LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN070273.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.537	190	204	220	rBV	216024	394194	4.16%	0.716%
2	3.845	674	692	721	rVB4	54321	166804	1.76%	0.303%
3	4.256	819	845	882	rBV8	32598	151948	1.60%	0.276%
4	5.374	1233	1262	1303	rBV3	281440	1027935	10.86%	1.867%
5	5.618	1326	1353	1395	rVB3	307259	1106952	11.69%	2.010%
6	6.495	1651	1680	1705	rVV4	85603	335068	3.54%	0.608%
7	7.219	1929	1950	1972	rBV4	72952	217711	2.30%	0.395%
8	7.783	2142	2160	2168	rBV5	38945	97430	1.03%	0.177%
9	7.844	2170	2183	2207	rVB2	134350	333815	3.53%	0.606%
10	8.021	2225	2249	2260	rBV	630924	1502420	15.87%	2.728%
11	8.086	2261	2273	2294	rVB	1112156	2503564	26.44%	4.547%
12	8.177	2299	2307	2333	rVB9	42881	108449	1.15%	0.197%
13	8.437	2384	2404	2422	rBV	778976	1846325	19.50%	3.353%
14	8.534	2422	2440	2461	rBV	4103007	9467396	100.00%	17.193%
15	8.968	2580	2602	2632	rBV2	1820332	3989828	42.14%	7.246%
16	9.196	2675	2687	2699	rBV2	72635	149212	1.58%	0.271%
17	9.424	2757	2772	2784	rBV6	54681	126718	1.34%	0.230%
18	9.732	2870	2887	2902	rBV3	60828	129805	1.37%	0.236%
19	9.880	2929	2942	2958	rVB2	122299	247370	2.61%	0.449%
20	9.971	2960	2976	2986	rBV	477400	958923	10.13%	1.741%
21	10.202	3044	3062	3065	rBV2	1046225	1661067	17.55%	3.017%
22	10.234	3067	3074	3100	rVB	1893997	3696736	39.05%	6.713%
23	10.440	3135	3151	3176	rBV	2592445	4893004	51.68%	8.886%
24	10.550	3177	3192	3216	rBV	2035628	3998143	42.23%	7.261%
25	10.856	3293	3306	3326	rVV2	233184	476648	5.03%	0.866%
26	11.089	3378	3393	3404	rBV2	187318	372954	3.94%	0.677%
27	11.213	3426	3439	3467	rVB2	369992	899111	9.50%	1.633%
28	11.621	3575	3591	3618	rBV5	336772	873651	9.23%	1.587%
29	11.744	3619	3637	3666	rVV	2917705	5664592	59.83%	10.287%
30	11.862	3667	3681	3706	rVB3	312262	682432	7.21%	1.239%
31	11.964	3707	3719	3737	rVB7	69701	143621	1.52%	0.261%
32	12.042	3738	3748	3759	rBV3	79062	130086	1.37%	0.236%
33	12.358	3854	3866	3877	rBV3	83458	160409	1.69%	0.291%
34	12.538	3919	3933	3960	rBV6	102491	276564	2.92%	0.502%
35	12.731	3988	4005	4030	rVB	1612868	2962304	31.29%	5.380%
36	12.846	4036	4048	4060	rBV5	113129	235237	2.48%	0.427%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

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\82N120221W.M
Title : SW846 8260

37	13.675	4340	4357	4380	rBV	1559586	2807306	29.65%	5.098%
38	13.919	4436	4448	4463	rVB	168591	269279	2.84%	0.489%

