LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 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\82N083022W.M
Title : SW846 8260

Signal : TIC: VN074246.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	50	59	63	rBV4	13207	26058	1.72%	0.178%
2	2.399	79	87	94	rBV	70060	120587	7.98%	0.824%
3	2.704	135	139	150	rVB8	20873	47986	3.18%	0.328%
4	3.081	195	203	214	rBV2	185393	421039	27.87%	2.877%
5	3.451	258	266	275	rBV2	29941	72093	4.77%	0.493%
6	3.928	337	347	356	rBV3	16145	43919	2.91%	0.300%
7	4.193	381	392	394	rBV4	13238	36026	2.38%	0.246%
8	4.222	396	397	408	rVB2	11117	21404	1.42%	0.146%
9	4.993	517	528	535	rBV3	46182	168939	11.18%	1.154%
10	5.087	538	544	545	rBV3	16023	23811	1.58%	0.163%
11	5.281	567	577	579	rBV3	16194	32950	2.18%	0.225%
12	5.534	606	620	633	rBV2	202263	711915	47.12%	4.864%
13	6.416	756	770	781	rBV2	216536	700530	46.36%	4.787%
14	6.516	781	787	794	rVB7	8082	23140	1.53%	0.158%
15	6.816	828	838	846	rBV4	8436	27881	1.85%	0.191%
16	6.969	854	864	865	rBV3	12731	25158	1.67%	0.172%
17	7.069	869	881	890	rVV3	92263	274981	18.20%	1.879%
18	7.245	904	911	912	rBV4	10160	17702	1.17%	0.121%
19	7.951	1021	1031	1036	rBV	207311	479684	31.75%	3.278%
20	8.016	1036	1042	1051	rVV	400431	974541	64.50%	6.659%
21	8.104	1051	1057	1065	rVB6	26969	71461	4.73%	0.488%
22	8.286	1082	1088	1094	rVB4	9637	18492	1.22%	0.126%
23	8.375	1094	1103	1113	rBV3	276929	768387	50.86%	5.250%
24	8.475	1113	1120	1125	rBV5	31604	83821	5.55%	0.573%
25	8.545	1128	1132	1134	rBV	22702	32030	2.12%	0.219%
26	8.639	1143	1148	1155	rVB8	16052	35457	2.35%	0.242%
27	8.904	1184	1193	1206	rBV	535569	1113676	73.71%	7.610%
28	9.392	1262	1276	1283	rBV4	49221	158478	10.49%	1.083%
29	9.822	1343	1349	1357	rVB5	24190	54619	3.61%	0.373%
30	9.910	1357	1364	1367	rBV2	35323	73748	4.88%	0.504%
31	9.951	1367	1371	1380	rVB4	51259	104989	6.95%	0.717%
32	10.169	1395	1408	1417	rBV3	60211	188357	12.47%	1.287%
33	10.263	1419	1424	1429	rBV6	11456	20748	1.37%	0.142%
34	10.380	1436	1444	1451	rBV	793069	1484900	98.28%	10.146%
35	10.439	1451	1454	1459	rVV	61335	112914	7.47%	0.772%
36	10.486	1459	1462	1468	rVV2	59577	103414	6.84%	0.707%

LSC Area Percent Report

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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 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\82N083022W.M
Title : SW846 8260

37	10.580	1468	1478	1485	rVV	115425	220060	14.56%	1.504%
38	10.657	1485	1491	1500	rVB	122011	213245	14.11%	1.457%
39	10.798	1510	1515	1524	rVB5	23581	48581	3.22%	0.332%
40	11.027	1550	1554	1558	rBV3	11695	15634	1.03%	0.107%
41	11.069	1558	1561	1567	rVB3	15409	23122	1.53%	0.158%
42	11.157	1571	1576	1579	rVV6	10295	20124	1.33%	0.138%
43	11.557	1634	1644	1654	rBV2	45913	113488	7.51%	0.775%
44	11.686	1658	1666	1676	rVV	841384	1510908	100.00%	10.324%
45	11.786	1676	1683	1693	rVV4	90360	186896	12.37%	1.277%
46	11.898	1694	1702	1712	rVB	100664	192655	12.75%	1.316%
47	12.221	1748	1757	1761	rBV6	13942	32233	2.13%	0.220%
48	12.292	1764	1769	1774	rBV4	14881	25222	1.67%	0.172%
49	12.516	1802	1807	1815	rVV2	47595	86811	5.75%	0.593%
50	12.592	1815	1820	1824	rVB7	10546	16275	1.08%	0.111%
51	12.669	1825	1833	1844	rBV	669937	1135150	75.13%	7.756%
52	12.780	1846	1852	1857	rVV5	25212	47762	3.16%	0.326%
53	12.863	1857	1866	1873	rVB2	55587	111763	7.40%	0.764%
54	12.951	1873	1881	1884	rBV5	12587	28348	1.88%	0.194%
55	12.998	1884	1889	1895	rVB7	20459	41898	2.77%	0.286%
56	13.163	1911	1917	1923	rVB	24723	40176	2.66%	0.275%
57	13.310	1936	1942	1945	rVB5	9674	15166	1.00%	0.104%
58	13.610	1986	1993	2004	rBV	762063	1364486	90.31%	9.323%
59	13.774	2018	2021	2024	rBV3	24401	34523	2.28%	0.236%
60	13.816	2024	2028	2037	rVB	89057	154409	10.22%	1.055%
61	14.010	2053	2061	2065	rVB10	10344	20752	1.37%	0.142%
62	14.151	2079	2085	2092	rVB4	17250	34006	2.25%	0.232%
63	14.268	2099	2105	2110	rVB2	48557	78579	5.20%	0.537%
64	14.392	2120	2126	2133	rBV9	13531	28272	1.87%	0.193%
65	14.474	2136	2140	2145	rBV5	14610	27039	1.79%	0.185%
66	14.751	2183	2187	2191	rBV6	13492	20189	1.34%	0.138%
67	14.868	2203	2207	2212	rVB5	17008	30426	2.01%	0.208%
68	14.921	2212	2216	2227	rVB5	9379	21470	1.42%	0.147%
69	15.127	2247	2251	2254	rBV6	13164	19798	1.31%	0.135%

