LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

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_Y\methods\82Y010623S.M
Title : SW846 8260

Signal : TIC: VY012115.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	227	235	252	rVB	105973	238433	10.13%	2.470%
2	3.948	340	349	365	rBV	15115	42319	1.80%	0.438%
3	4.716	463	475	484	rBV3	14868	44001	1.87%	0.456%
4	6.990	836	848	856	rBV	11180	30938	1.31%	0.321%
5	7.716	956	967	973	rBV	140018	333678	14.17%	3.457%
6	7.789	973	979	992	rVB	243138	548947	23.31%	5.687%
7	8.143	1027	1037	1050	rBV	129463	291431	12.38%	3.019%
8	8.691	1117	1127	1138	rBV	361232	716500	30.43%	7.423%
9	9.136	1192	1200	1215	rVB	1286542	2354484	100.00%	24.393%
10	9.283	1216	1224	1234	rVB	106309	205695	8.74%	2.131%
11	9.447	1244	1251	1261	rBV	81174	149657	6.36%	1.550%
12	10.179	1363	1371	1380	rBV	601799	1015674	43.14%	10.522%
13	10.606	1431	1441	1452	rBV2	24744	49886	2.12%	0.517%
14	10.831	1469	1478	1489	rBV	101098	162481	6.90%	1.683%
15	10.935	1489	1495	1501	rBV2	29354	49838	2.12%	0.516%
16	11.490	1578	1586	1597	rBV	553906	889127	37.76%	9.211%
17	11.886	1641	1651	1663	rBV	98294	159818	6.79%	1.656%
18	12.105	1680	1687	1697	rBV	234592	391049	16.61%	4.051%
19	12.483	1742	1749	1760	rVB	458197	721489	30.64%	7.475%
20	13.087	1842	1848	1856	rVV	167745	246649	10.48%	2.555%
21	13.166	1856	1861	1866	rVB	91449	131194	5.57%	1.359%
22	13.428	1897	1904	1911	rBV	561184	854260	36.28%	8.850%
23	13.520	1911	1919	1927	rVB4	10010	24876	1.06%	0.258%

