LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

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\82N031824W.M
Title : SW846 8260

Signal : TIC: VN081730.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.024	9	12	30	rVB	341969	730155	6.01%	1.203%
2	2.289	52	57	67	rVB	145802	266867	2.20%	0.440%
3	2.818	140	147	161	rVB2	128197	363071	2.99%	0.598%
4	4.418	405	419	432	rBV	901364	2726706	22.46%	4.491%
5	5.512	589	605	631	rBV	2631375	9264714	76.31%	15.260%
6	7.435	918	932	938	rBV	4284136	12140218	100.00%	19.996%
7	7.835	983	1000	1018	rBV	1360287	3498034	28.81%	5.762%
8	8.165	1046	1056	1060	rBV	268152	618018	5.09%	1.018%
9	8.224	1060	1066	1081	rVB	557839	1277382	10.52%	2.104%
10	8.582	1113	1127	1135	rBV2	293694	850701	7.01%	1.401%
11	8.665	1135	1141	1157	rVB7	149990	497570	4.10%	0.820%
12	9.100	1206	1215	1228	rBV	786652	1632424	13.45%	2.689%
13	10.441	1433	1443	1451	rBV3	51512	131197	1.08%	0.216%
14	10.571	1457	1465	1471	rBV	1012921	1866747	15.38%	3.075%
15	10.635	1471	1476	1488	rVB3	149677	427944	3.53%	0.705%
16	11.171	1557	1567	1578	rBV	246845	480347	3.96%	0.791%
17	11.776	1662	1670	1675	rVV5	49201	137755	1.13%	0.227%
18	11.865	1675	1685	1694	rVV	1096233	2126895	17.52%	3.503%
19	11.965	1694	1702	1708	rVV3	126683	296666	2.44%	0.489%
20	12.070	1710	1720	1730	rVB2	169137	445413	3.67%	0.734%
21	12.400	1765	1776	1781	rBV2	127307	250286	2.06%	0.412%
22	12.853	1845	1853	1860	rVB	709705	1270002	10.46%	2.092%
23	13.194	1903	1911	1919	rVB7	68821	165328	1.36%	0.272%
24	13.482	1948	1960	1974	rVB3	85813	246583	2.03%	0.406%
25	13.612	1974	1982	1987	rBV3	111557	218356	1.80%	0.360%
26	13.729	1997	2002	2006	rBV	114929	181190	1.49%	0.298%
27	13.794	2006	2013	2020	rVV	1076999	1952183	16.08%	3.215%
28	13.859	2020	2024	2036	rVB3	329447	669549	5.52%	1.103%
29	14.000	2042	2048	2061	rVB4	67351	158304	1.30%	0.261%
30	14.247	2084	2090	2094	rBV2	242513	432837	3.57%	0.713%
31	14.300	2094	2099	2110	rVB	598984	1083152	8.92%	1.784%
32	14.447	2115	2124	2133	rBV5	84317	222820	1.84%	0.367%
33	14.676	2157	2163	2169	rVV	1675037	2764866	22.77%	4.554%
34	14.935	2202	2207	2215	rBV7	87343	174897	1.44%	0.288%
35	15.023	2217	2222	2227	rBV7	69530	138852	1.14%	0.229%
36	15.100	2229	2235	2241	rVV	260601	445095	3.67%	0.733%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

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\82N031824W.M
Title : SW846 8260

37	15.206	2243	2253	2258	rVB6	62192	163067	1.34%	0.269%
38	15.276	2258	2265	2267	rBV5	220934	492369	4.06%	0.811%
39	15.329	2268	2274	2290	rVB2	2994335	7399455	60.95%	12.187%
40	15.517	2301	2306	2312	rVB2	216245	363716	3.00%	0.599%
41	15.641	2317	2327	2335	rVB	527371	1093689	9.01%	1.801%
42	15.800	2350	2354	2371	rVB4	109919	300551	2.48%	0.495%
43	16.011	2382	2390	2401	rBV2	336791	747835	6.16%	1.232%

