H6N2O	004549-40-0	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

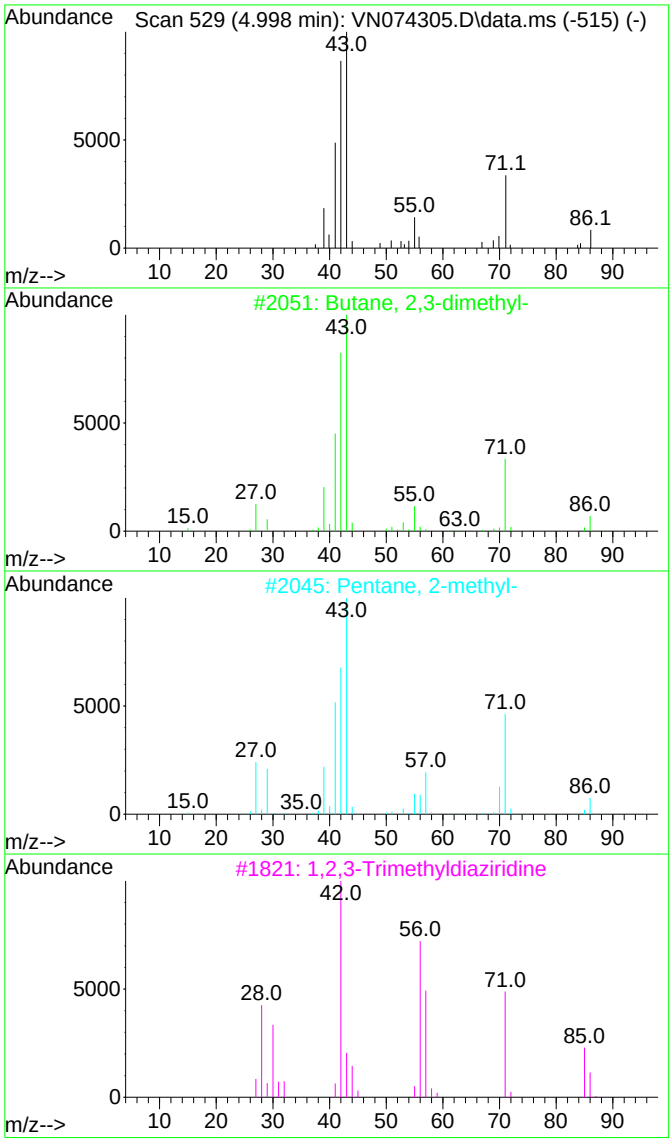
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

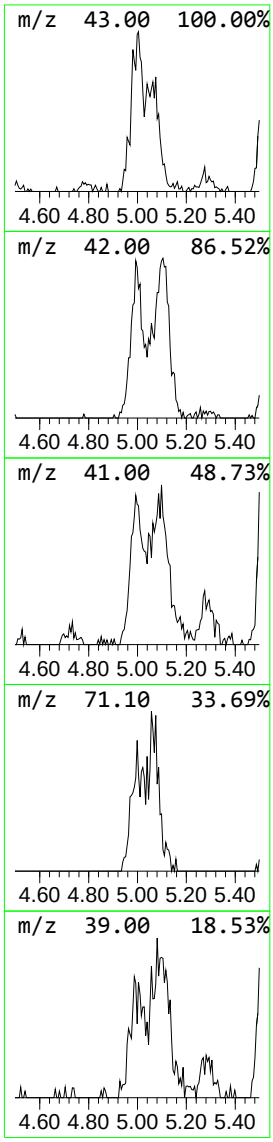
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	6.75 ug/l	130852	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	42
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	36
4	1-Pentene	70	C5H10	000109-67-1	28
5	4-Penten-2-one	84	C5H8O	013891-87-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

