LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

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\82N072822W.M
Title : SW846 8260

Signal : TIC: VN073716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	48	54	62	rBV3	13450	33832	1.71%	0.217%
2	2.346	67	78	79	rBV2	17179	40562	2.05%	0.261%
3	2.493	100	103	109	rVB3	15990	23214	1.18%	0.149%
4	2.710	132	140	147	rVB5	24030	76648	3.88%	0.492%
5	3.081	194	203	222	rVB	629901	1431564	72.47%	9.197%
6	3.452	256	266	276	rBV	64678	151383	7.66%	0.973%
7	3.652	291	300	311	rVB5	6968	19758	1.00%	0.127%
8	4.234	380	399	414	rBV2	22884	88869	4.50%	0.571%
9	4.510	435	446	466	rBV	95643	307418	15.56%	1.975%
10	4.993	516	528	529	rBV2	27623	60640	3.07%	0.390%
11	5.528	607	619	633	rBV2	31325	112166	5.68%	0.721%
12	6.381	754	764	775	rBV3	10668	33220	1.68%	0.213%
13	6.522	777	788	797	rBV4	10390	31656	1.60%	0.203%
14	7.063	869	880	890	rBV2	124109	369474	18.71%	2.374%
15	7.345	920	928	940	rVB	20182	52717	2.67%	0.339%
16	7.622	966	975	986	rVB5	10266	28716	1.45%	0.184%
17	7.951	1021	1031	1036	rBV	257592	610770	30.92%	3.924%
18	8.022	1036	1043	1052	rVB	452179	1063937	53.86%	6.835%
19	8.375	1093	1103	1114	rBV2	288086	736897	37.31%	4.734%
20	8.904	1184	1193	1207	rBV	623112	1293089	65.46%	8.307%
21	9.369	1261	1272	1273	rBV5	10011	20984	1.06%	0.135%
22	9.392	1273	1276	1283	rVB4	14789	29114	1.47%	0.187%
23	9.910	1357	1364	1369	rBV4	20107	37382	1.89%	0.240%
24	10.380	1436	1444	1452	rBV	911765	1649979	83.53%	10.600%
25	10.445	1452	1455	1460	rVV2	23556	42081	2.13%	0.270%
26	10.580	1473	1478	1484	rVB6	11619	24382	1.23%	0.157%
27	11.233	1583	1589	1598	rBV2	33874	64068	3.24%	0.412%
28	11.686	1658	1666	1677	rBV	905600	1574020	79.69%	10.112%
29	11.786	1677	1683	1691	rVV	78743	144800	7.33%	0.930%
30	11.898	1691	1702	1713	rVB2	42248	82096	4.16%	0.527%
31	12.222	1750	1757	1764	rBV	45549	75923	3.84%	0.488%
32	12.522	1798	1808	1814	rBV	94292	168027	8.51%	1.079%
33	12.674	1827	1834	1843	rVB	756583	1259774	63.78%	8.093%
34	12.863	1858	1866	1873	rBV	187139	303326	15.36%	1.949%
35	12.957	1873	1882	1886	rVV	71205	125830	6.37%	0.808%
36	12.998	1886	1889	1895	rVB4	18847	29191	1.48%	0.188%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

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\82N072822W.M
Title : SW846 8260

37	13.163	1908	1917	1929	rBV	338710	548715	27.78%	3.525%
38	13.310	1935	1942	1948	rBV	13265	21051	1.07%	0.135%
39	13.616	1986	1994	2005	rBV2	971949	1975259	100.00%	12.690%
40	13.710	2006	2010	2016	rVV	42033	68583	3.47%	0.441%
41	13.780	2016	2022	2024	rVV	35543	57655	2.92%	0.370%
42	13.816	2024	2028	2033	rVV	123612	203222	10.29%	1.306%
43	13.857	2033	2035	2046	rVV3	13788	26039	1.32%	0.167%
44	14.010	2056	2061	2067	rVB	19403	28611	1.45%	0.184%
45	14.157	2081	2086	2092	rVB	50689	77393	3.92%	0.497%
46	14.268	2100	2105	2112	rVB2	46467	79415	4.02%	0.510%
47	14.398	2122	2127	2134	rVB2	12997	20655	1.05%	0.133%
48	14.480	2134	2141	2146	rBV	29669	50360	2.55%	0.324%
49	14.745	2181	2186	2195	rVB2	26596	43804	2.22%	0.281%
50	14.868	2197	2207	2213	rBV3	67125	131888	6.68%	0.847%
51	15.433	2297	2303	2310	rBV	21333	35434	1.79%	0.228%