Sum of corrected areas: 55065011

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Data File : VN070273.D
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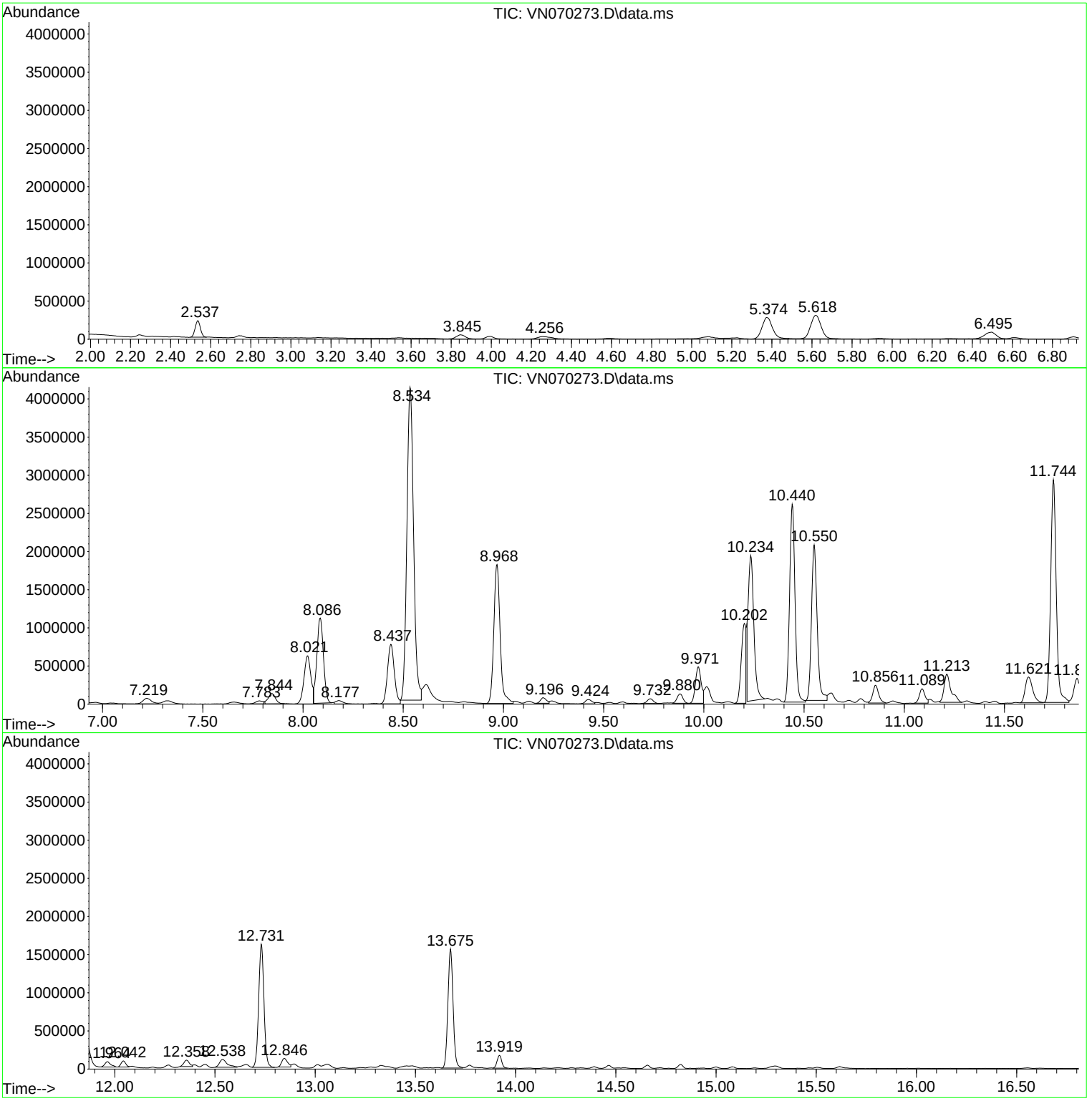
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

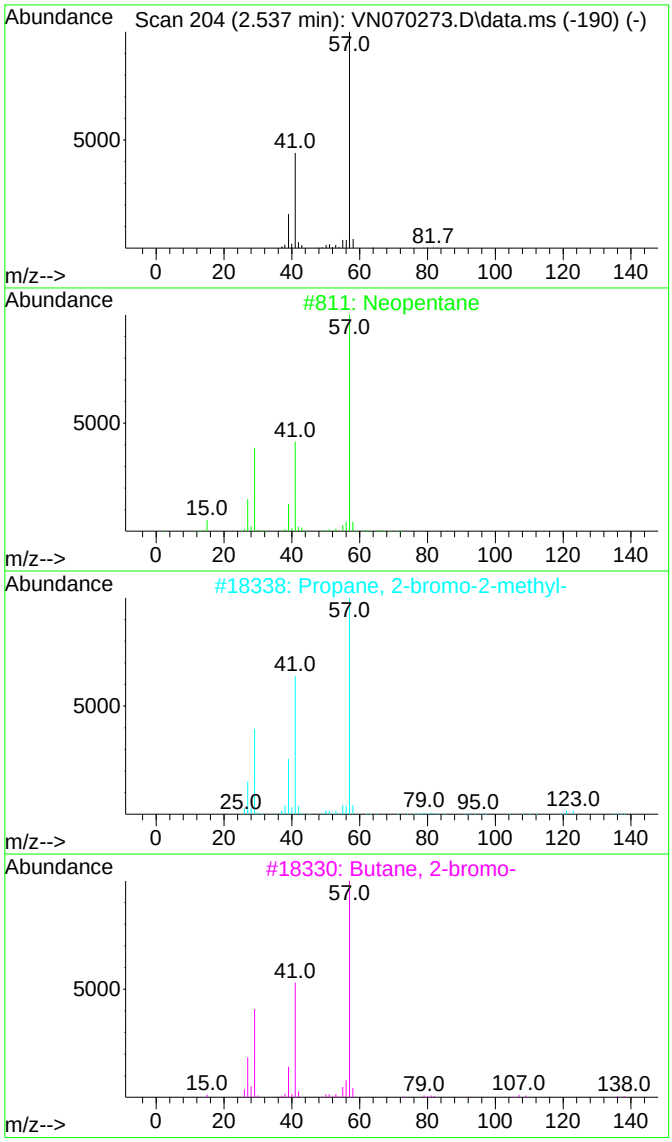
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