Sum of corrected areas: 14635301

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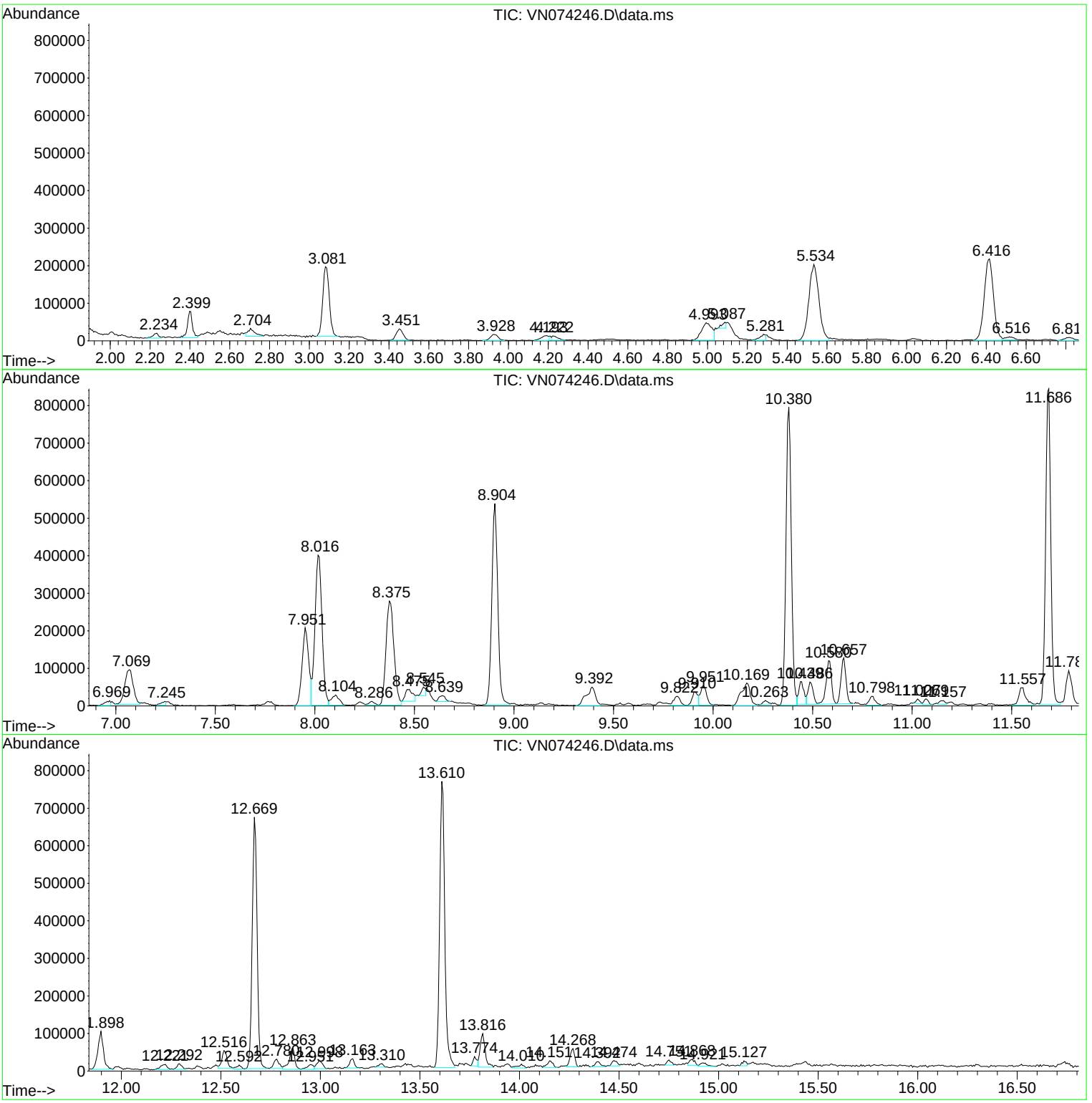
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
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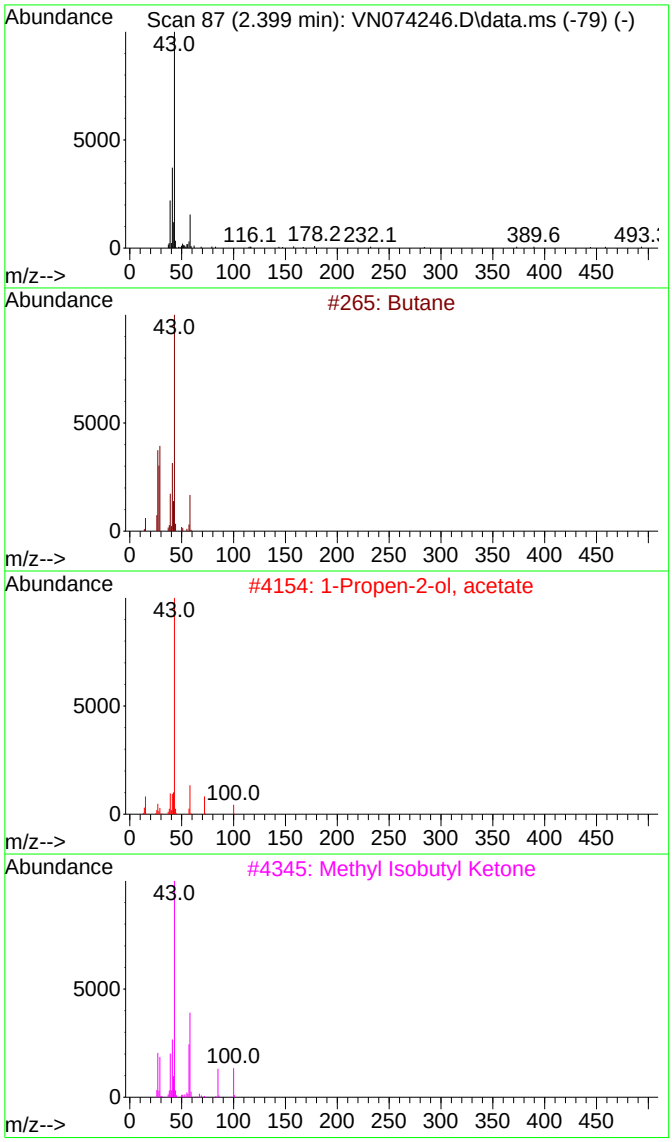
Quant Title : SW846 8260