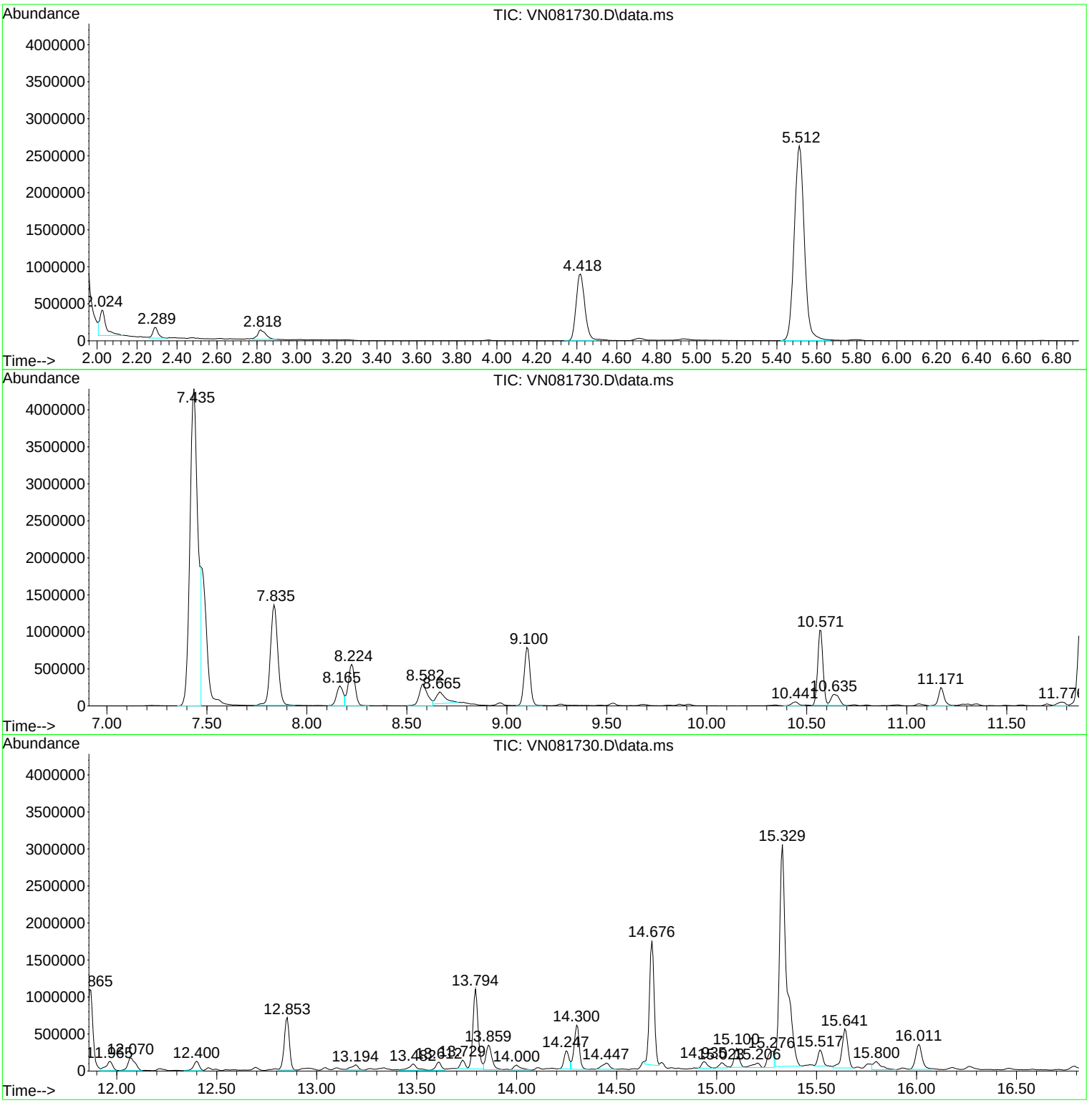
Sum of corrected areas: 60713806

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

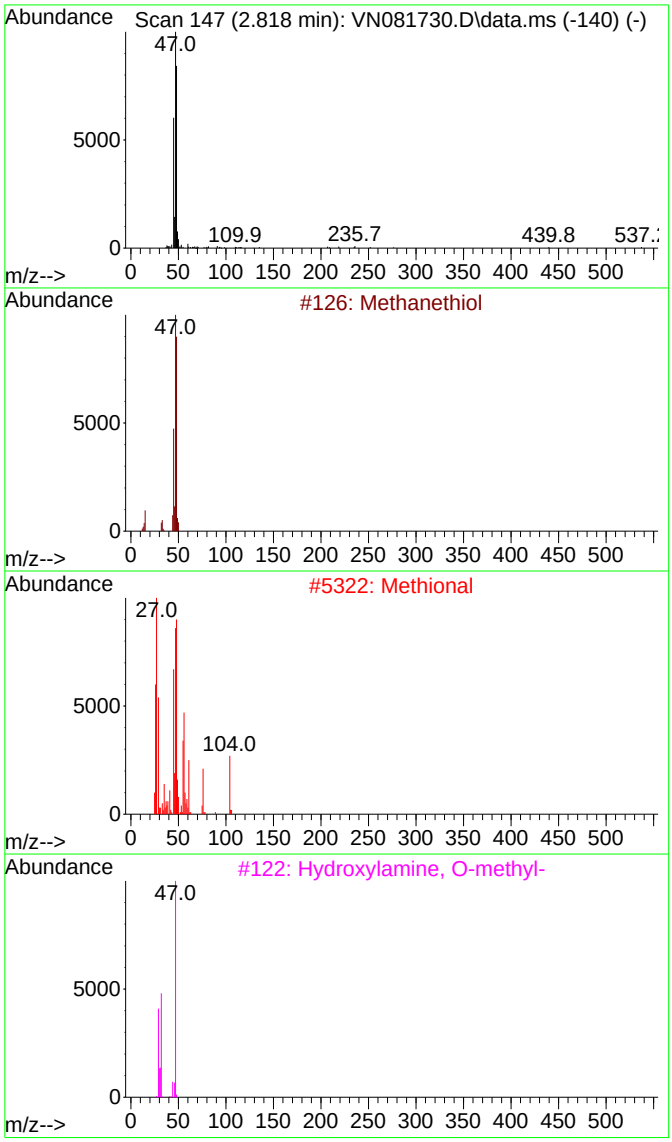
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