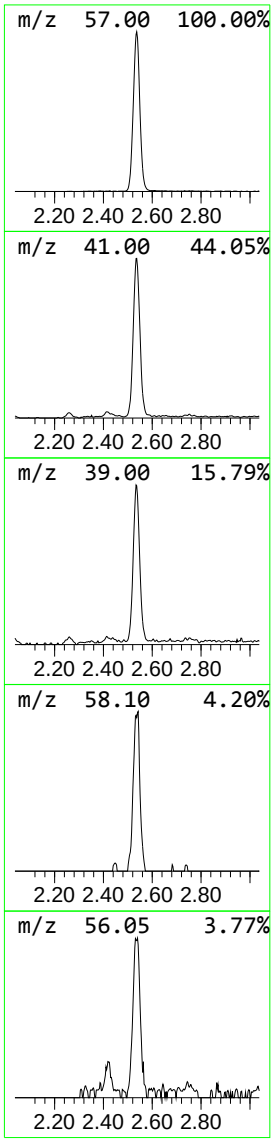
****

Peak Number 1 Neopentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.537	7.87 ug/l	394194	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentane	72	C5H12	000463-82-1	72
2	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	72
3	Butane, 2-bromo-	136	C4H9Br	000078-76-2	39
4	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	36
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	9





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Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

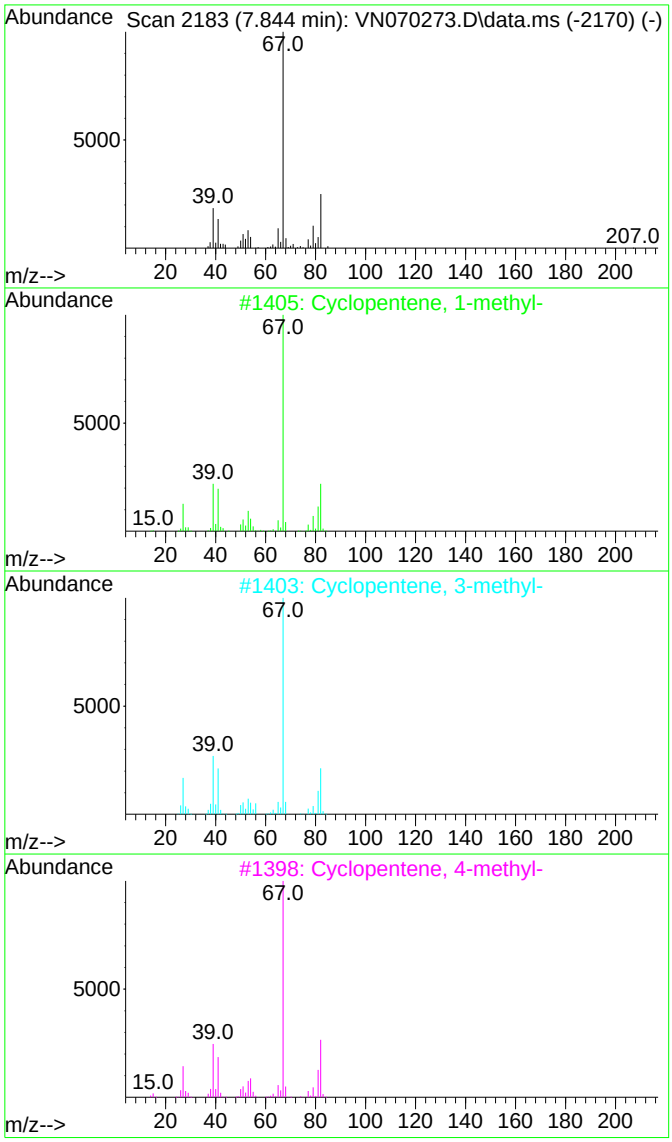
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

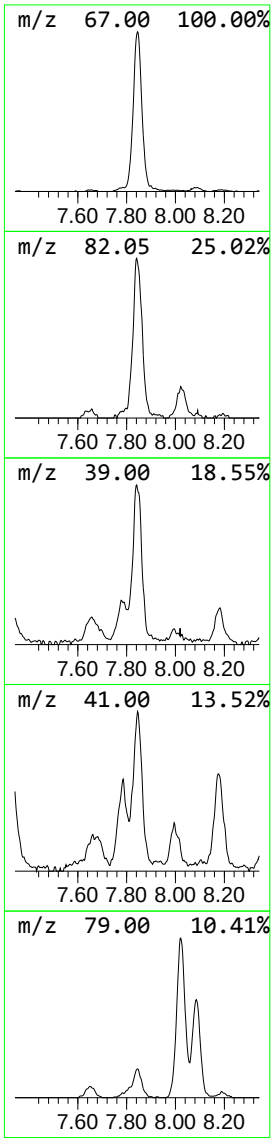
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.844	6.67 ug/l	333815	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	83
2	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	80
3	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	80
4	Cyclopentane, methylene-	82	C6H10	001528-30-9	64
5	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