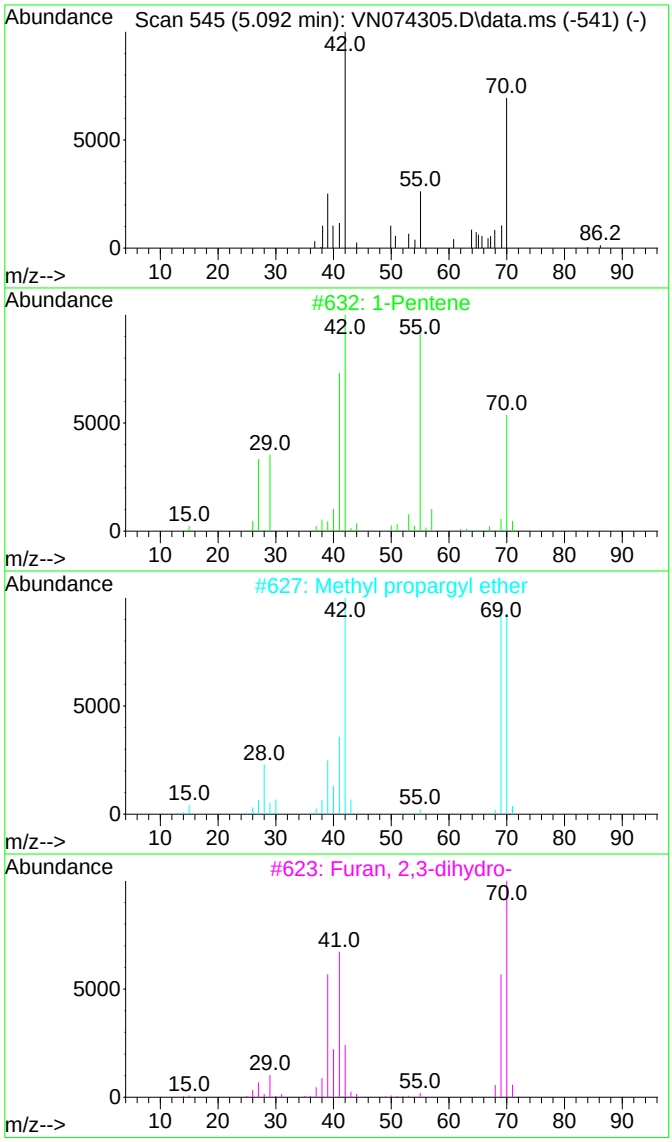
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

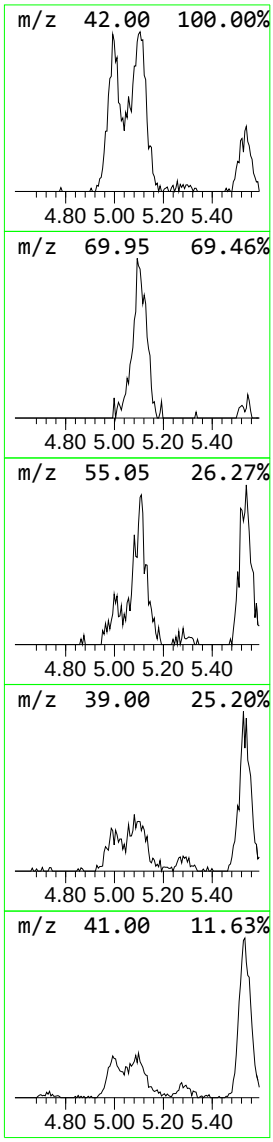
****

Peak Number 5 unknown5.092 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	7.60 ug/l	147246	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	45
2	Methyl propargyl ether	70	C4H6O	000627-41-8	40
3	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	9
4	Diaziridine, 3-ethyl-3-methyl-	86	C4H10N2	004901-75-1	9
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	9