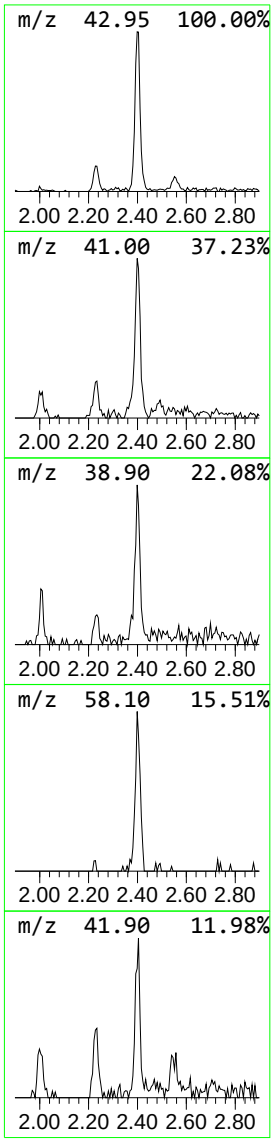
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	6.19 ug/l	120587	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	58
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	36
3	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	23
4	Isobutane	58	C4H10	000075-28-5	9
5	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

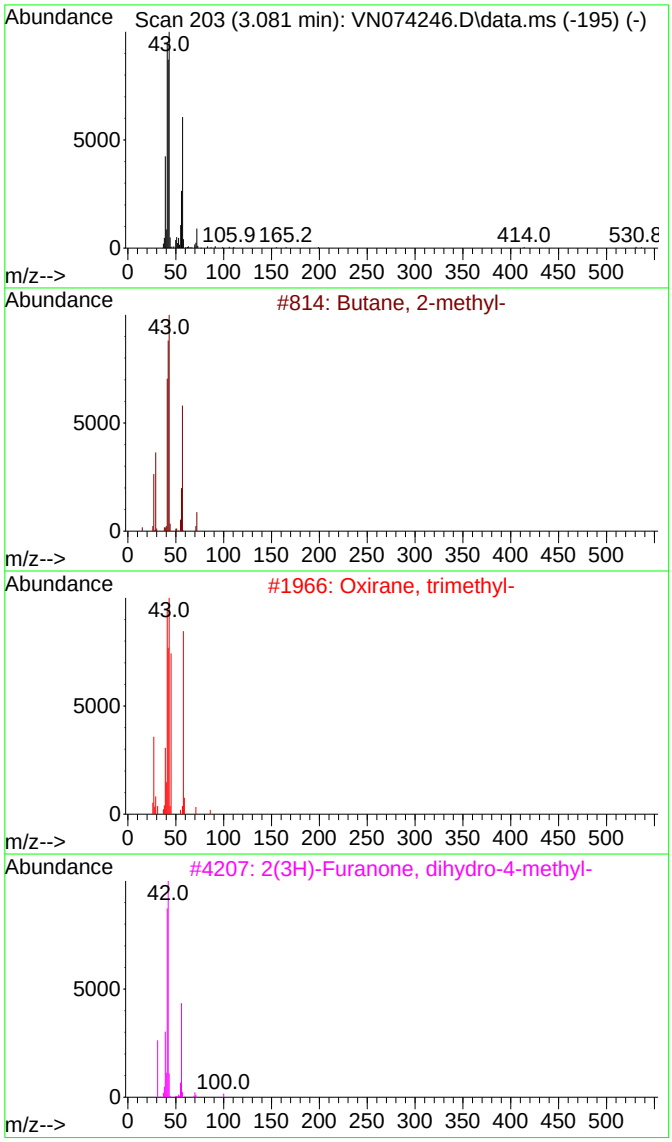
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