Sum of corrected areas: 15565591

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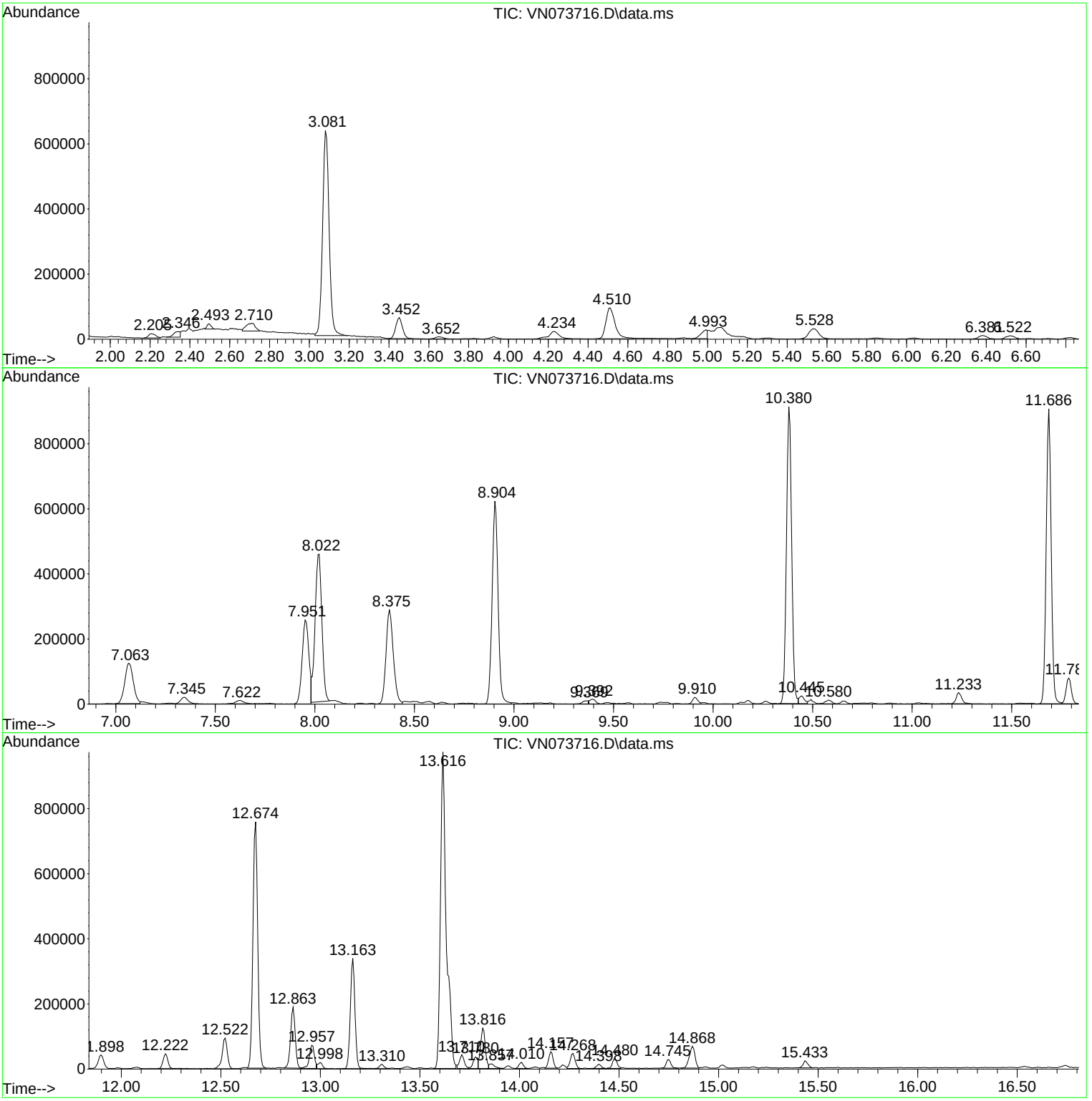
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

