LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

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_X\Method\82X051123W.M
Title : SW846 8260

Signal : TIC: VX035792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.294	193	198	209	rVB	56375	95711	4.41%	0.965%
2	5.385	692	705	720	rBV2	132519	392778	18.08%	3.960%
3	5.550	720	732	744	rBV	220614	632949	29.14%	6.381%
4	5.958	788	799	818	rBV	169443	453745	20.89%	4.574%
5	6.763	920	931	943	rBV	356989	859587	39.57%	8.665%
6	7.123	982	990	1004	rBV	113664	252489	11.62%	2.545%
7	7.574	1056	1064	1075	rBV	91080	186788	8.60%	1.883%
8	8.647	1233	1240	1250	rBV	722887	1105917	50.91%	11.149%
9	9.275	1336	1343	1351	rBV	137242	203251	9.36%	2.049%
10	9.518	1377	1383	1405	rBV	1621798	2172457	100.00%	21.901%
11	10.055	1465	1471	1484	rVB	746000	1017185	46.82%	10.254%
12	10.854	1597	1602	1614	rBV	153008	191525	8.82%	1.931%
13	11.079	1634	1639	1648	rBV	607486	771810	35.53%	7.781%
14	11.616	1724	1727	1733	rBV	18753	25297	1.16%	0.255%
15	11.927	1772	1778	1788	rBV	196397	239021	11.00%	2.410%
16	12.018	1788	1793	1802	rVB	741954	925055	42.58%	9.325%
17	12.591	1882	1887	1900	rBV	53338	83917	3.86%	0.846%
18	12.853	1925	1930	1945	rBV	81842	111447	5.13%	1.123%
19	14.255	2155	2160	2170	rBV	105057	167956	7.73%	1.693%
20	14.993	2274	2281	2290	rBV2	18258	30777	1.42%	0.310%