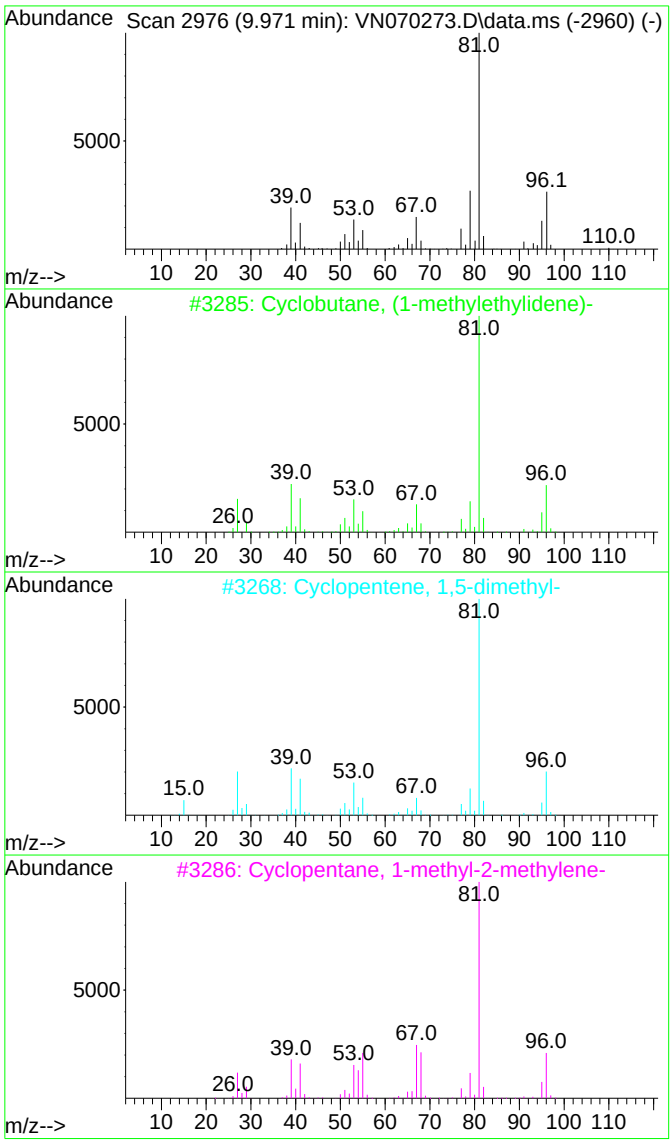
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

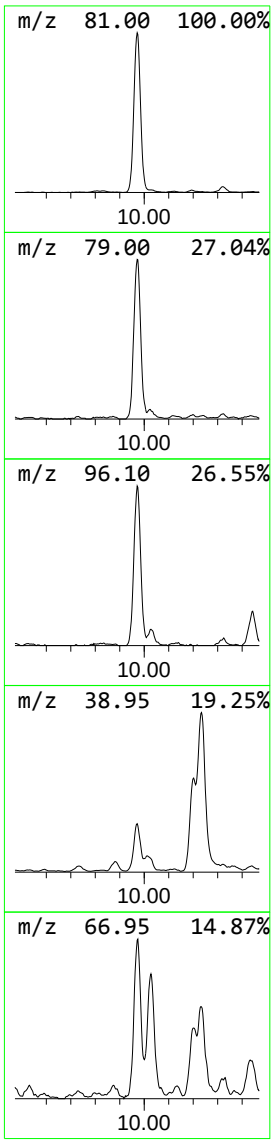
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclobutane, (1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.971	12.02 ug/l	958923	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	90
3	Cyclopentane, 1-methyl-2-methylene-	96	C7H12	041158-41-2	72
4	2,3-Dimethyl-1,4-pentadiene	96	C7H12	000758-86-1	72
5	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

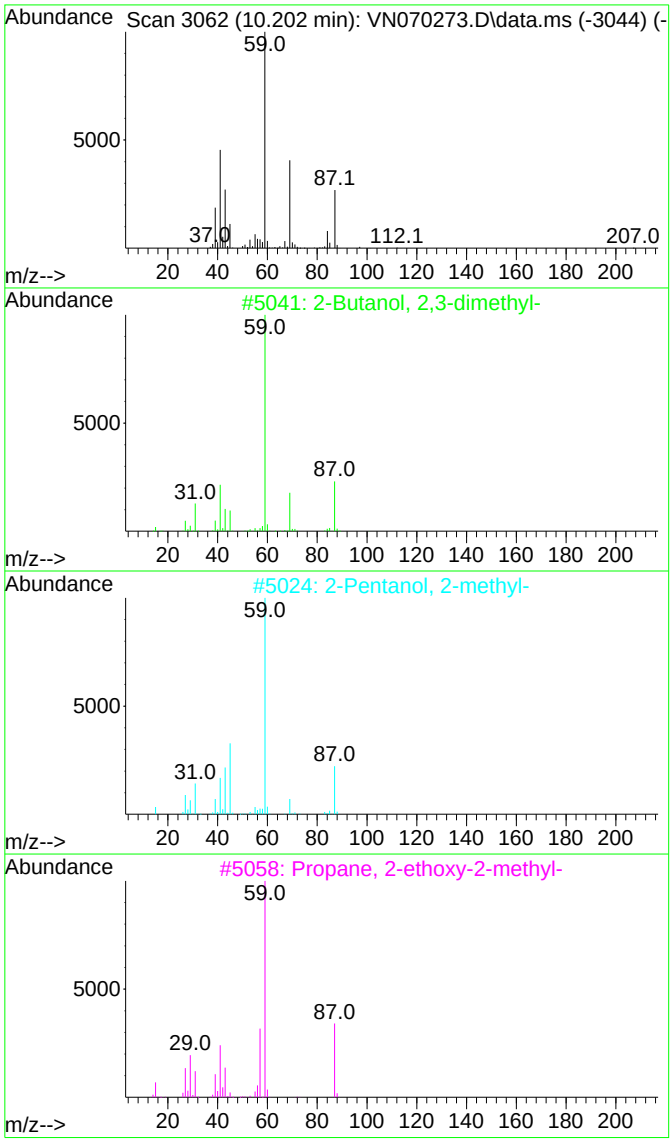
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