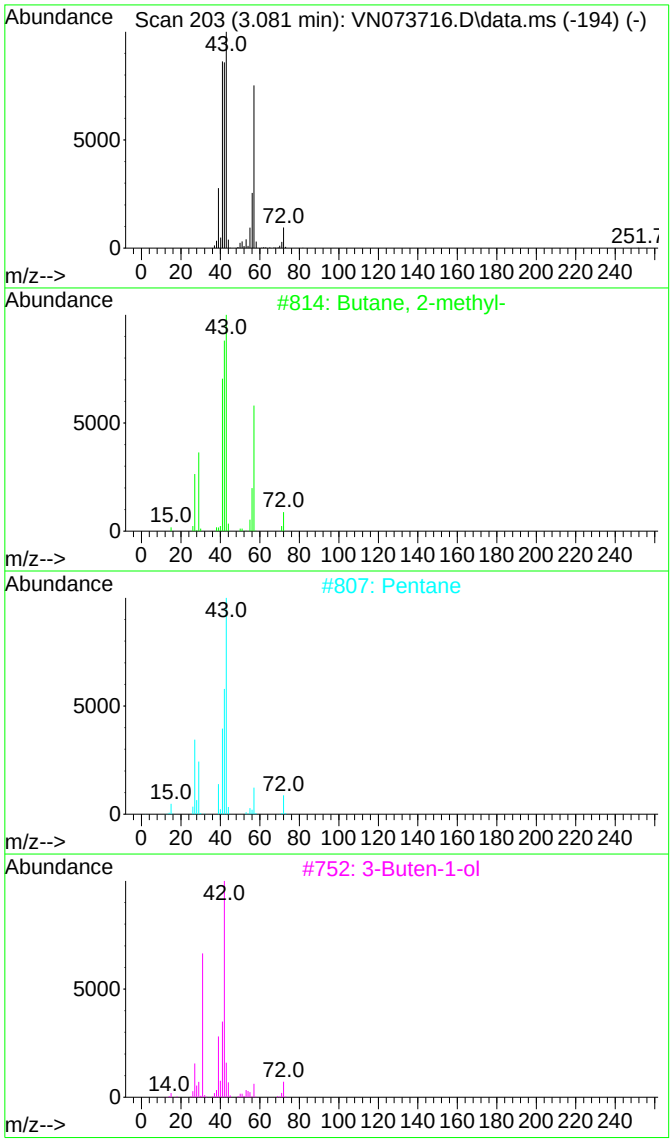
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

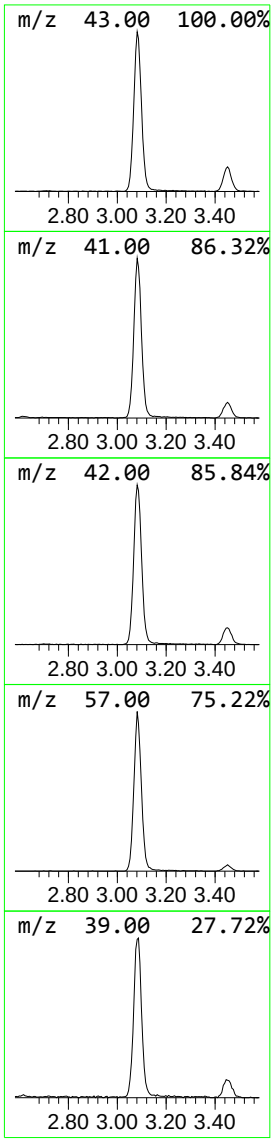
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	67.28 ug/l	1431560	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	45
3	3-Buten-1-ol	72	C4H8O	000627-27-0	43
4	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	17
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