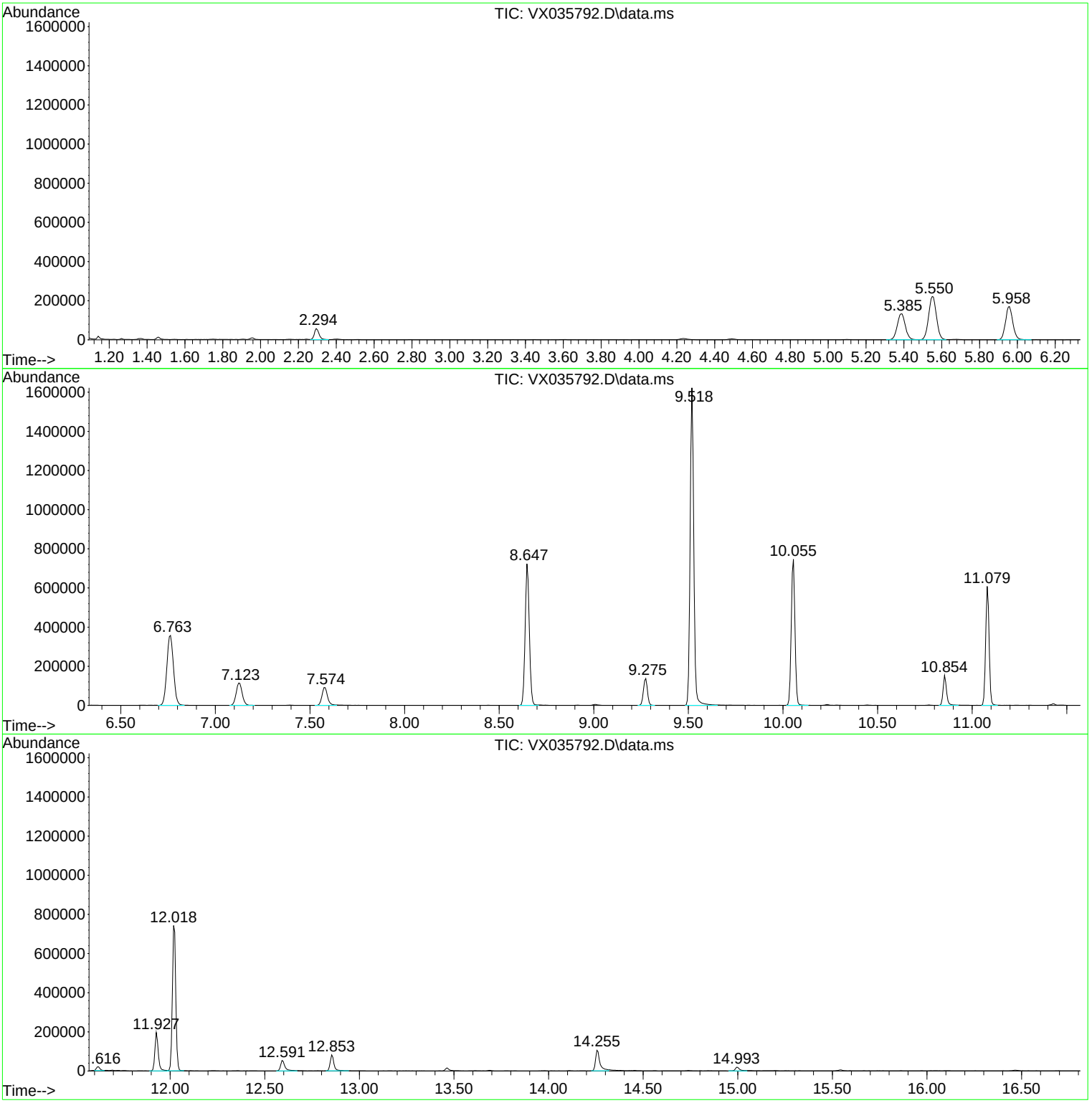
Sum of corrected areas: 9919662

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

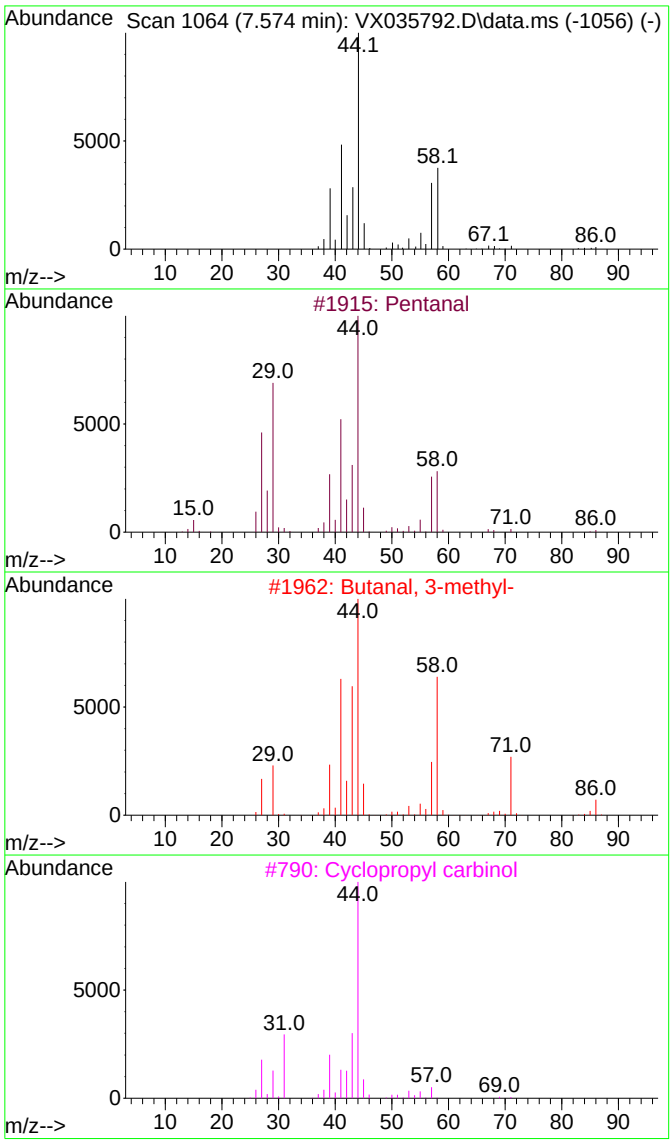
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