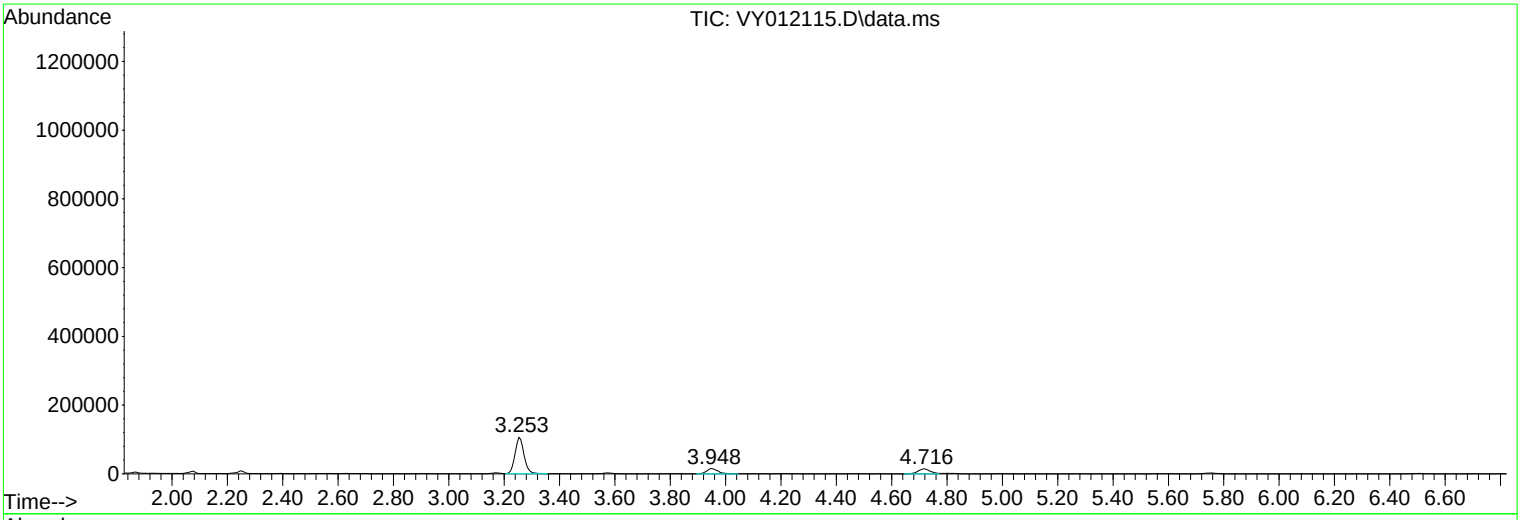
Sum of corrected areas: 9652424

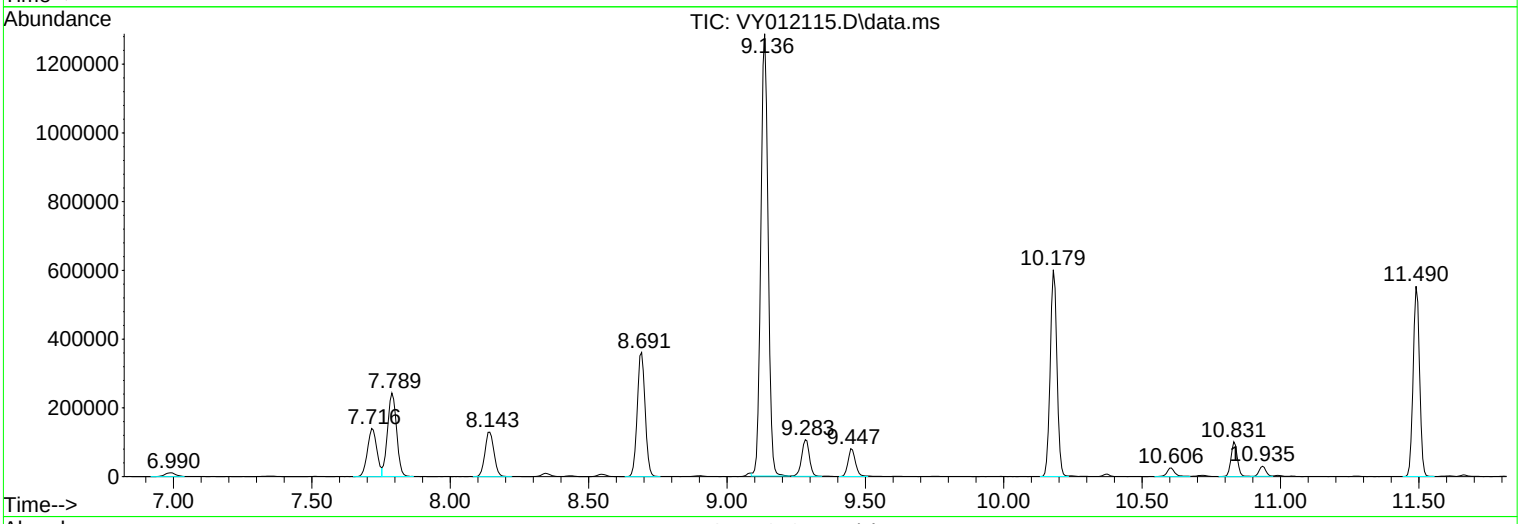
Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

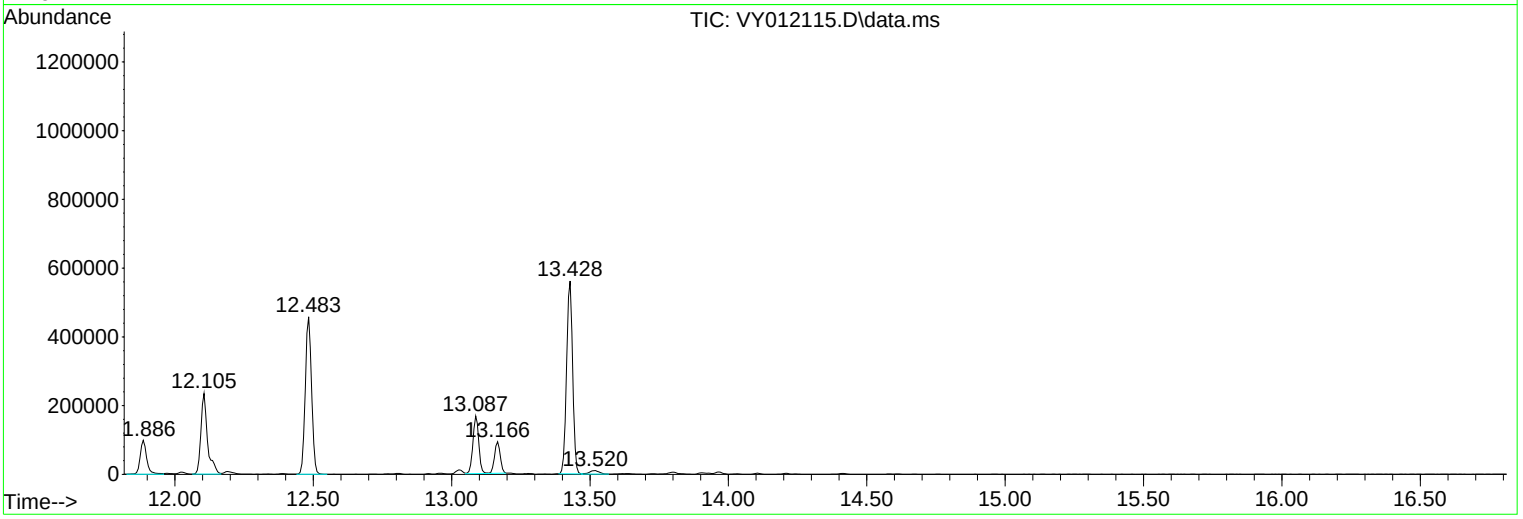
Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