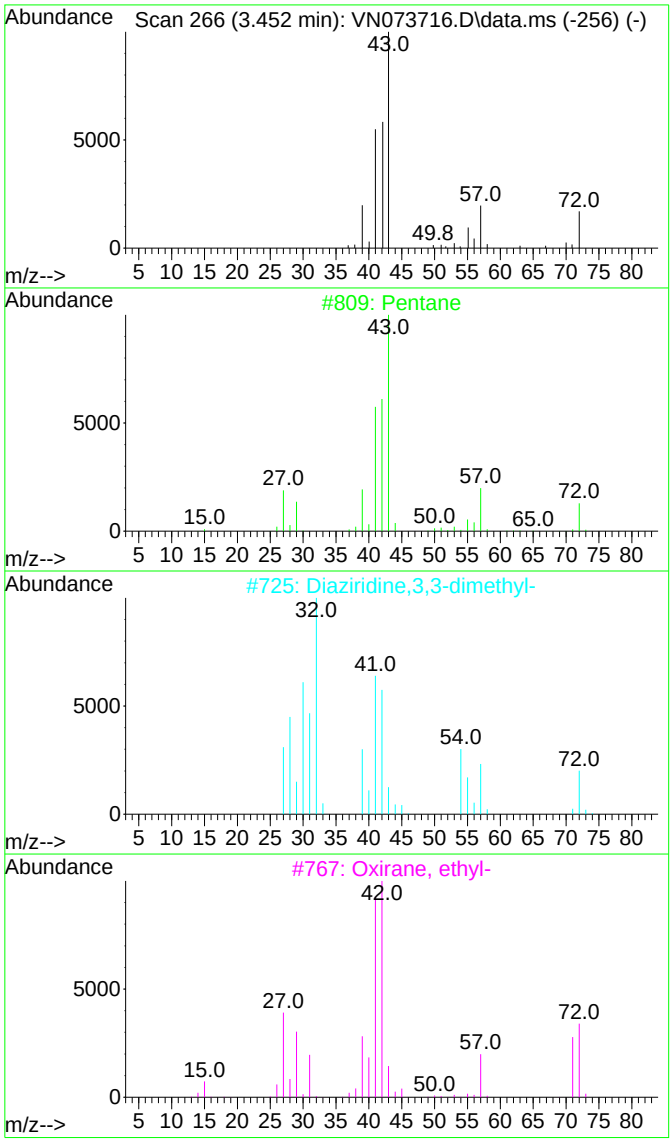
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

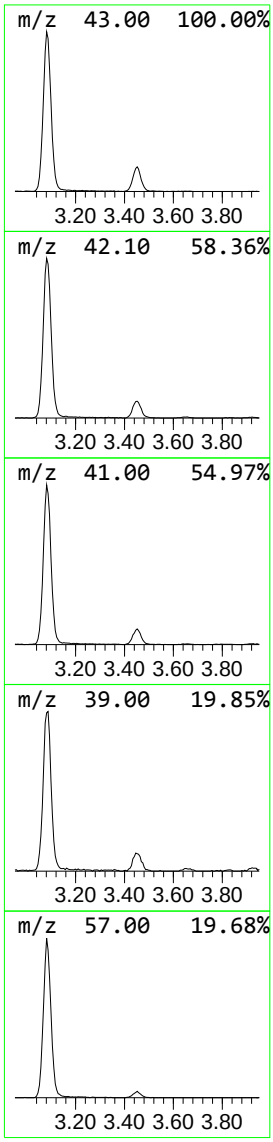
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.452	7.11 ug/l	151383	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	42
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	25
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

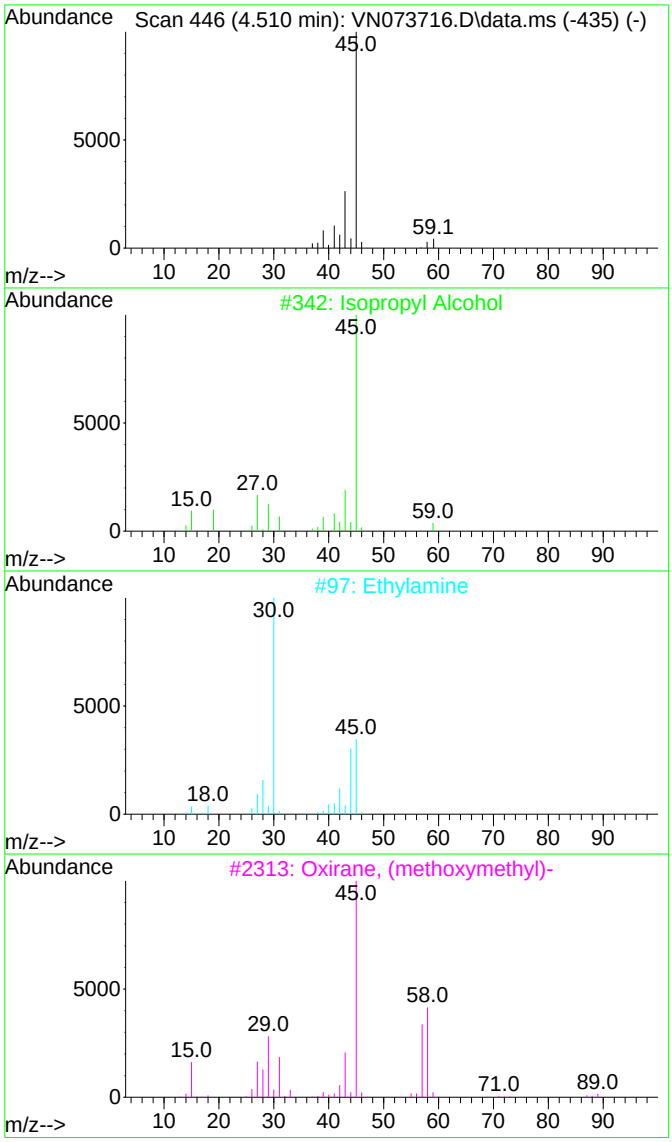
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