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

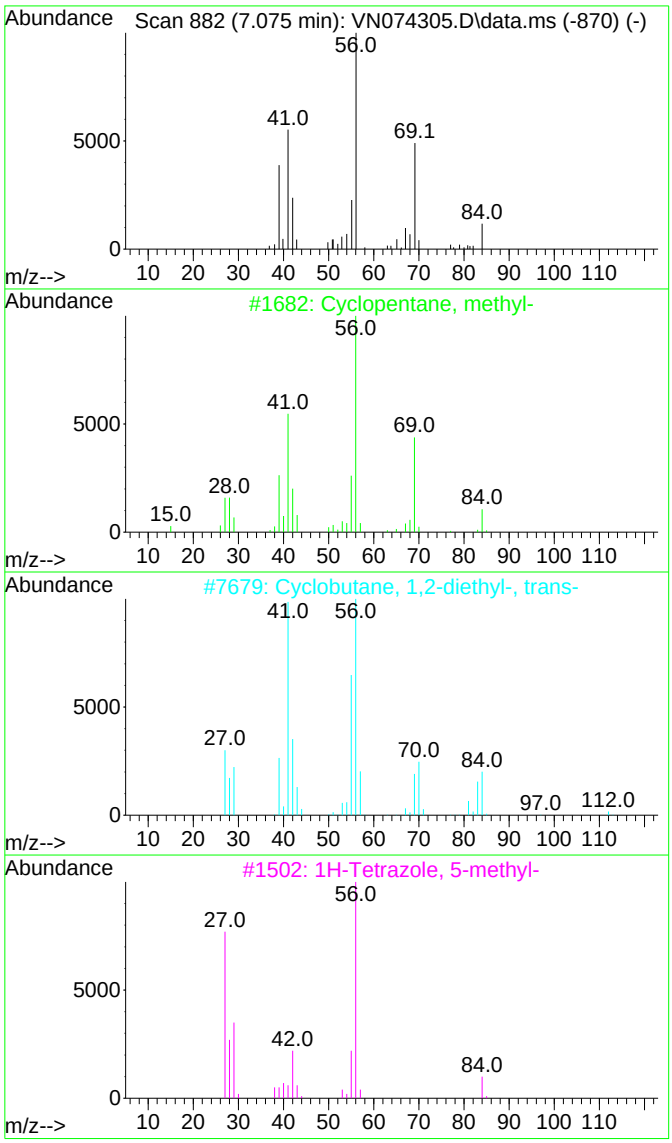
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

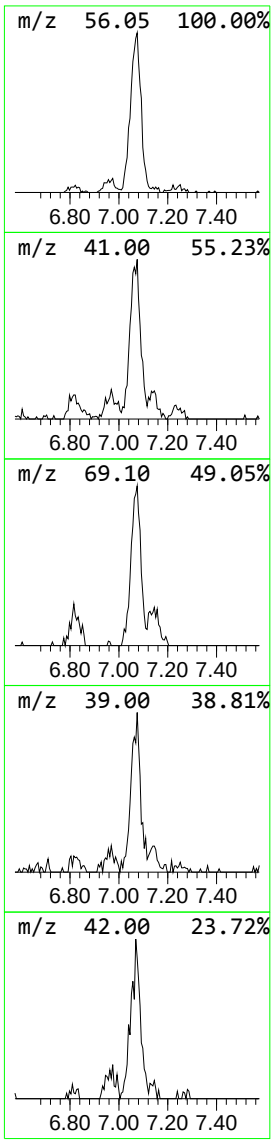
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.075	11.12 ug/l	215595	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	62
2	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	47
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	43
4	1-Pentanol, 3-methyl-	102	C6H14O	000589-35-5	33
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	25





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Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