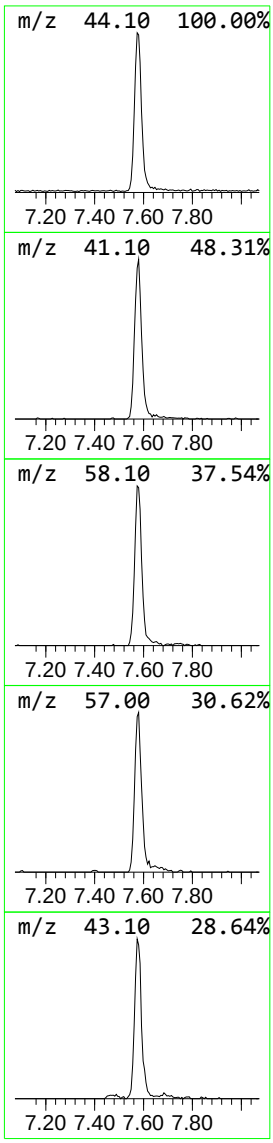
****

Peak Number 1 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	10.87 ug/l	186788	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	87
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	64
4	Glycidol	74	C3H6O2	000556-52-5	38
5	Succindialdehyde	86	C4H6O2	000638-37-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

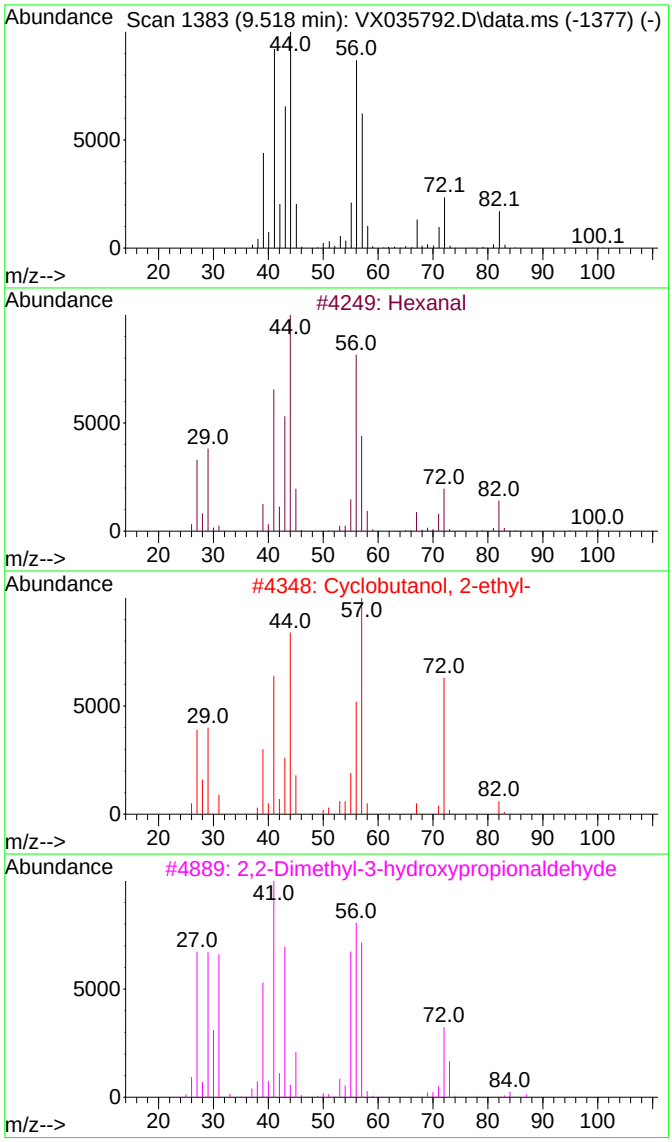
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