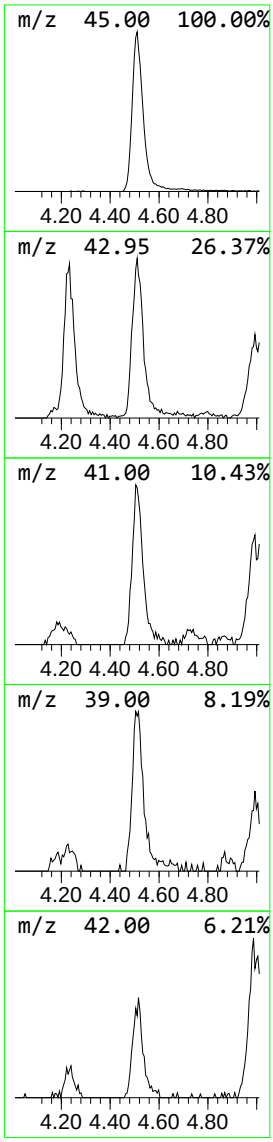
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	14.45 ug/l	307418	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2	Ethylamine	45	C2H7N	000075-04-7	5
3	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
4	4-Penten-2-ol	86	C5H10O	000625-31-0	4
5	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

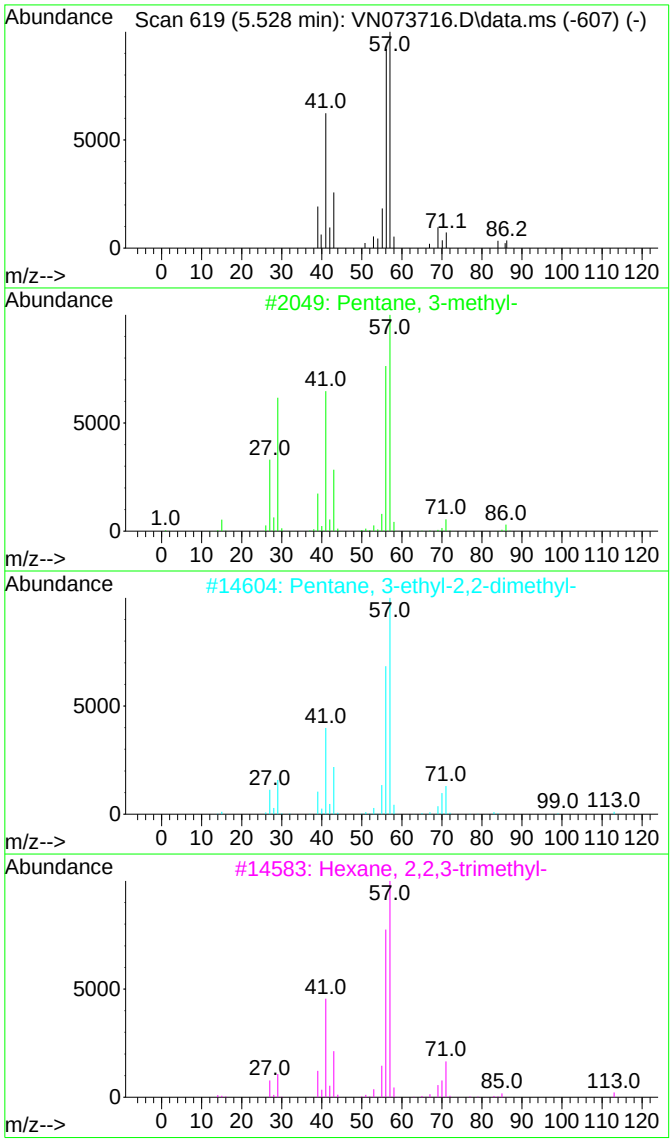
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