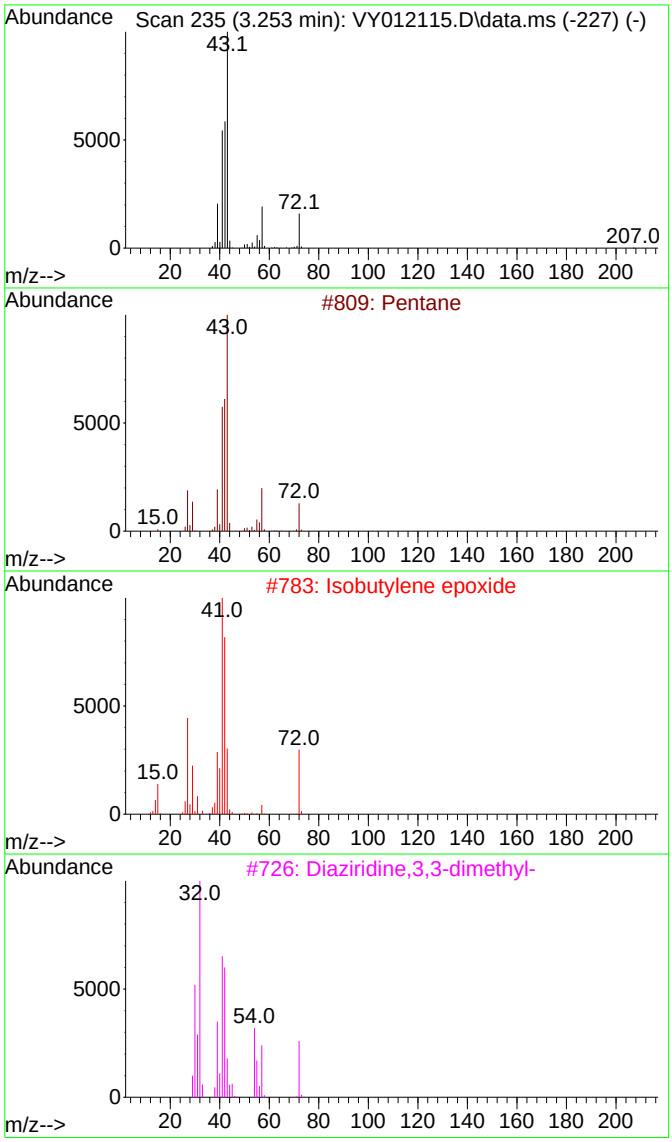
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