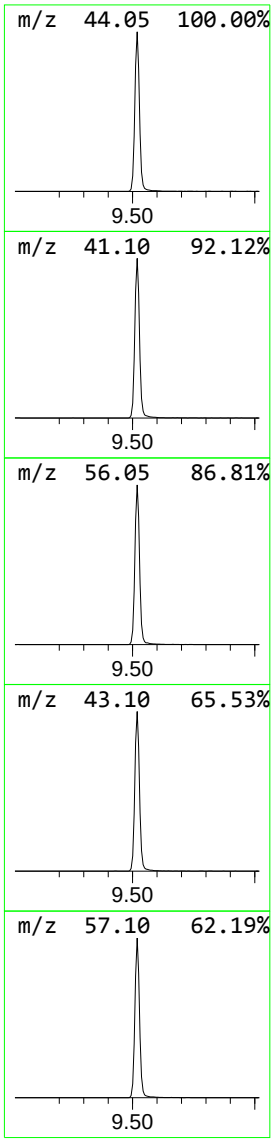
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.518	106.79 ug/l	2172460	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	72
2	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
3	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
4	Glutaraldehyde	100	C5H8O2	000111-30-8	30
5	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

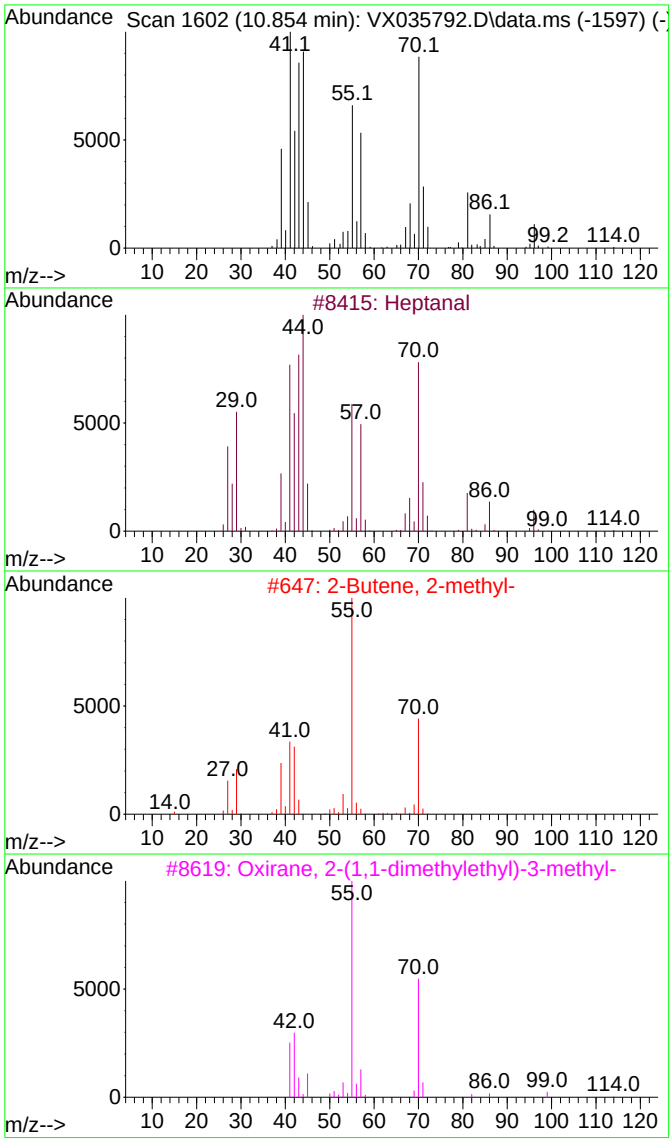
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

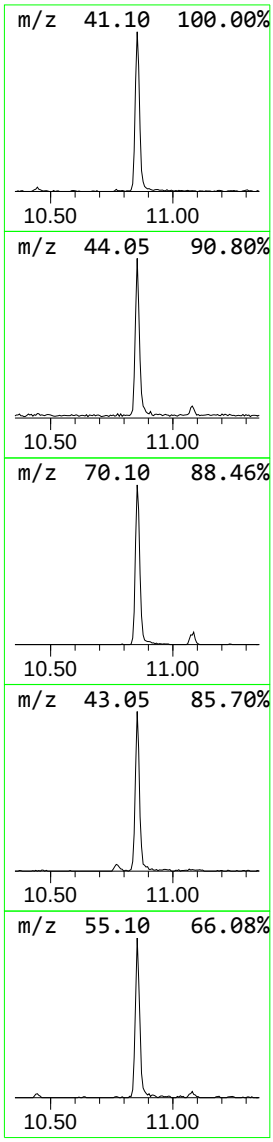
****

Peak Number 3 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	9.41 ug/l	191525	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	96
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	38
3	Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	38
4	2-Methyl-1-butene	70	C5H10	000563-46-2	38
5	Hexanal, 3-methyl-	114	C7H14O	019269-28-4	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