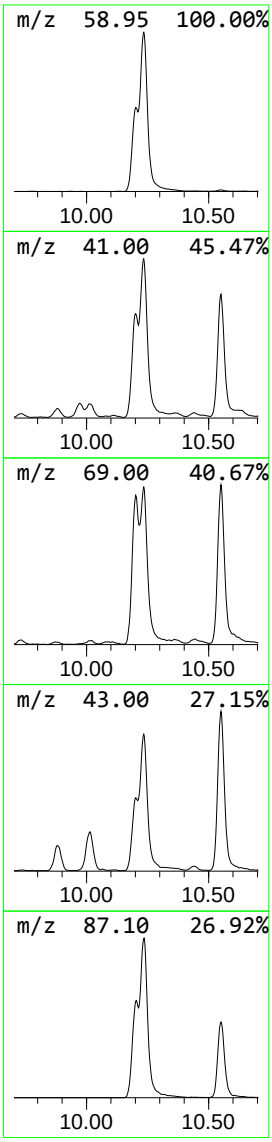
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.202	20.82 ug/l	1661070	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	42
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

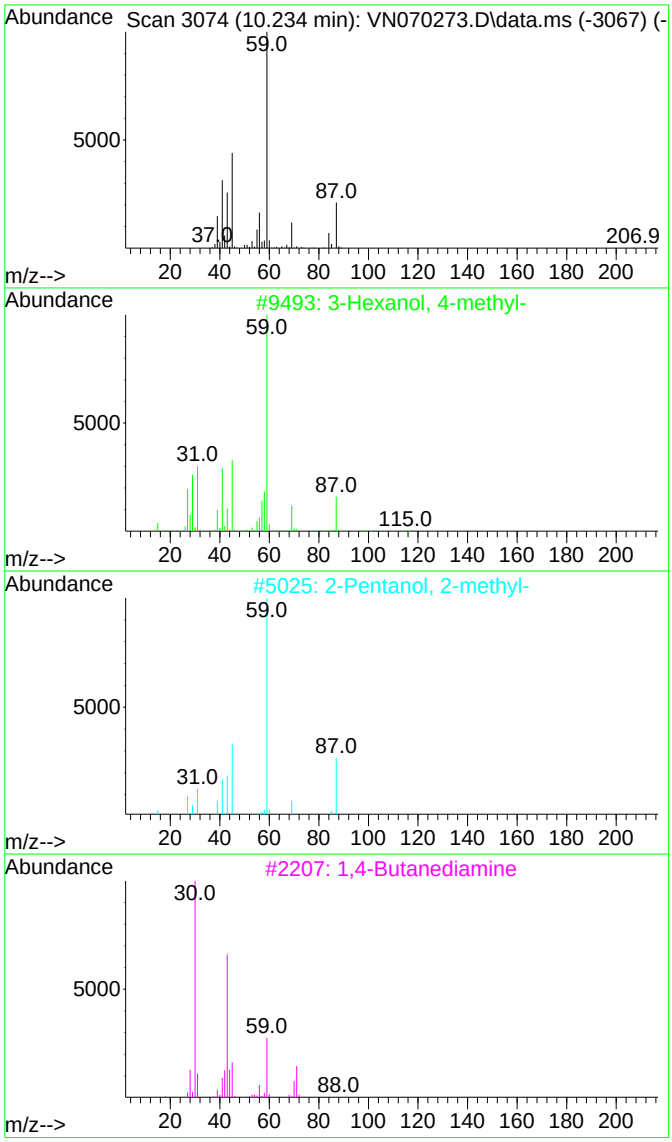
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

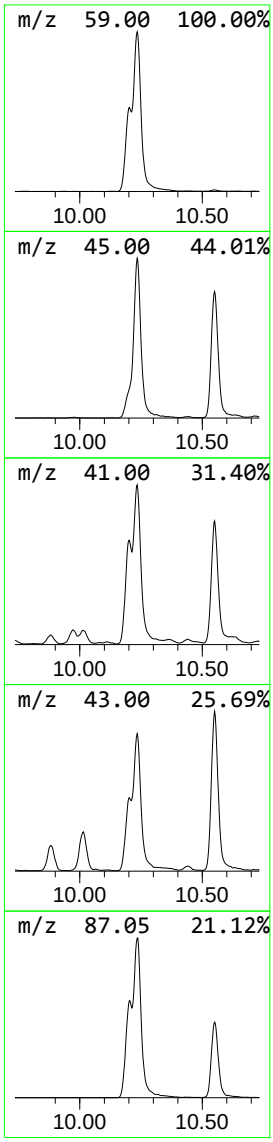
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Hexanol, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.234	46.33 ug/l	3696740	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	42
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	40
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	37