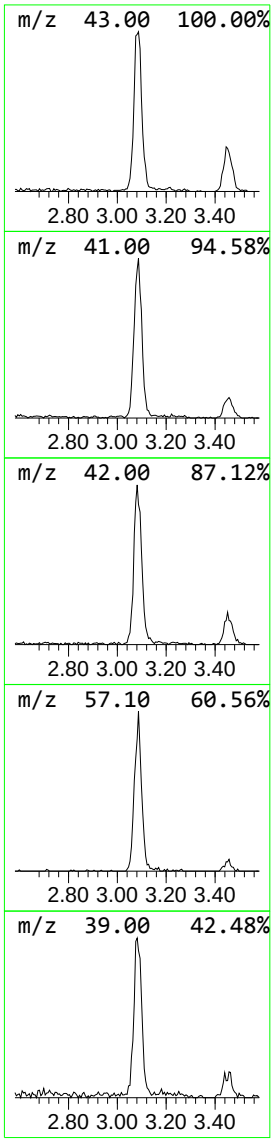
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	21.60 ug/l	421039	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	58
2	Oxirane, trimethyl-	86	C5H10O	005076-19-7	32
3	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	25
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

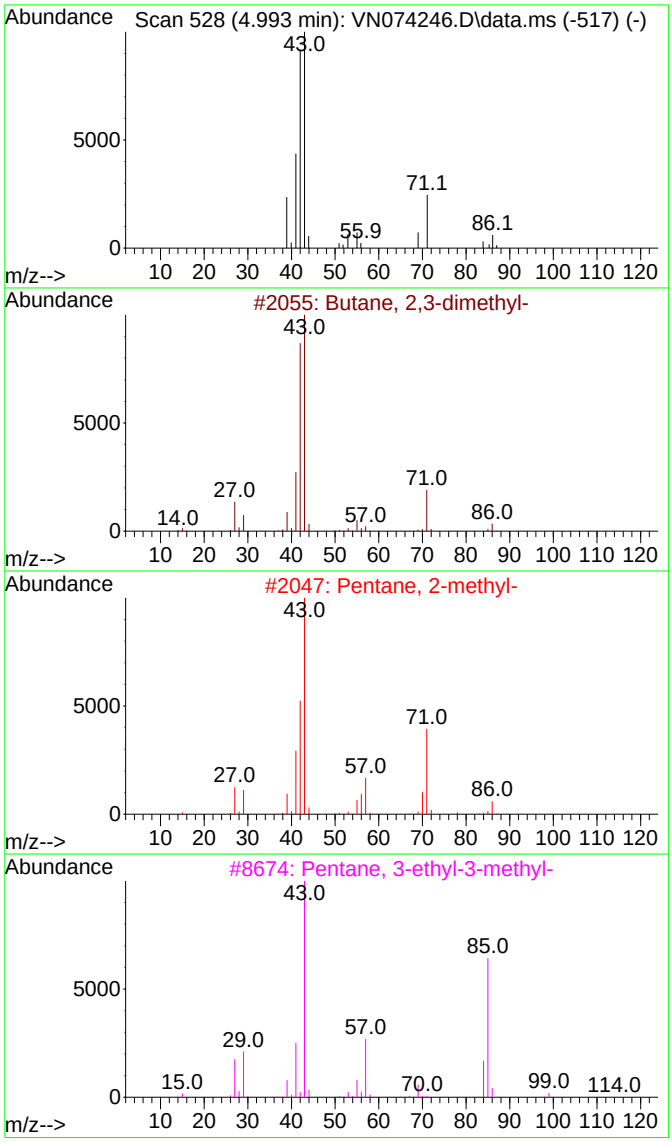
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