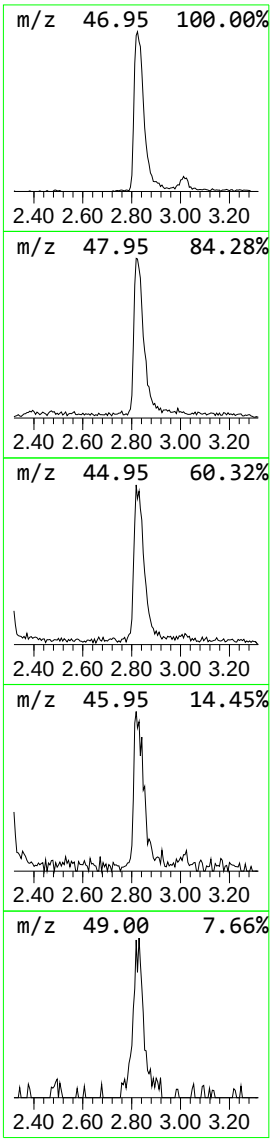
****

Peak Number 2 Methanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.818	14.21 ug/l	363071	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Methional	104	C4H8OS	003268-49-3	9
3	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	5
4	Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	5
5	Methane, nitroso-	45	CH3NO	000865-40-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

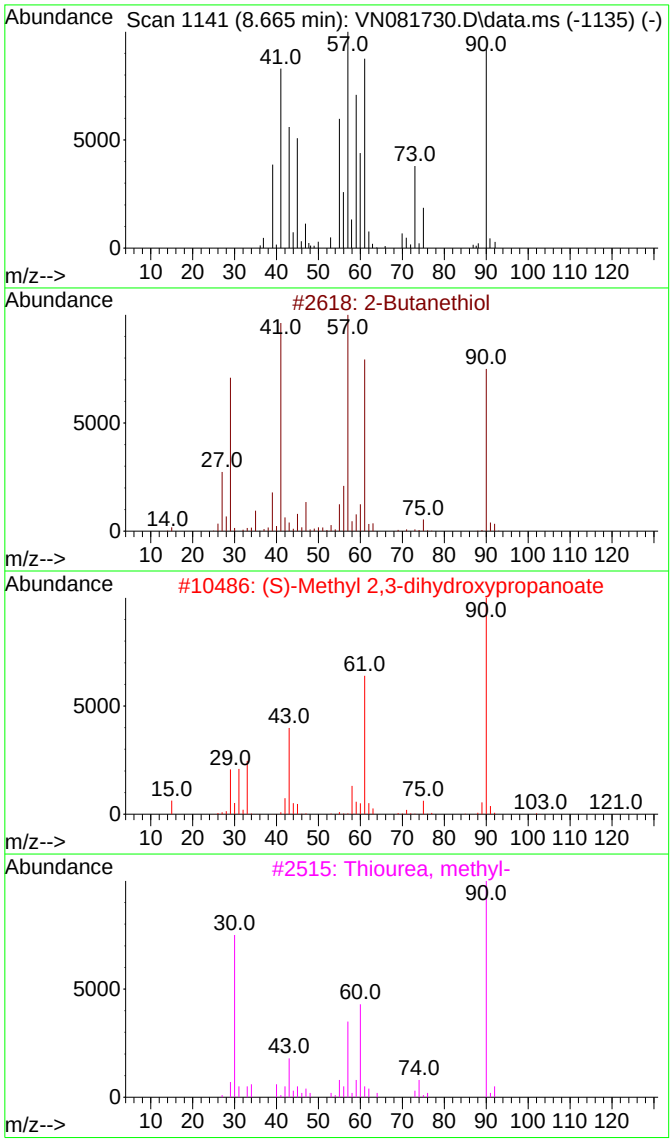
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