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

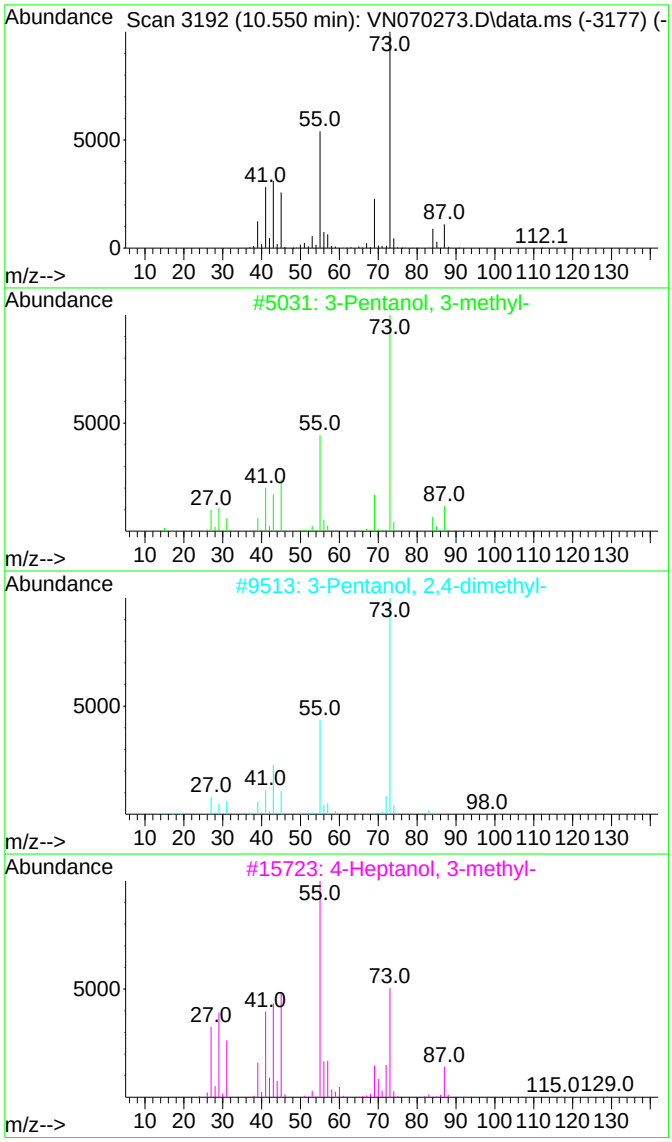
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

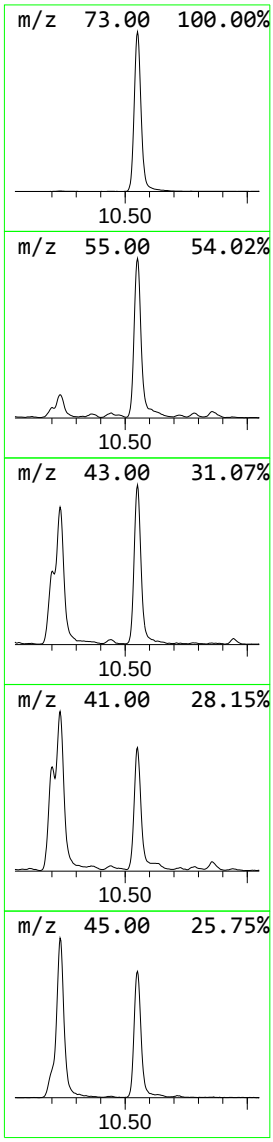
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.550	35.29 ug/l	3998140	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	42
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37





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Operator : JC/MD
Sample : M5039-10
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

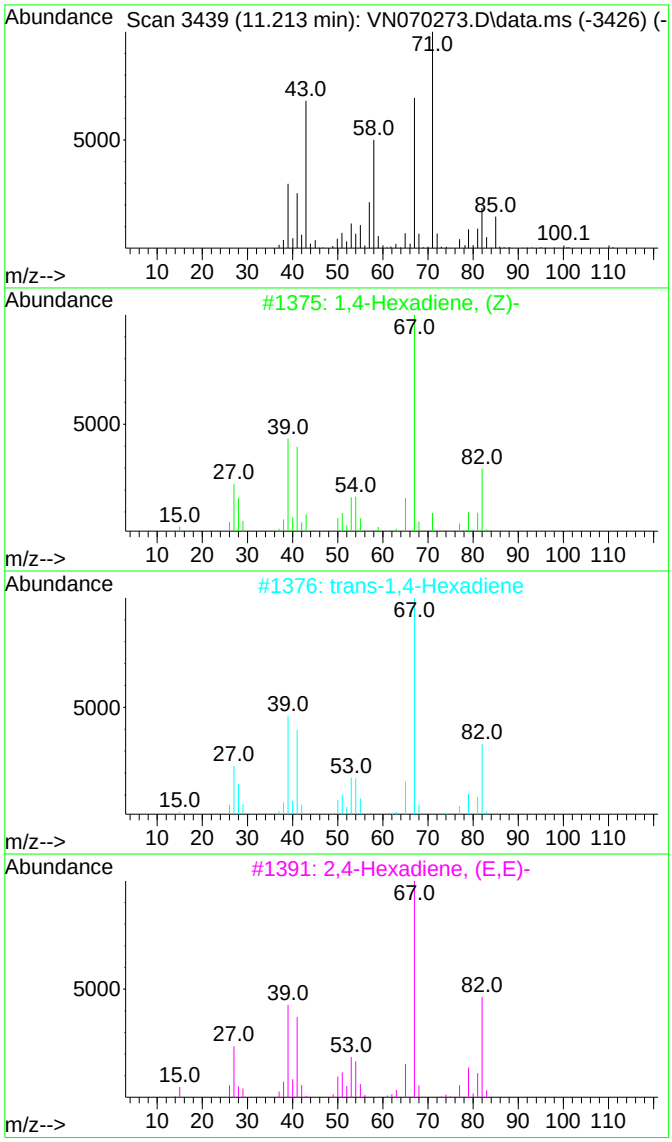
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