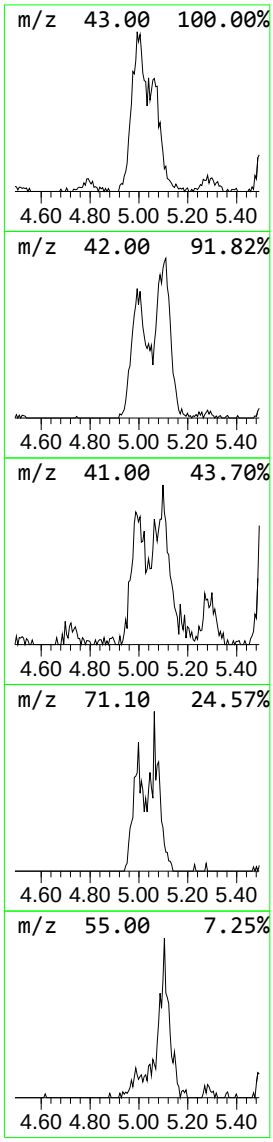
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	8.67 ug/l	168939	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	23
3	Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	9
4	Hexane, 2-bromo-	164	C6H13Br	003377-86-4	9
5	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
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Acq On : 01 Sep 2022 16:43
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Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

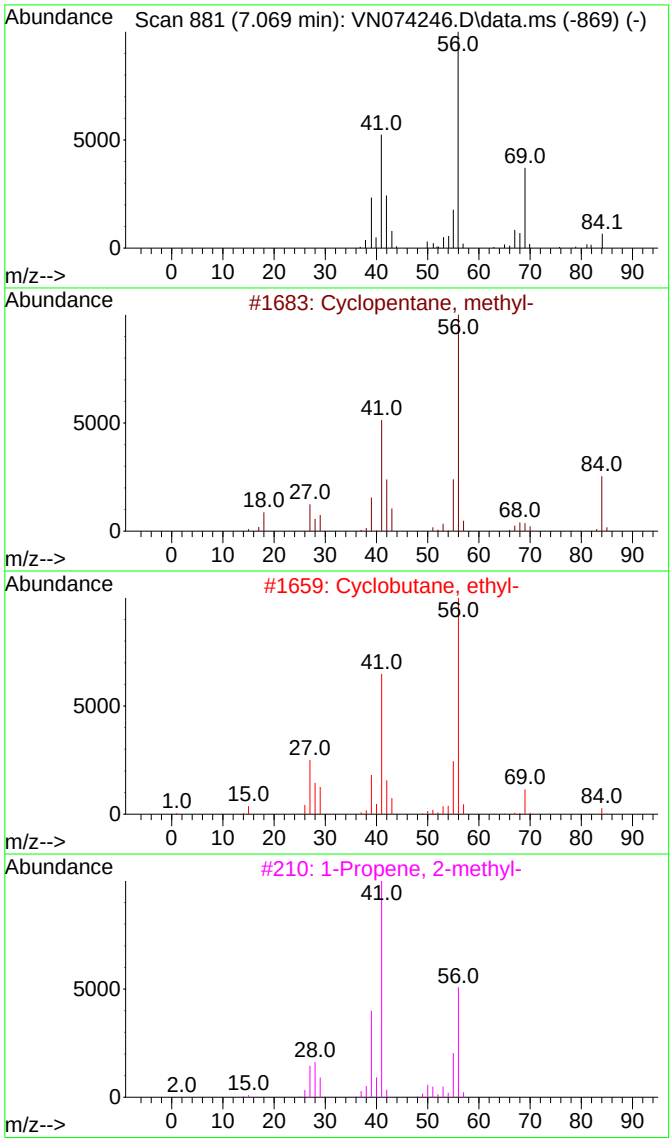
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

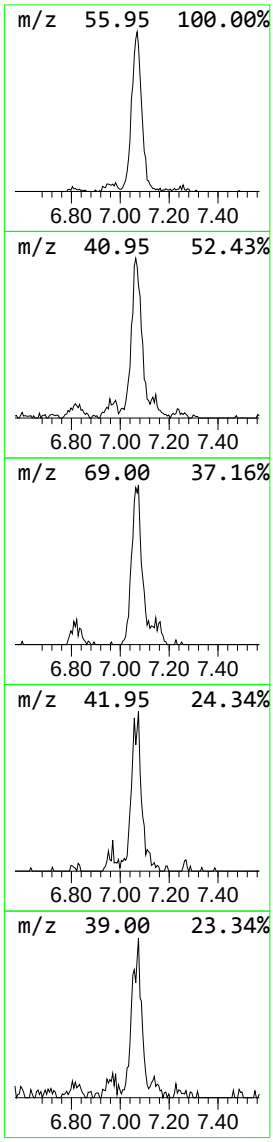
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	14.11 ug/l	274981	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	40
4	Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	39
5	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	39