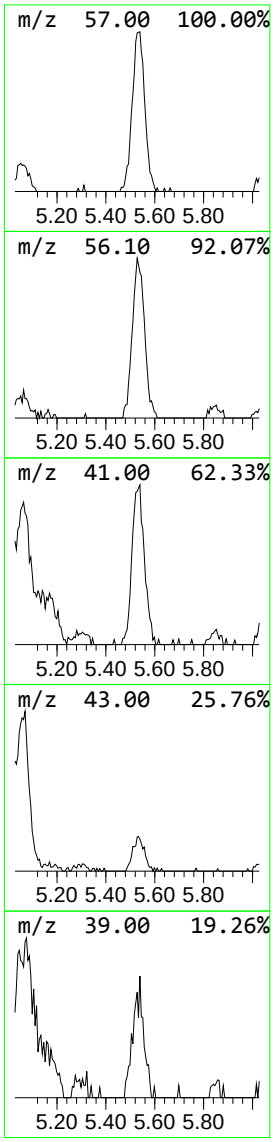
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.528	5.27 ug/l	112166	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	72
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
4	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	50
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

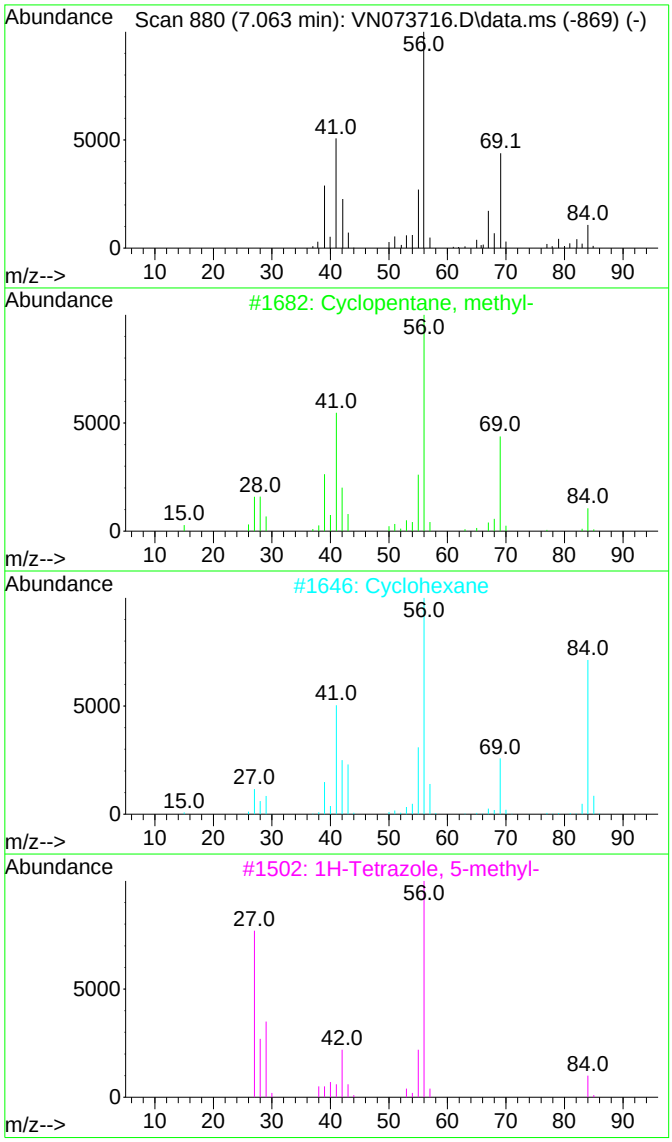
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