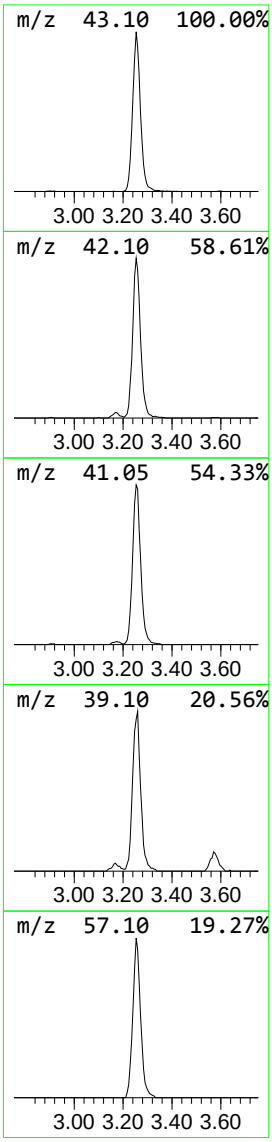
****

Peak Number 1 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.253	21.72 ug/l	238433	Pentafluorobenzene	7.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Isobutylene epoxide	72	C4H8O	000558-30-5	47
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
5	Tetrahydrofuran	72	C4H8O	000109-99-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

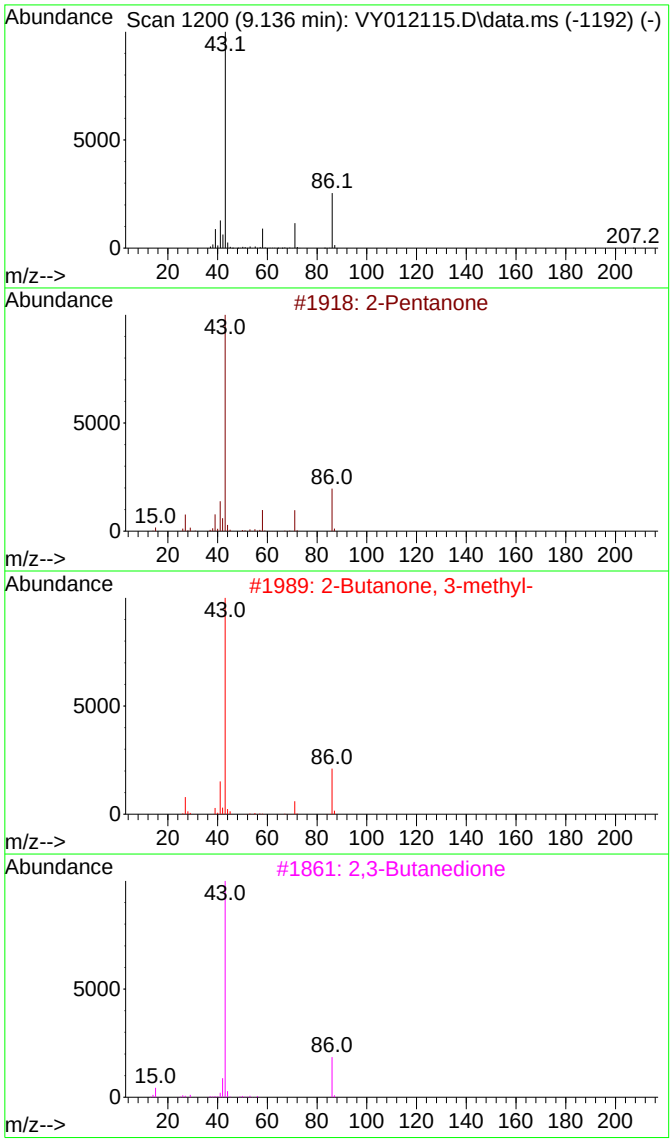
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

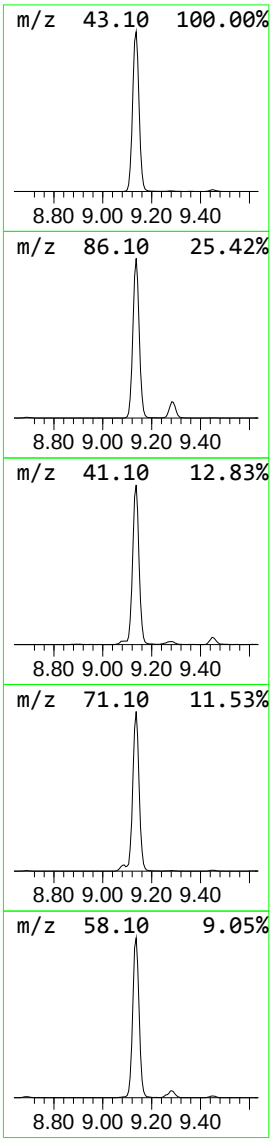
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.136	164.31 ug/l	2354480	1,4-Difluorobenzene	8.691