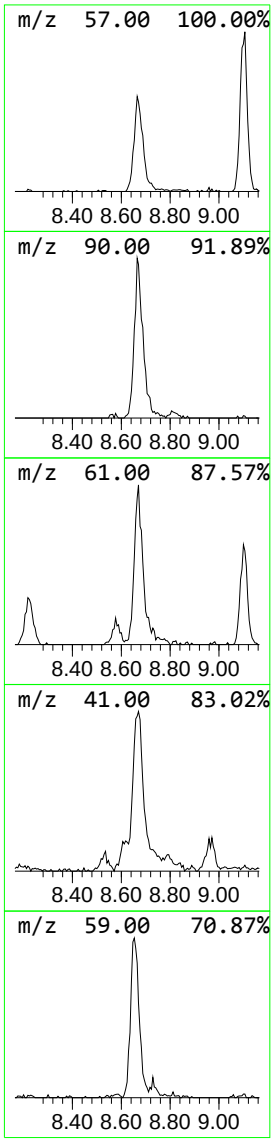
****

Peak Number 3 2-Butanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.665	15.24 ug/l	497570	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanethiol	90	C4H10S	000513-53-1	76
2	(S)-Methyl 2,3-dihydroxypropanoate	120	C4H8O4	010303-88-5	53
3	Thiourea, methyl-	90	C2H6N2S	000598-52-7	40
4	3-Thietanol	90	C3H6OS	010304-16-2	40
5	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

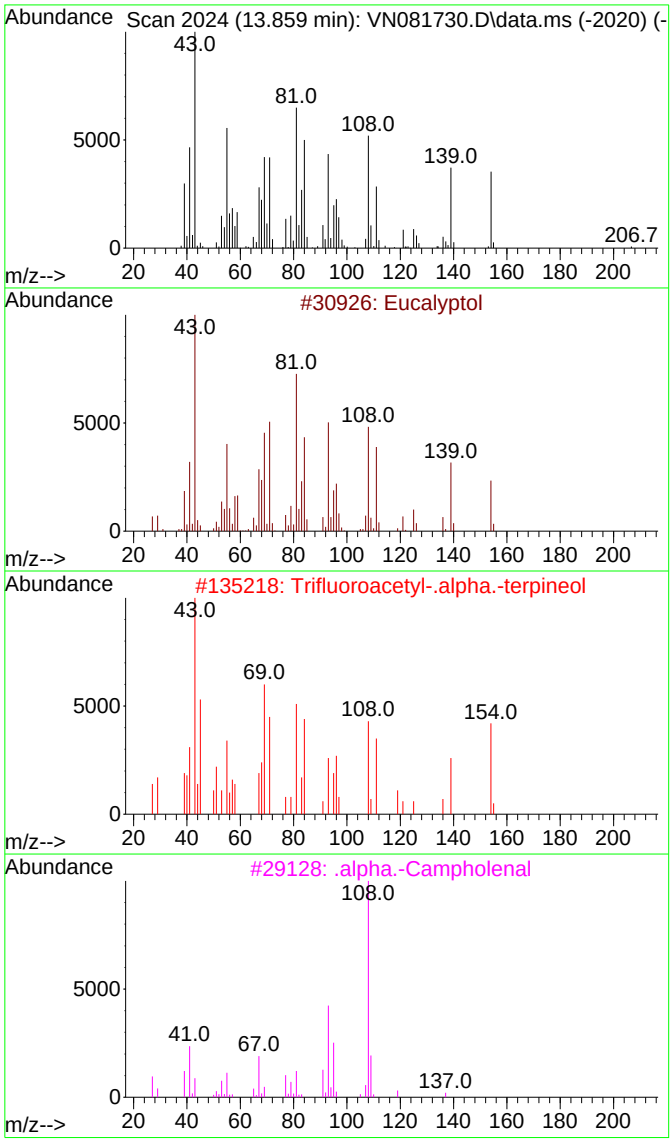
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

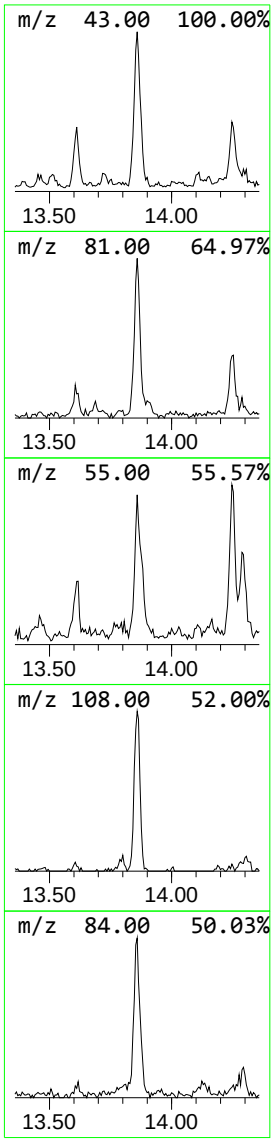
****

Peak Number 4 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	17.15 ug/l	669549	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	91
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	86
3	.alpha.-Campholenal	152	C10H16O	004501-58-0	22
4	3-Cyclohexene-1-methanol, 6-methyl-	126	C8H14O	005259-31-4	22
5	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