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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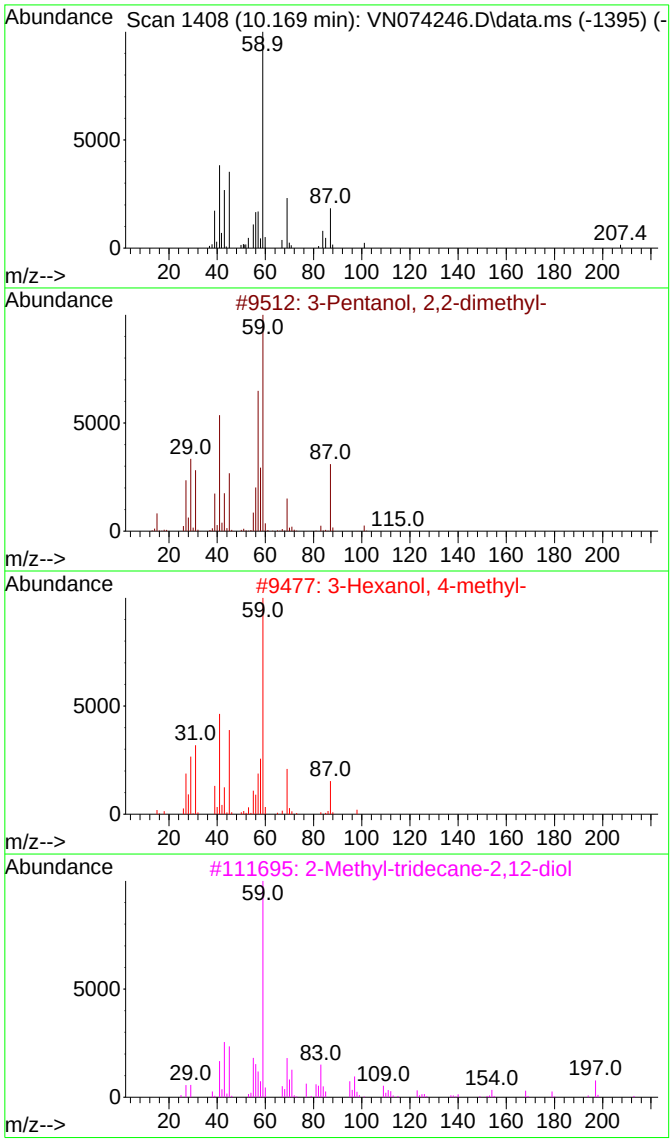
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

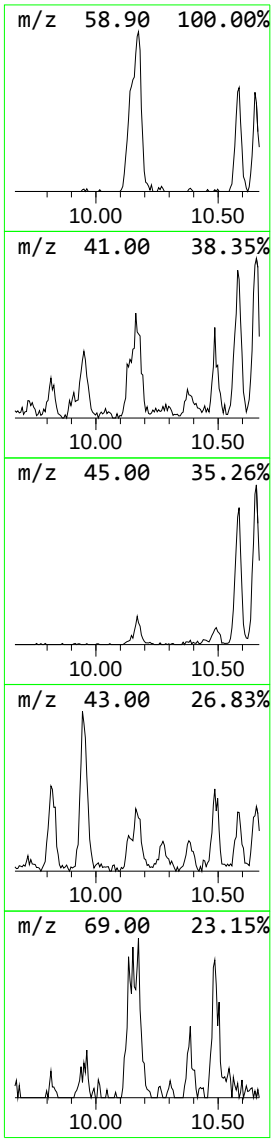
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanol, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.169	8.46 ug/l	188357	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	56
3	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	56
4	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
5	Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	50





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

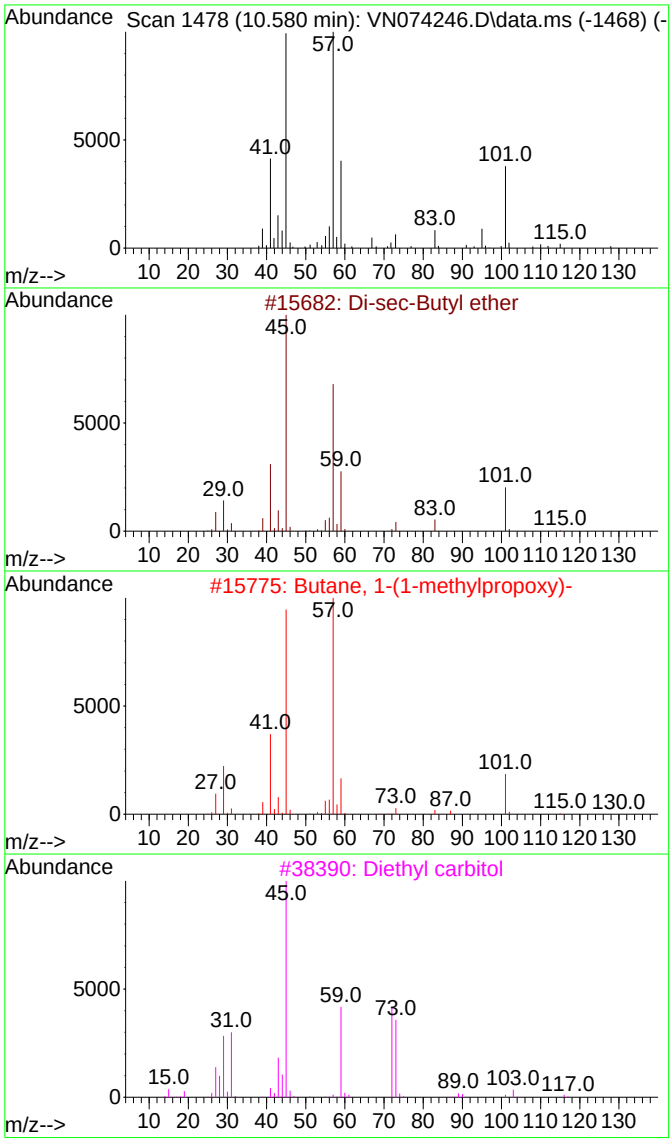
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