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3	2,3-Butanedione	86	C4H6O2	000431-03-8	49
4	Butane	58	C4H10	000106-97-8	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

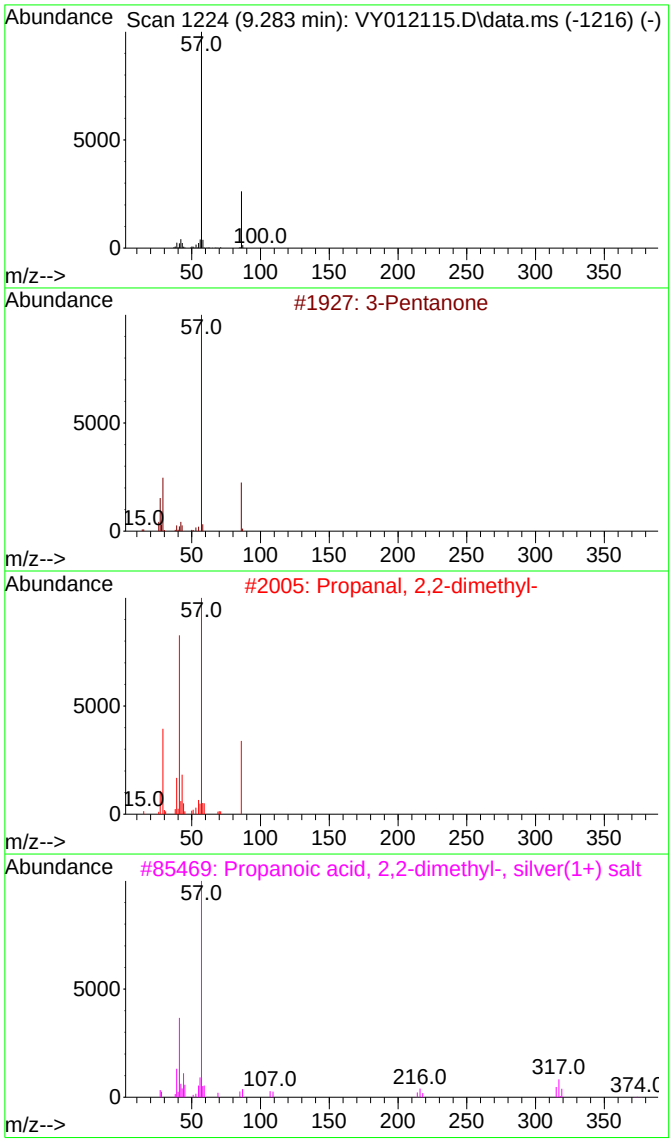
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

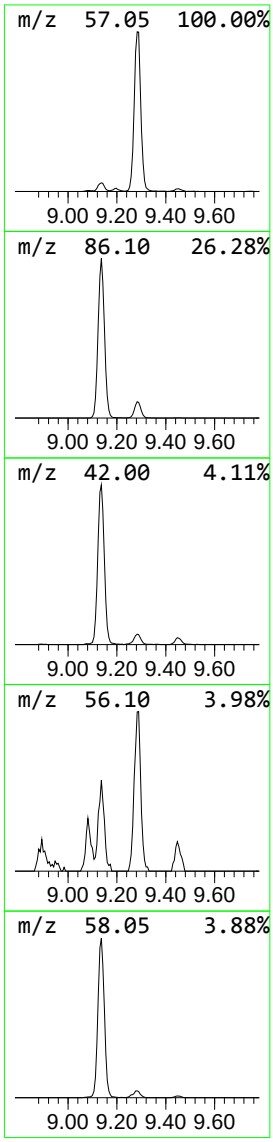
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.283	14.35 ug/l	205695	1,4-Difluorobenzene	8.691

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	39
3	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
4	Neopentane	72	C5H12	000463-82-1	9
5	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