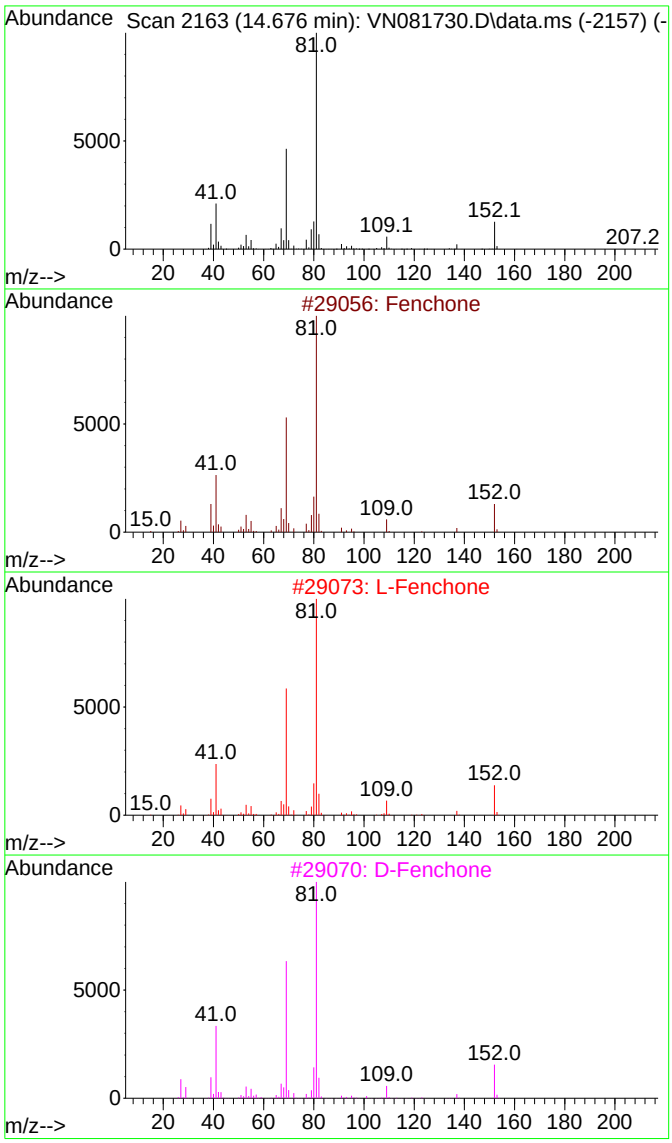
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

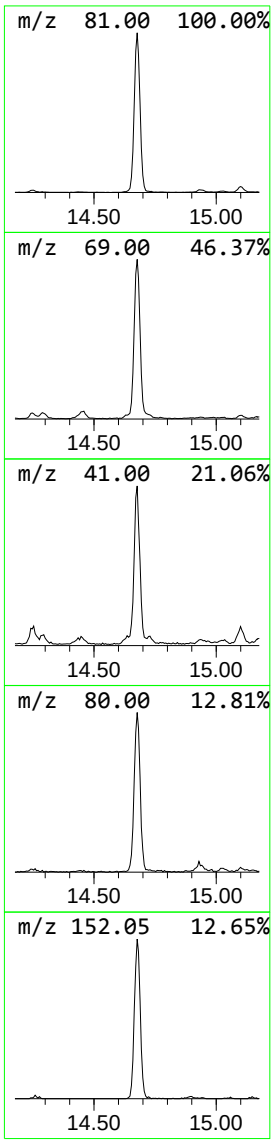
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	70.81 ug/l	2764870	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fenchone	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	94
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	38
5	Formic acid, cis-4-methylcyclohe...	142	C8H14O2	1000368-24-7	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

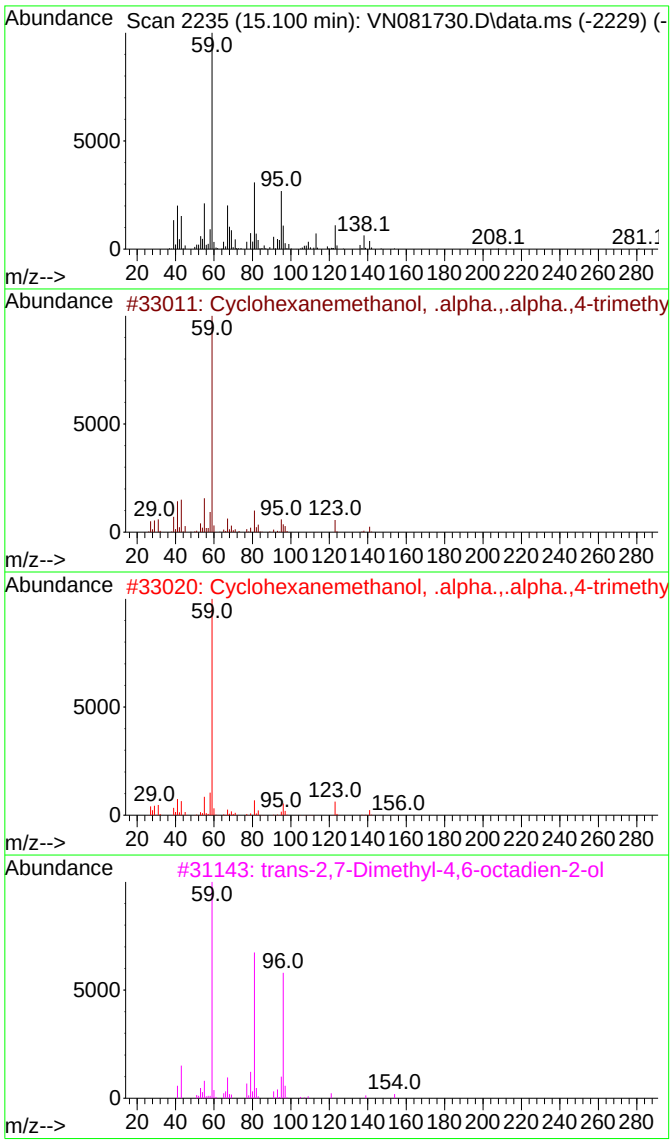
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