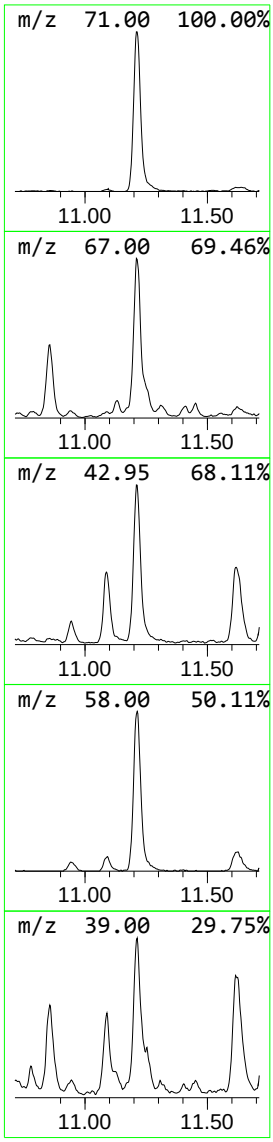
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown11.213 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.213	7.94 ug/l	899111	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Hexadiene, (Z)-	82	C6H10	007318-67-4	38
2	trans-1,4-Hexadiene	82	C6H10	007319-00-8	30
3	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	25
4	2,4-Hexadiene, (E,Z)-	82	C6H10	005194-50-3	25
5	(Z),(Z)-2,4-Hexadiene	82	C6H10	006108-61-8	25





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Sample : M5039-10
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

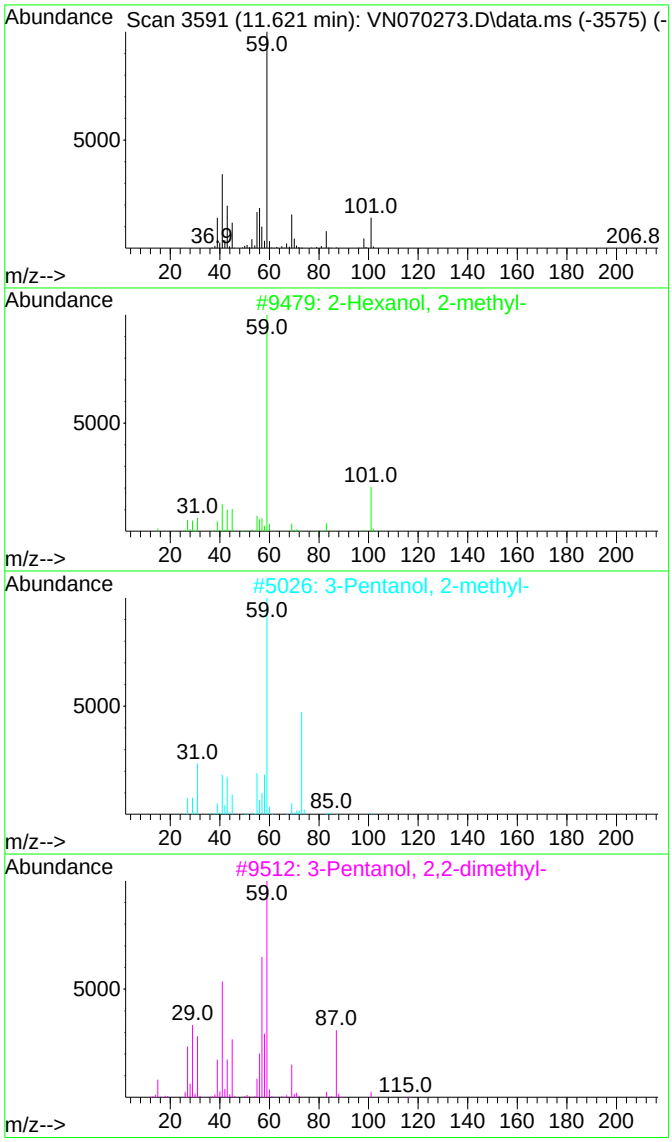
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