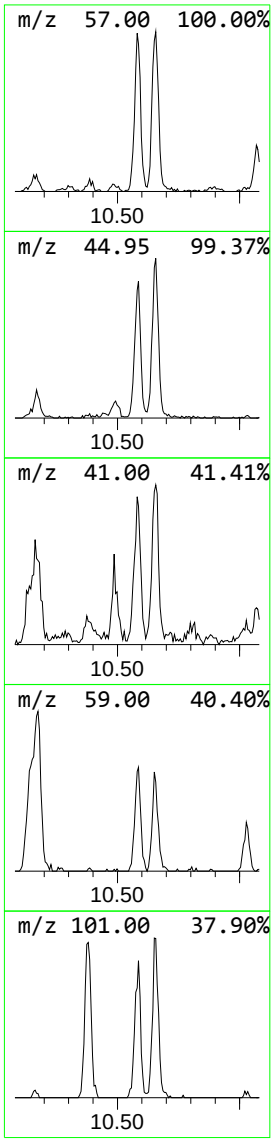
****

Peak Number 6 Di-sec-Butyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	7.28 ug/l	220060	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
3	Diethyl carbitol	162	C8H18O3	000112-36-7	50
4	2-Butanol, (R)-	74	C4H10O	014898-79-4	42
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

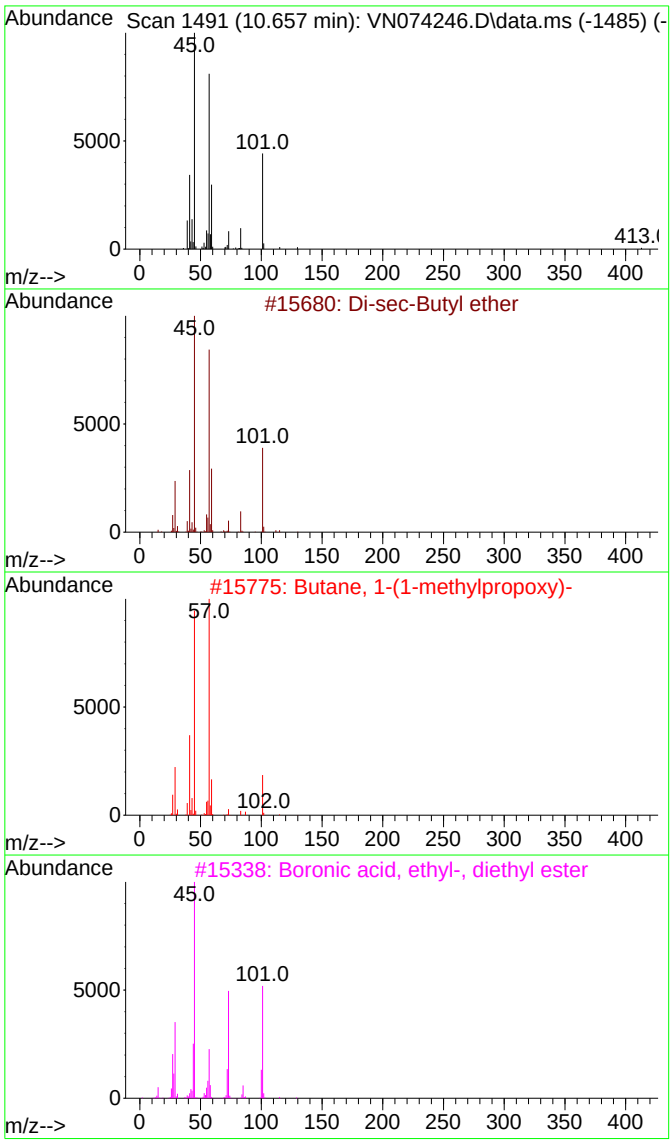
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

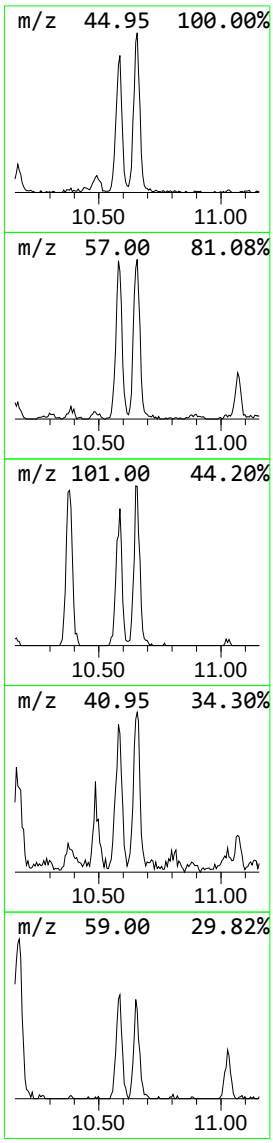
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butane, 1-(1-methylpropoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	7.06 ug/l	213245	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	56
3	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	40
4	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	33
5	Propane, 1,1'-[ethylidenebis(oxy...	174	C10H22O2	005669-09-0	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