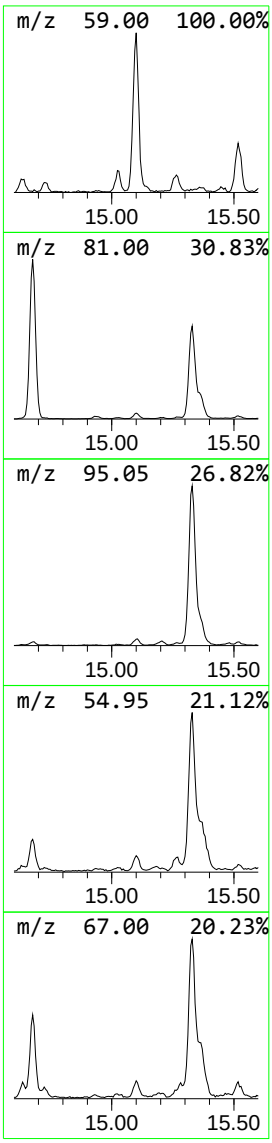
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	11.40 ug/l	445095	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	50
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	50
3	trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1010281-69-5	47
4	Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	42
5	Succinic acid, tridec-2-yn-1-yl ...	354	C20H34O5	1000390-75-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

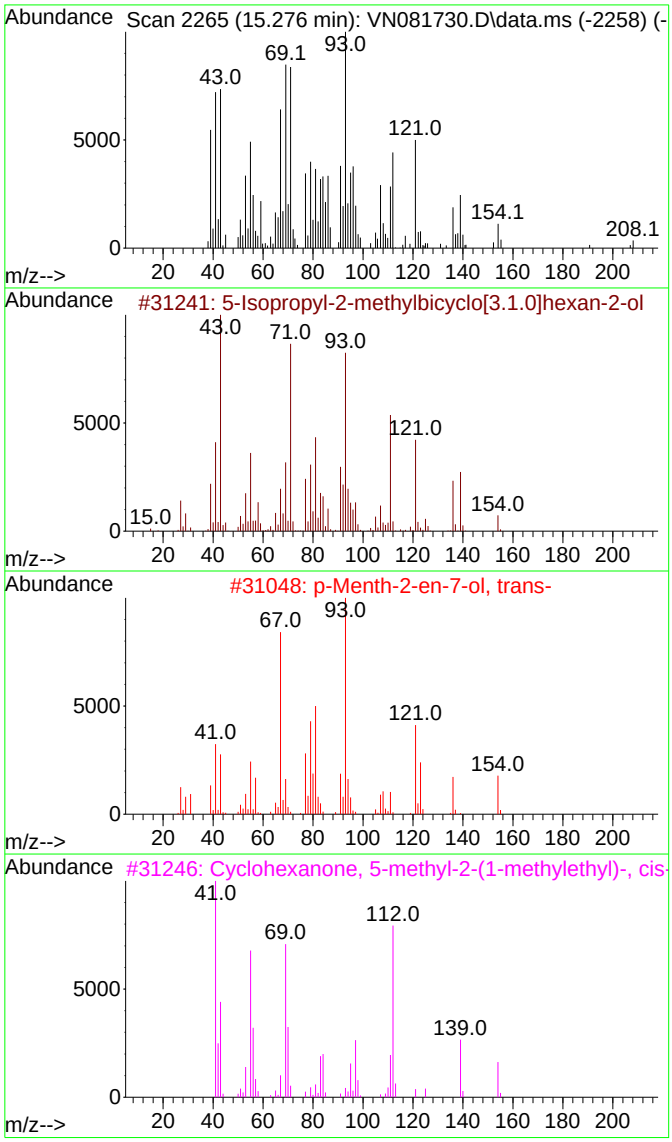
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