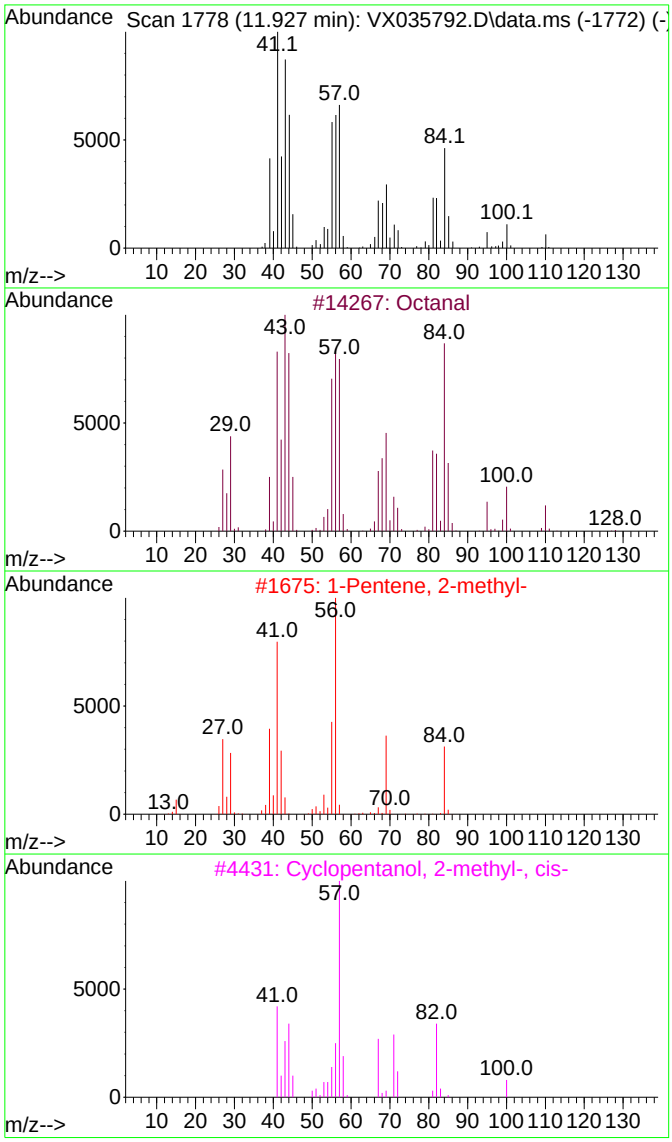
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

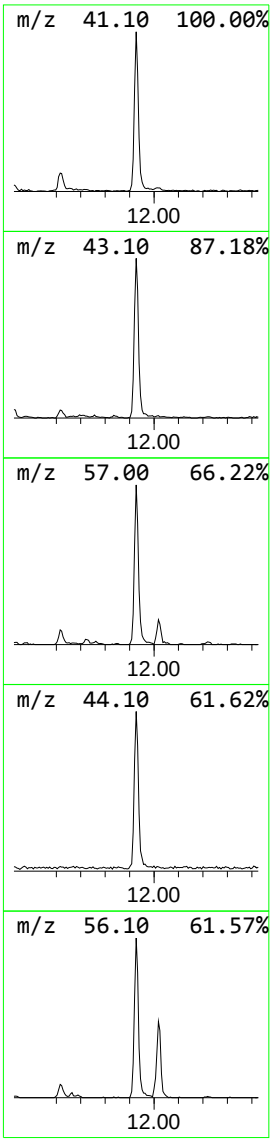
****

Peak Number 4 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	12.92 ug/l	239021	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	83
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	27
3	Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	25
4	Cyclopentanol, 2-methyl-, trans-	100	C6H12O	025144-04-1	25
5	6-Amino-1-hexyl phosphate	197	C6H16NO4P	007564-68-3	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