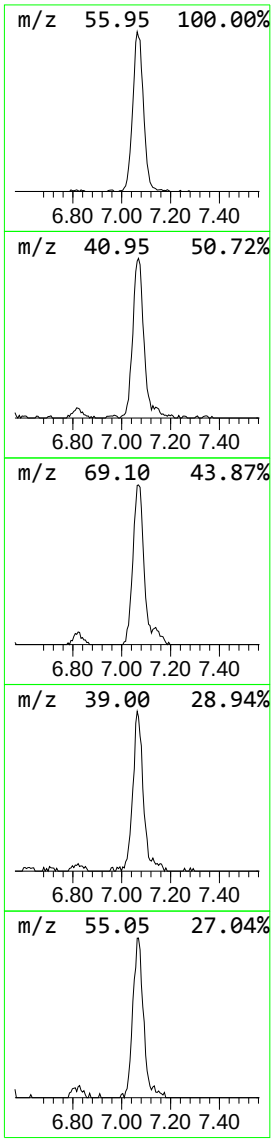
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	17.36 ug/l	369474	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclohexane	84	C6H12	000110-82-7	72
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

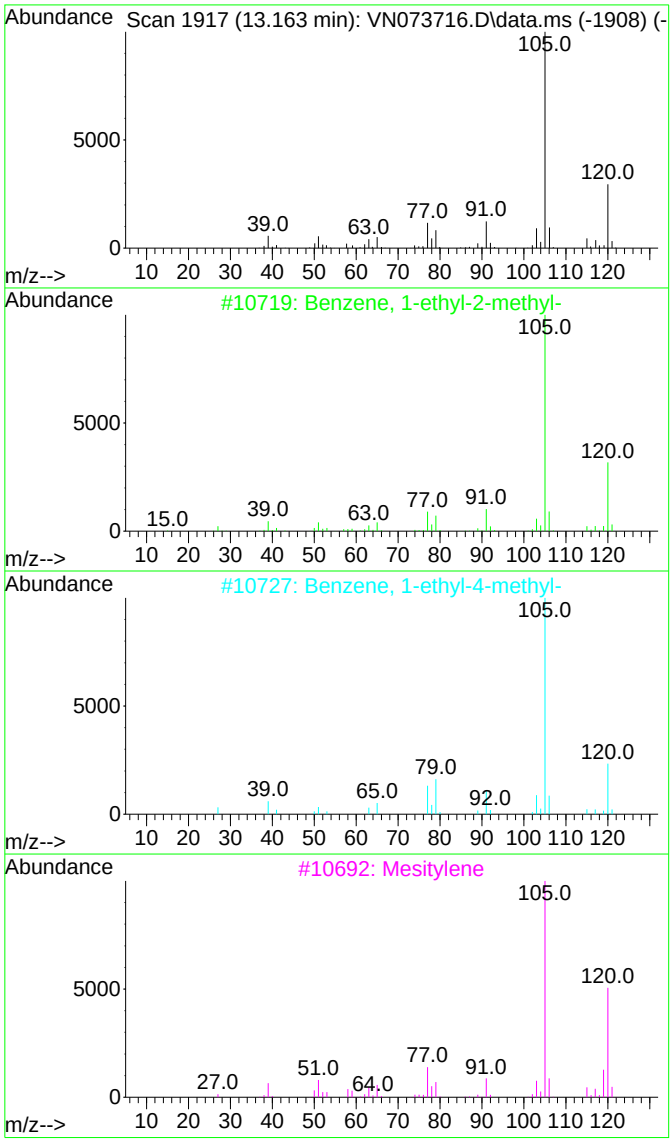
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

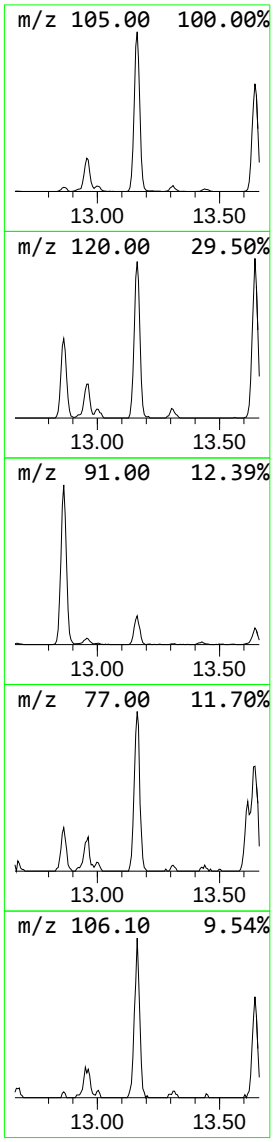
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	13.89 ug/l	548715	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
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Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