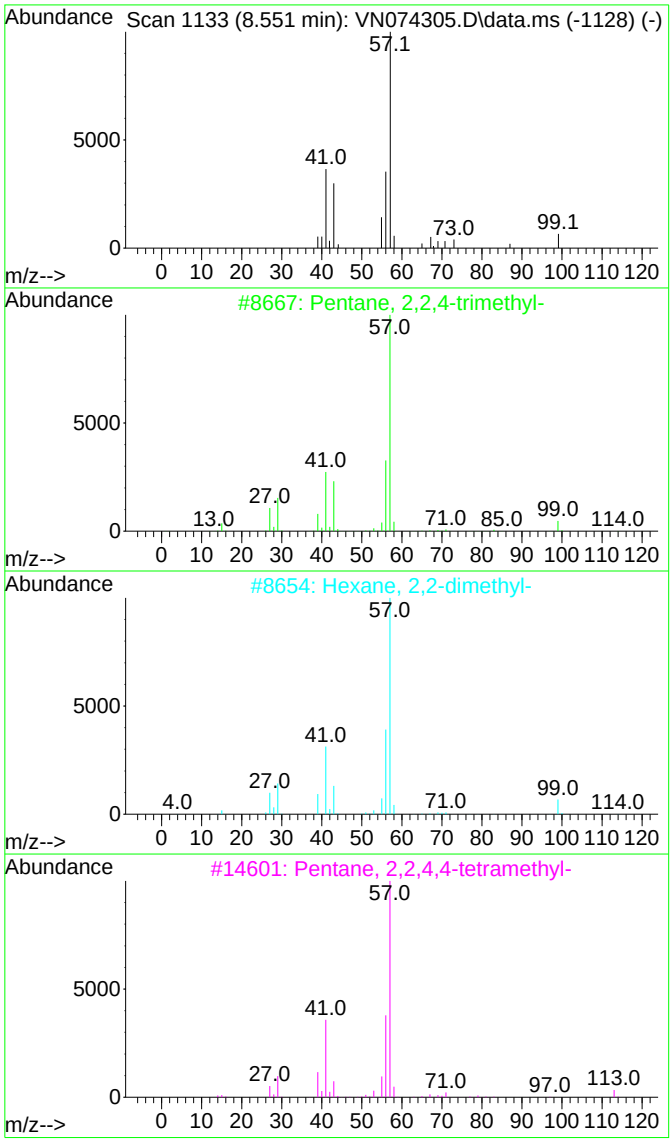
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

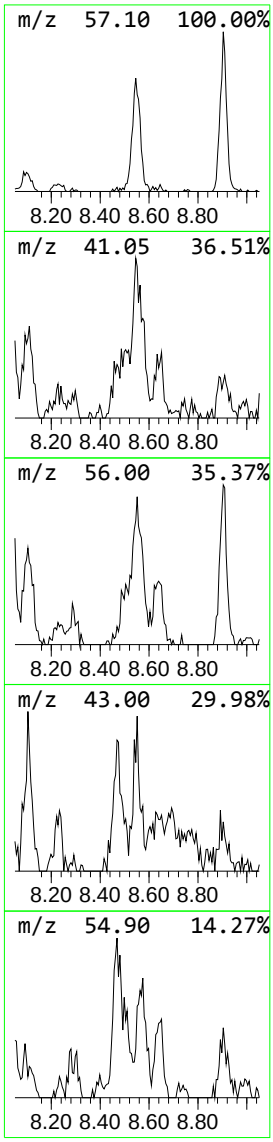
****

Peak Number 7 unknown8.551 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	5.88 ug/l	128247	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	45
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	45
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
4	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	40
5	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