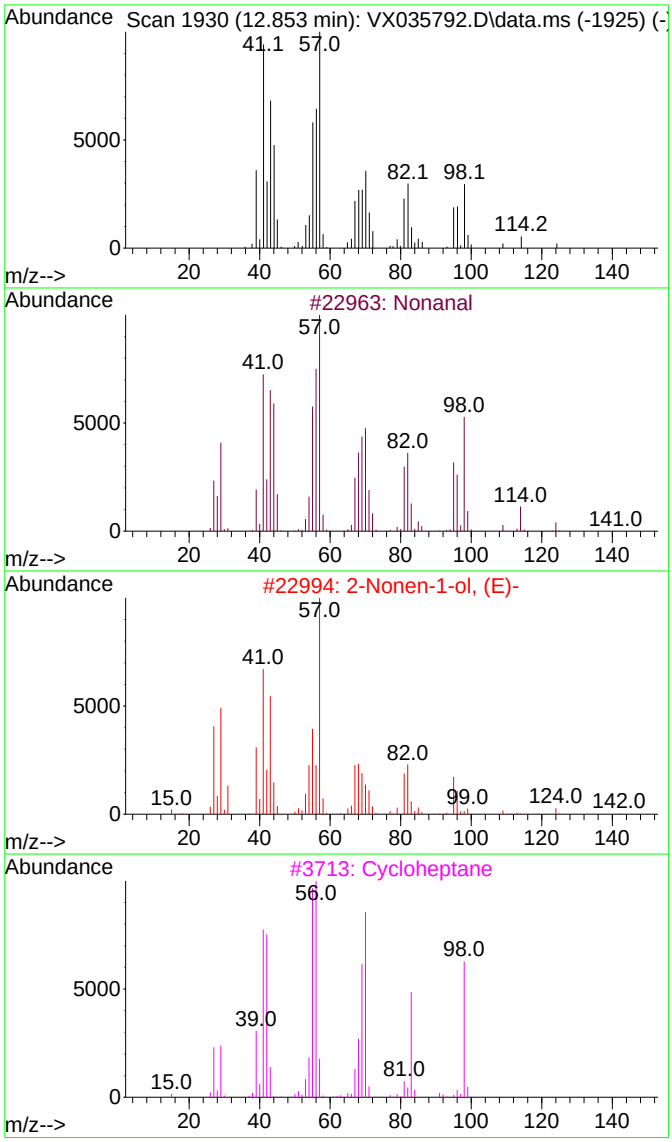
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

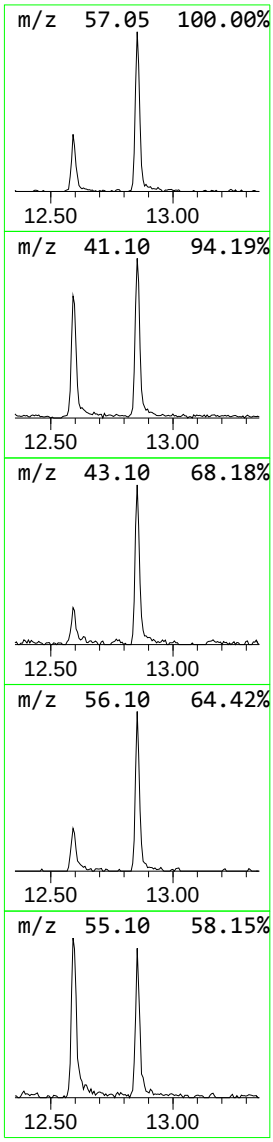
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Nonanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.853	6.02 ug/l	111447	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	83
2	2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	35
3	Cycloheptane	98	C7H14	000291-64-5	35
4	2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	35
5	Cycloheptanol	114	C7H14O	000502-41-0	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