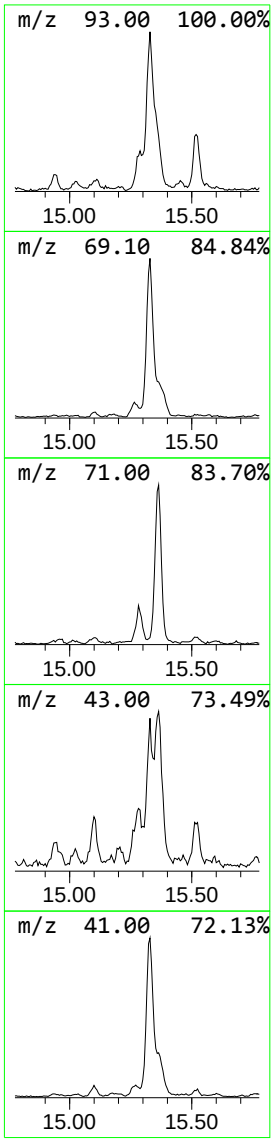
****

Peak Number 8 unknown15.276 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.276	12.61 ug/l	492369	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Isopropyl-2-methylbicyclo[3.1....	154	C10H18O	000546-79-2	43
2	p-Menth-2-en-7-ol, trans-	154	C10H18O	019898-87-4	25
3	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	25
4	Camphene	136	C10H16	000079-92-5	25
5	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

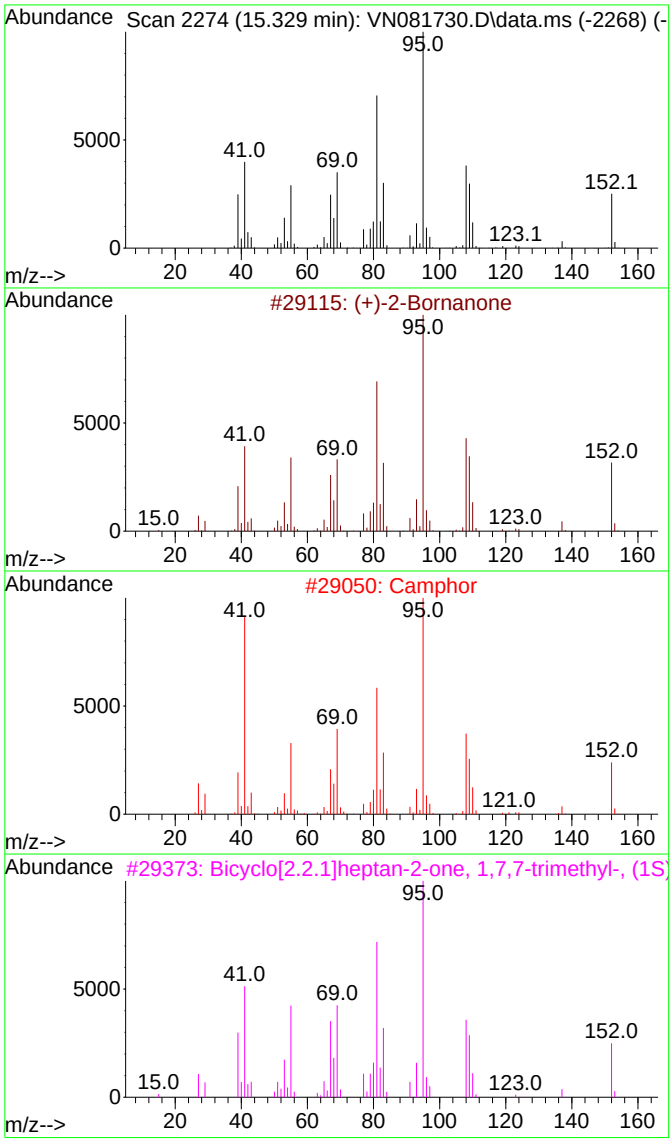
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

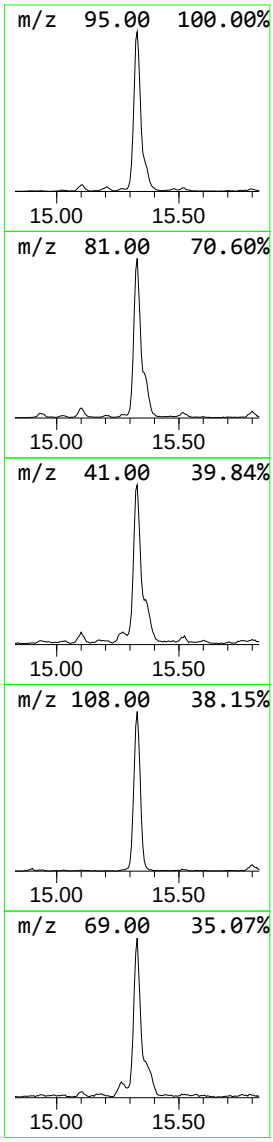
****

Peak Number 9 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.329	189.52 ug/l	7399460	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	52
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