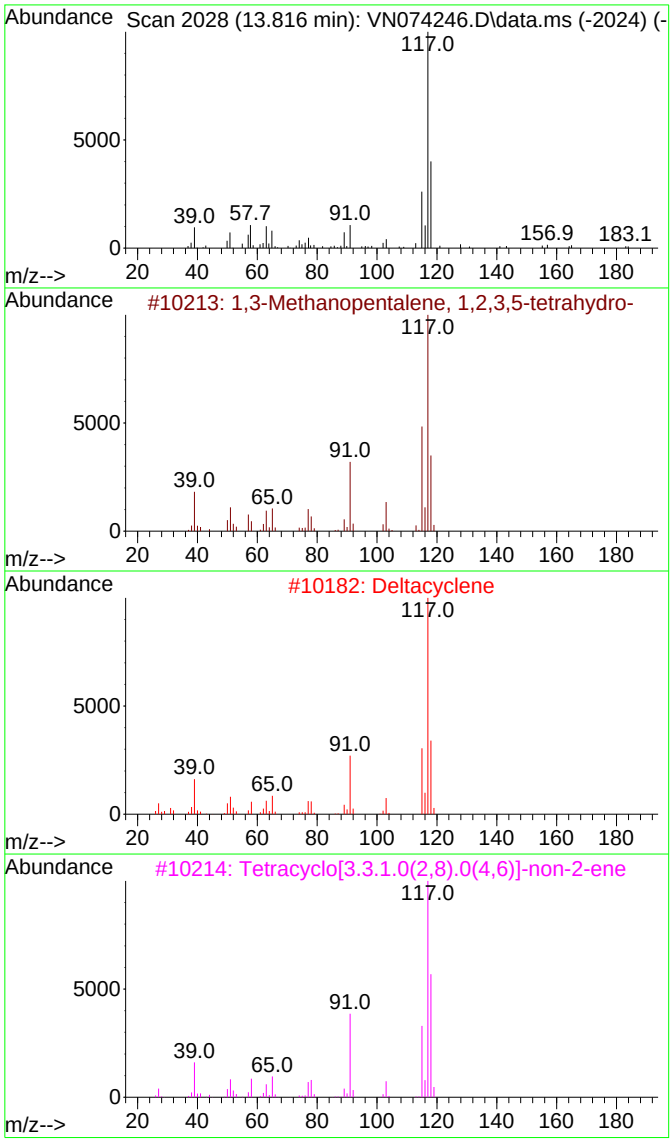
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

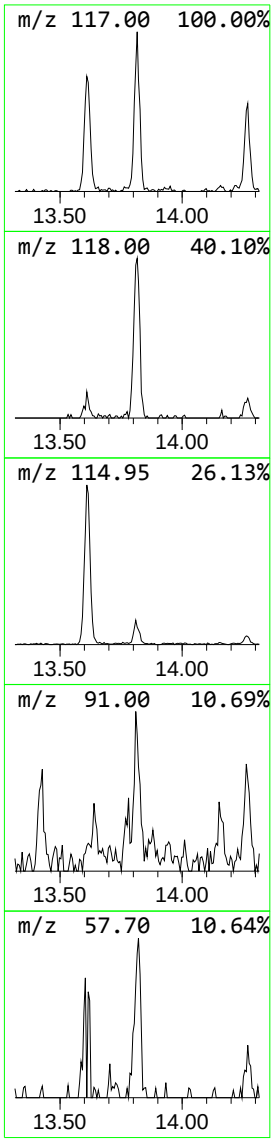
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Methanopentalene, 1,2,3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	5.66 ug/l	154409	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	64
2	Deltacyclene	118	C9H10	007785-10-6	64
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4	Benzene, 1-(chloromethyl)-3-ethe...	152	C9H9Cl	039833-65-3	59
5	Benzene, 1-(chloromethyl)-4-ethe...	152	C9H9Cl	001592-20-7	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074246.D
Acq On : 01 Sep 2022 16:43
Operator : JC\MD
Sample : N4329-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.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
Butane	2.399	6.2	ug/l	120587	1	8.022	974541	50.0
Butane, 2-methyl-	3.081	21.6	ug/l	421039	1	8.022	974541	50.0
Butane, 2,3-dim...	4.993	8.7	ug/l	168939	1	8.022	974541	50.0
Cyclopentane, m...	7.069	14.1	ug/l	274981	1	8.022	974541	50.0
3-Pentanol, 2,2...	10.169	8.5	ug/l	188357	2	8.904	1113680	50.0
Di-sec-Butyl ether	10.580	7.3	ug/l	220060	3	11.686	1510910	50.0
Butane, 1-(1-me...	10.657	7.1	ug/l	213245	3	11.686	1510910	50.0
1,3-Methanopent...	13.816	5.7	ug/l	154409	4	13.616	1364490	50.0