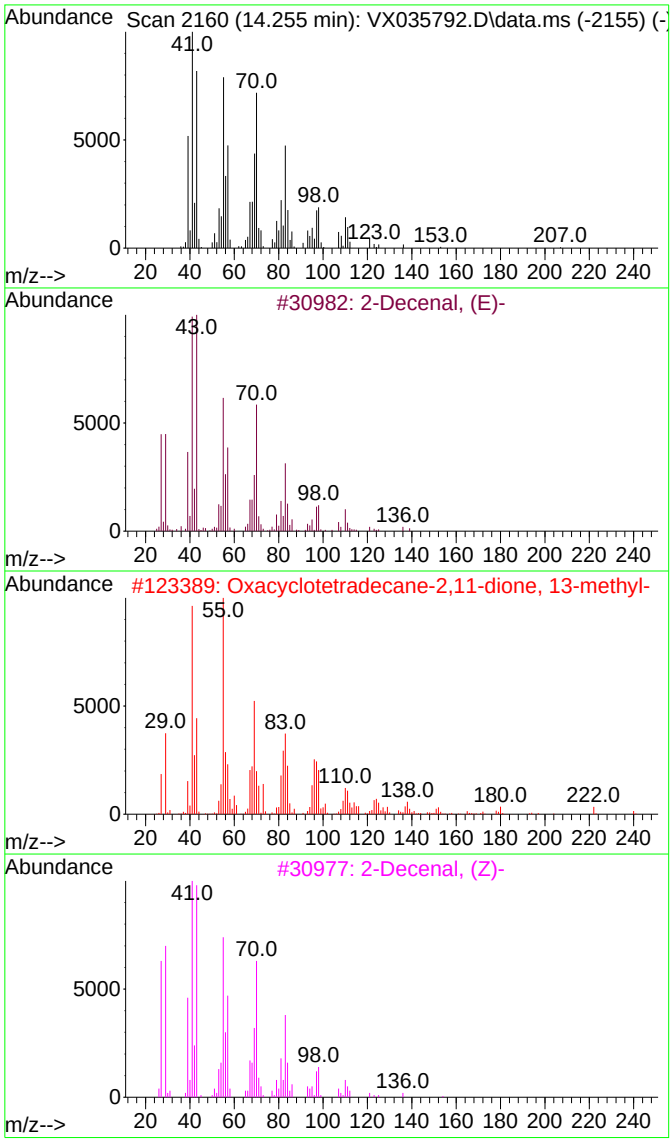
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

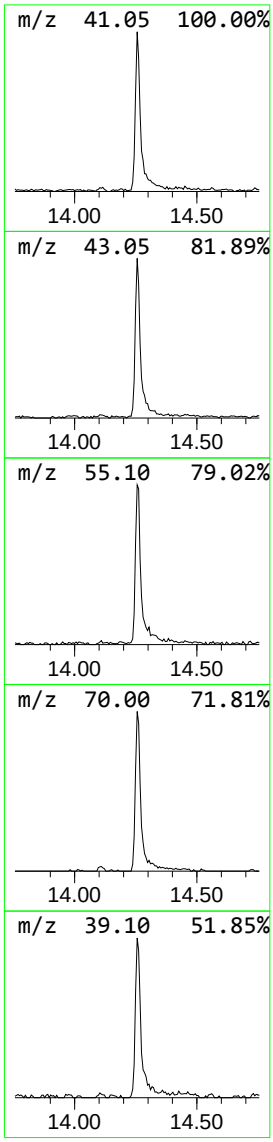
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Decenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.255	9.08 ug/l	167956	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (E)-	154	C10H18O	003913-81-3	64
2	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	58
3	2-Decenal, (Z)-	154	C10H18O	002497-25-8	58
4	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	49
5	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052223\
Data File : VX035792.D
Acq On : 22 May 2023 18:08
Operator : JC/MD
Sample : 02860-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-81-05112023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.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
Pentanal	7.574	10.9	ug/l	186788	2	6.763	859587	50.0
Hexanal	9.518	106.8	ug/l	2172460	3	10.055	1017190	50.0
Heptanal	10.854	9.4	ug/l	191525	3	10.055	1017190	50.0
Octanal	11.927	12.9	ug/l	239021	4	12.024	925055	50.0
Nonanal	12.853	6.0	ug/l	111447	4	12.024	925055	50.0
2-Decenal, (E)-	14.255	9.1	ug/l	167956	4	12.024	925055	50.0