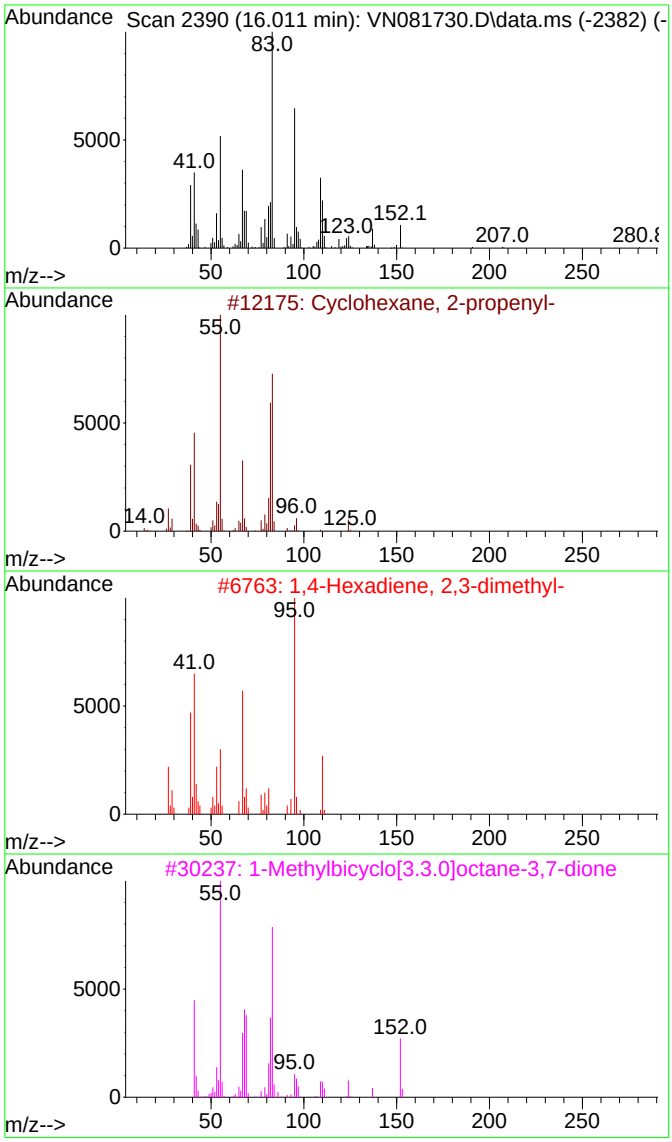
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

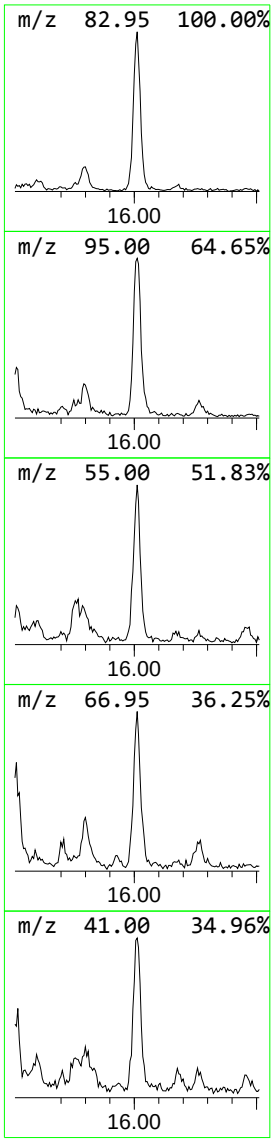
****

Peak Number 10 unknown16.011 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.011	19.15 ug/l	747835	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43
2	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	42
3	1-Methylbicyclo[3.3.0]octane-3,7...	152	C9H12O2	021170-08-1	38
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	35
5	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
Data File : VN081730.D
Acq On : 12 Apr 2024 20:07
Operator : JC\MD
Sample : P2075-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240410102-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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
Methanethiol	2.818	14.2	ug/l	363071	1	8.224	1277380	50.0
2-Butanethiol	8.665	15.2	ug/l	497570	2	9.100	1632420	50.0
Eucalyptol	13.859	17.1	ug/l	669549	4	13.794	1952180	50.0
Fenchone	14.676	70.8	ug/l	2764870	4	13.794	1952180	50.0
Cyclohexanemeth...	15.100	11.4	ug/l	445095	4	13.794	1952180	50.0
unknown15.276	15.276	12.6	ug/l	492369	4	13.794	1952180	50.0
(+)-2-Bornanone	15.329	189.5	ug/l	7399460	4	13.794	1952180	50.0
unknown16.011	16.011	19.1	ug/l	747835	4	13.794	1952180	50.0