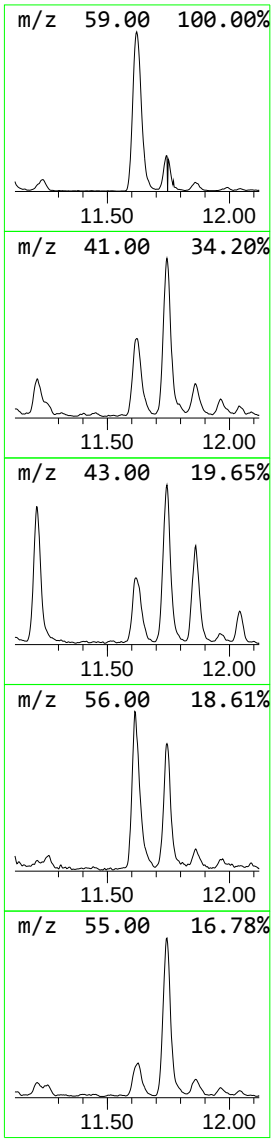
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Hexanol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.621	7.71 ug/l	873651	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	72
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	59
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	53
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	50
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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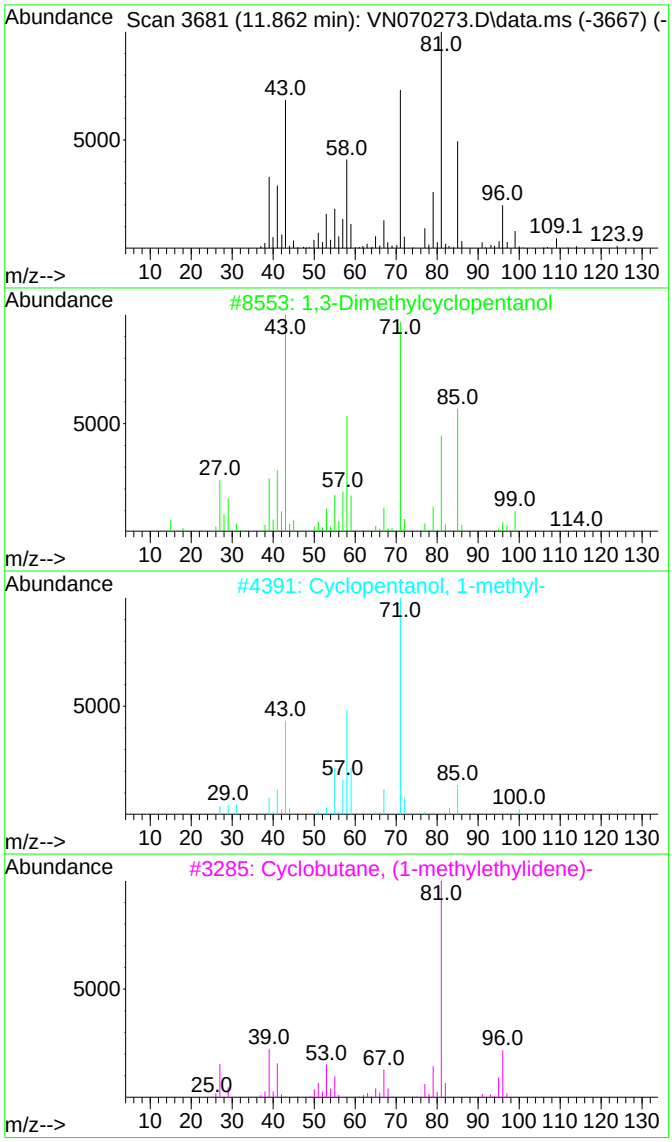
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

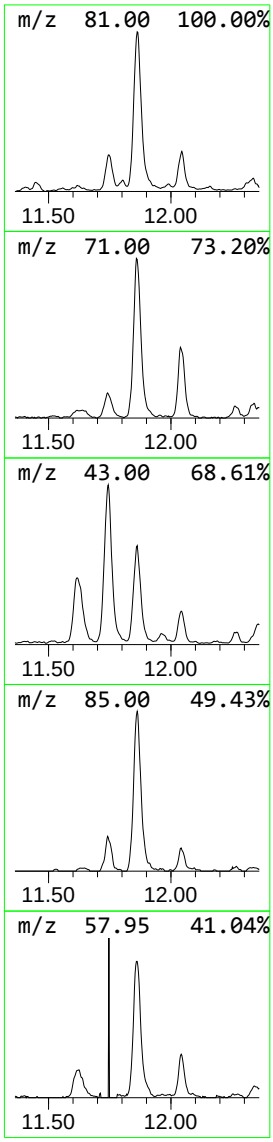
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,3-Dimethylcyclopentanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.862	6.02 ug/l	682432	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	90
2	Cyclopentanol, 1-methyl-	100	C6H12O	001462-03-9	27
3	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	25
4	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	25
5	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070273.D
Acq On : 21 Dec 2021 17:34
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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
Neopentane	2.537	7.9	ug/l	394194	1	8.086	2503560	50.0
Cyclopentene, 1...	7.844	6.7	ug/l	333815	1	8.086	2503560	50.0
Cyclobutane, (1...	9.971	12.0	ug/l	958923	2	8.968	3989830	50.0
2-Butanol, 2,3-...	10.202	20.8	ug/l	1661070	2	8.968	3989830	50.0
3-Hexanol, 4-me...	10.234	46.3	ug/l	3696740	2	8.968	3989830	50.0
3-Pentanol, 3-m...	10.550	35.3	ug/l	3998140	3	11.744	5664590	50.0
unknown11.213	11.213	7.9	ug/l	899111	3	11.744	5664590	50.0
2-Hexanol, 2-me...	11.621	7.7	ug/l	873651	3	11.744	5664590	50.0
1,3-Dimethylcyc...	11.862	6.0	ug/l	682432	3	11.744	5664590	50.0