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

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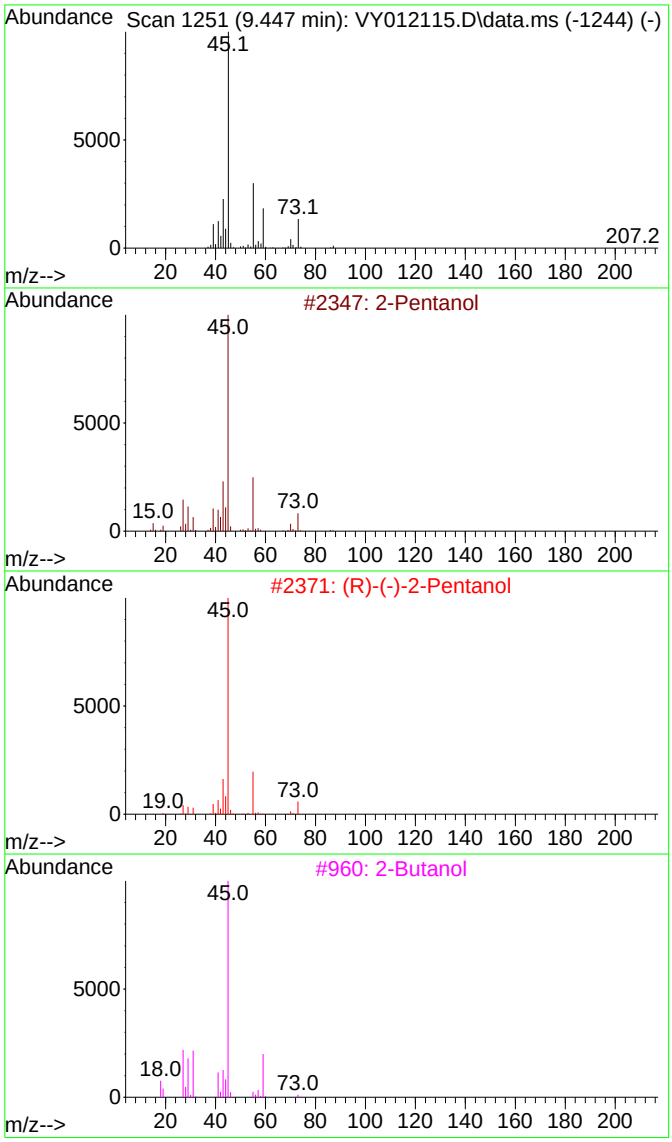
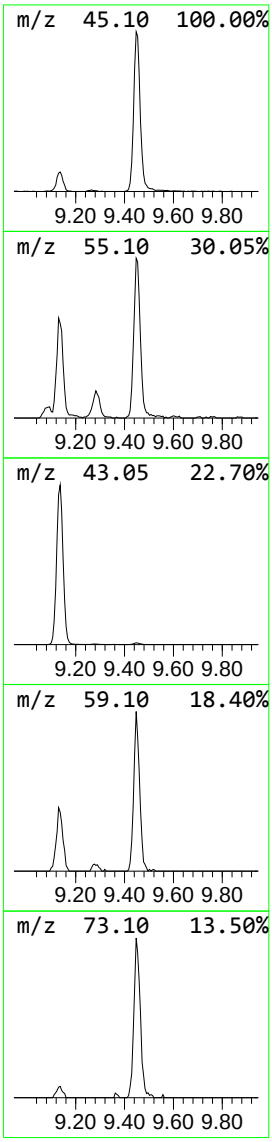
Peak Number 4 2-Pentanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.447	10.44 ug/l	149657	1,4-Difluorobenzene	8.691

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol	88	C5H12O	006032-29-7	72
2	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	72
3	2-Butanol	74	C4H10O	000078-92-2	64
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	59
5	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