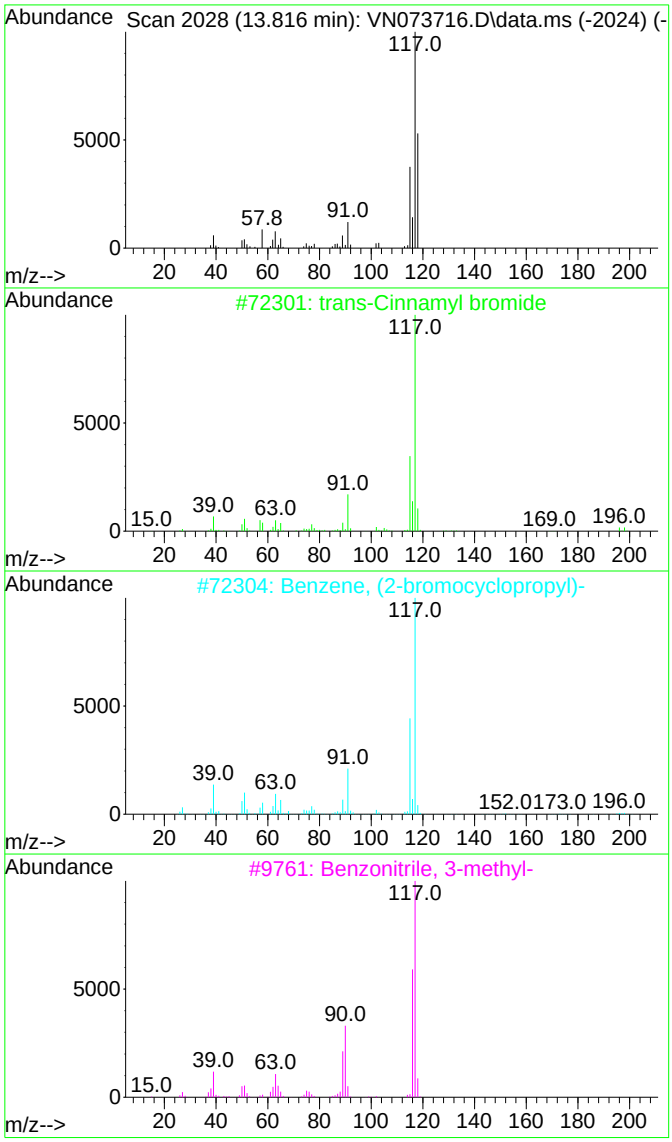
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

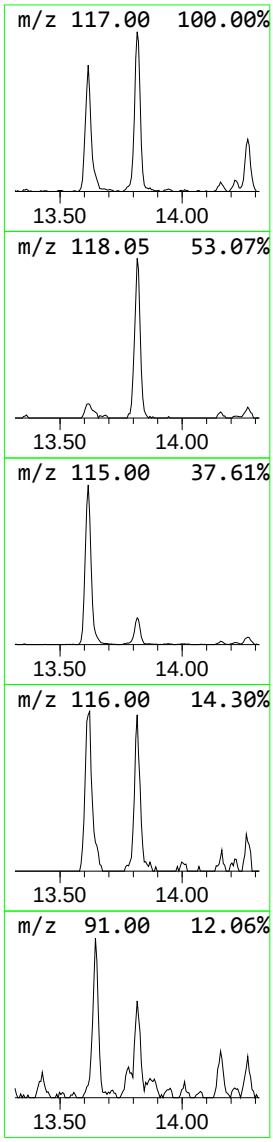
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 trans-Cinnamyl bromide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	5.14 ug/l	203222	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
2	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
3	Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	43
4	Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	38
5	Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073716.D
Acq On : 03 Aug 2022 17:03
Operator : JC\MD
Sample : N3972-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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-methyl-	3.081	67.3	ug/l	1431560	1	8.022	1063940	50.0
Pentane	3.452	7.1	ug/l	151383	1	8.022	1063940	50.0
Isopropyl Alcohol	4.510	14.4	ug/l	307418	1	8.022	1063940	50.0
Pentane, 3-methyl-	5.528	5.3	ug/l	112166	1	8.022	1063940	50.0
Cyclopentane, m...	7.063	17.4	ug/l	369474	1	8.022	1063940	50.0
Benzene, 1-ethy...	13.163	13.9	ug/l	548715	4	13.616	1975260	50.0
trans-Cinnamyl ...	13.816	5.1	ug/l	203222	4	13.616	1975260	50.0