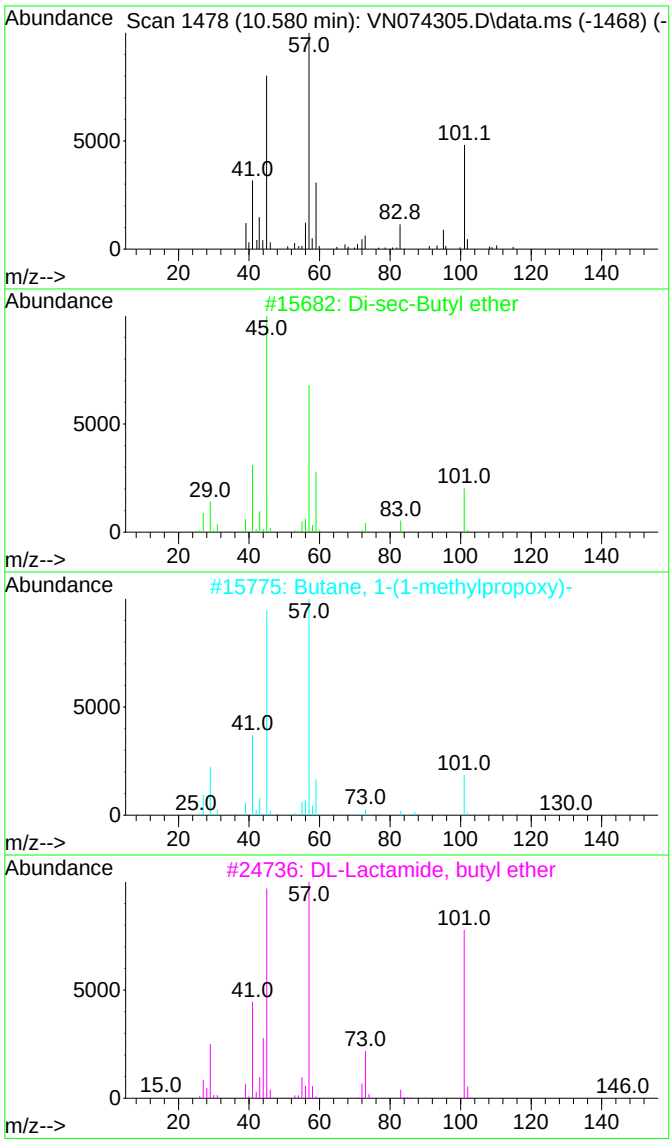
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

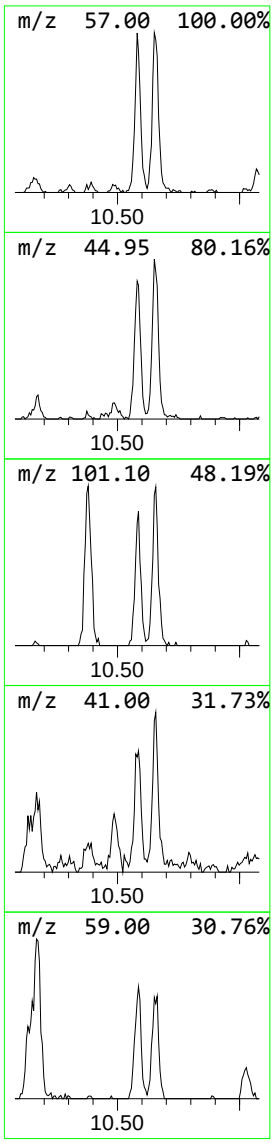
****

Peak Number 8 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	6.03 ug/l	180354	Chlorobenzene-d5	11.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	78
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	56
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	42
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	37
5	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