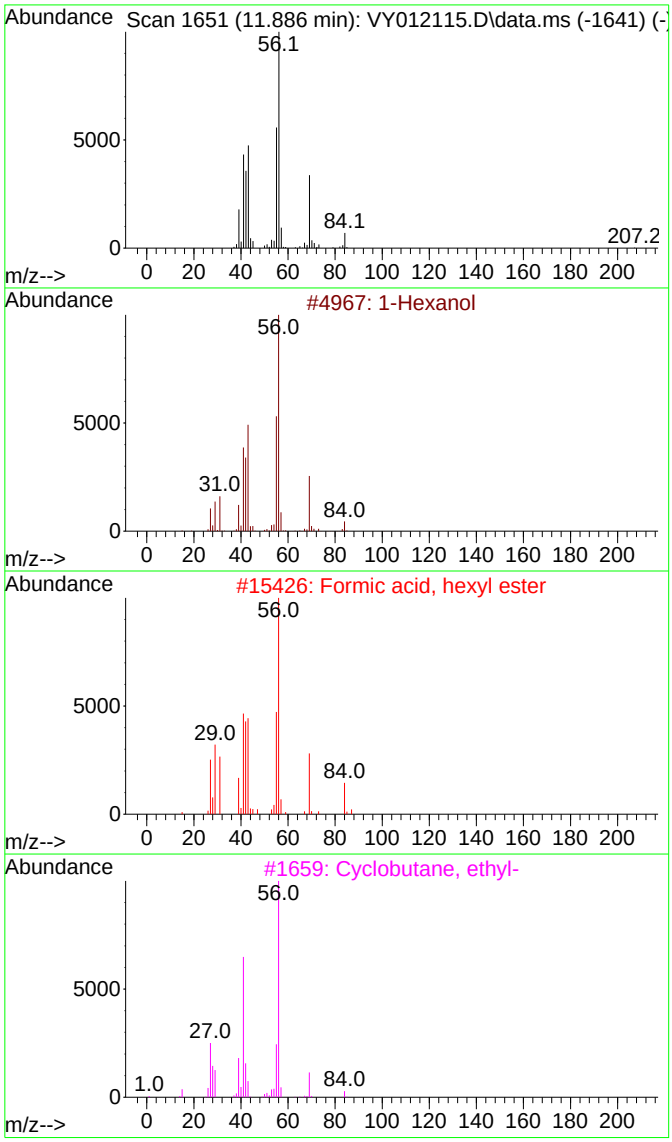
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

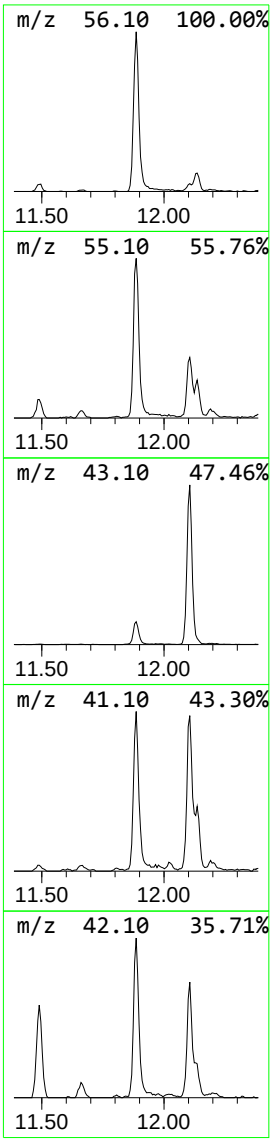
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	8.99 ug/l	159818	Chlorobenzene-d5	11.490

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	83
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	78
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

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

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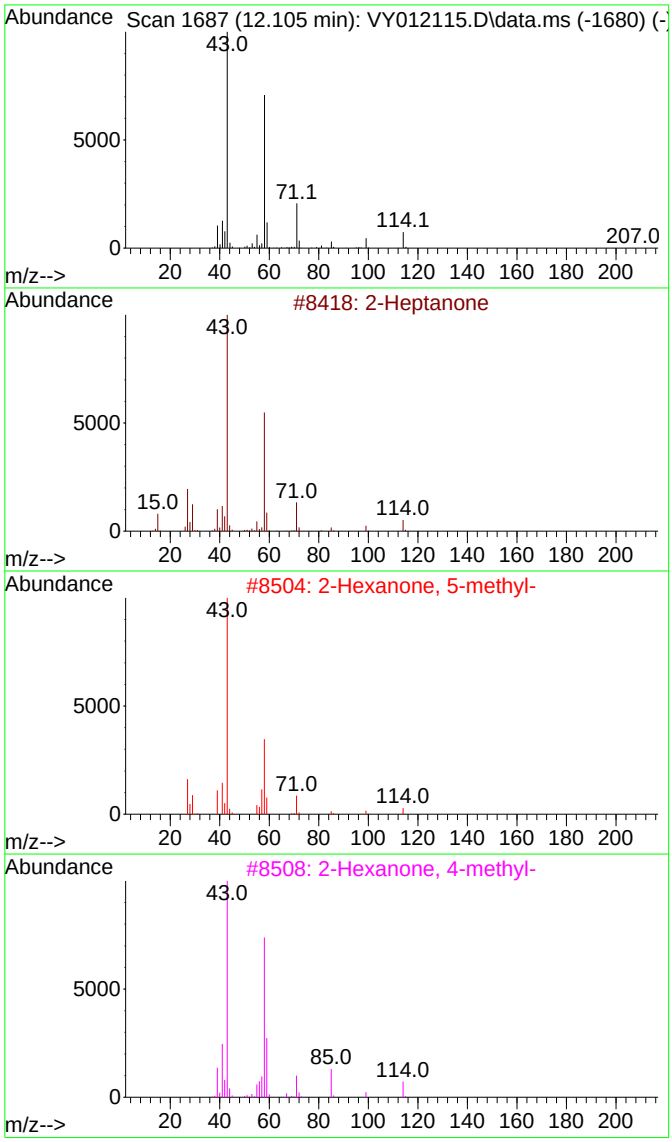
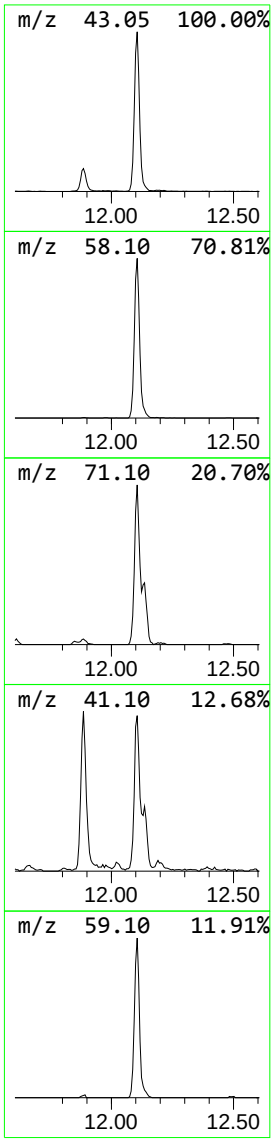
Peak Number 6 2-Heptanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	21.99 ug/l	391049	Chlorobenzene-d5	11.490