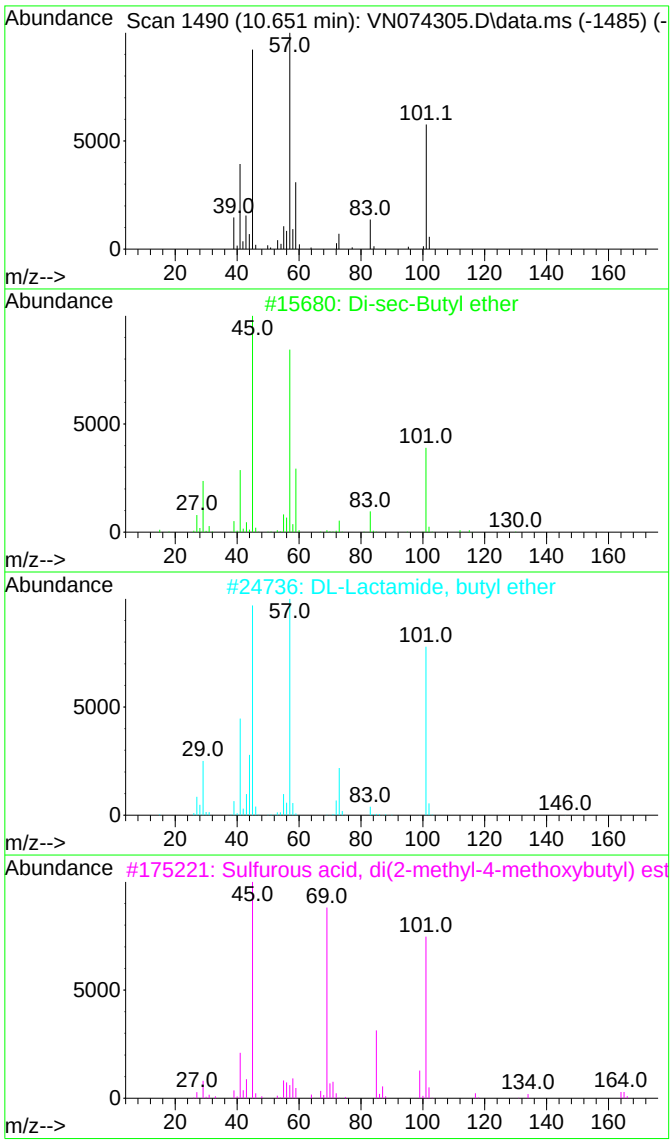
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

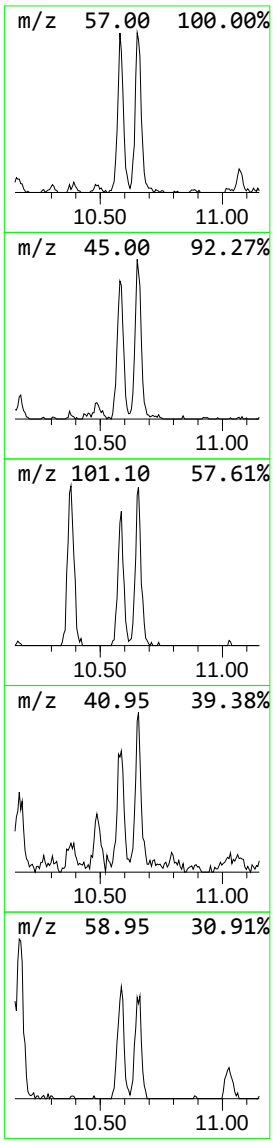
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 DL-Lactamide, butyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	5.63 ug/l	168447	Chlorobenzene-d5	11.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	64
3	Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	59
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5	trans-2-Hexenyl lactate	172	C9H16O3	1000431-56-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074305.D
Acq On : 02 Sep 2022 23:25
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.404	2.404	9.7	ug/l	188017	1	8.016	969319	50.0
Butane, 2-methyl-	3.087	56.9	ug/l	1103790	1	8.016	969319	50.0
Butane, 2,3-dim...	4.998	6.8	ug/l	130852	1	8.016	969319	50.0
unknown5.092	5.092	7.6	ug/l	147246	1	8.016	969319	50.0
Cyclopentane, m...	7.075	11.1	ug/l	215595	1	8.016	969319	50.0
unknown8.551	8.551	5.9	ug/l	128247	2	8.904	1090130	50.0
Di-sec-Butyl ether	10.580	6.0	ug/l	180354	3	11.680	1496610	50.0
DL-Lactamide, b...	10.651	5.6	ug/l	168447	3	11.680	1496610	50.0