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	83
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	47
5	5-Nonanone, 2,8-dimethyl-	170	C11H22O	002050-99-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

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

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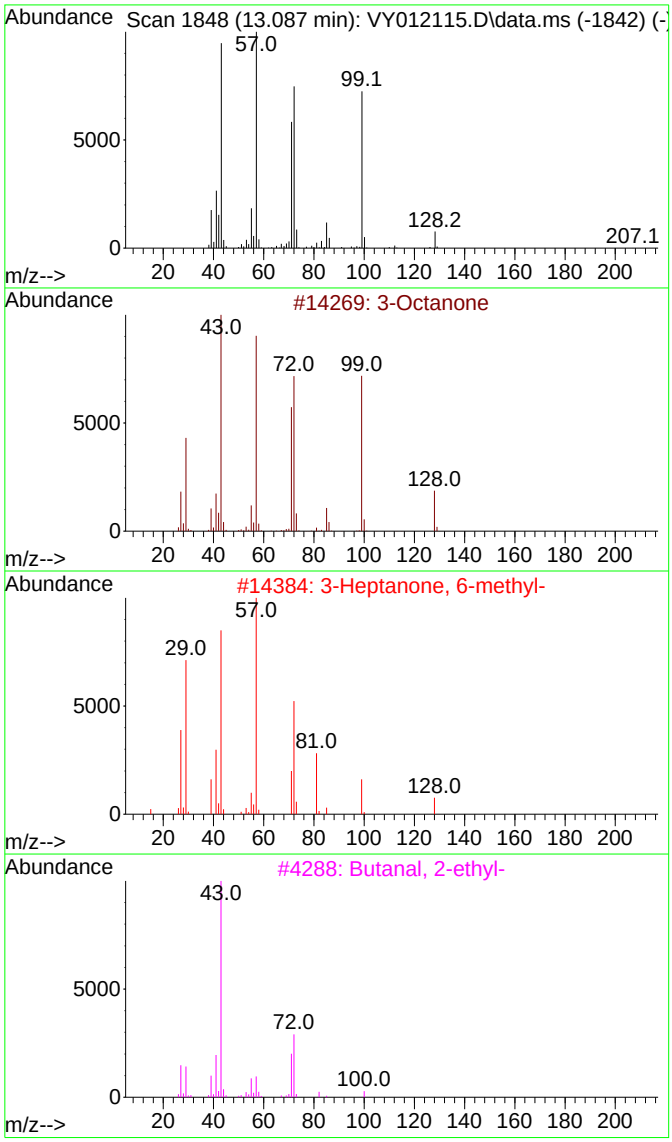
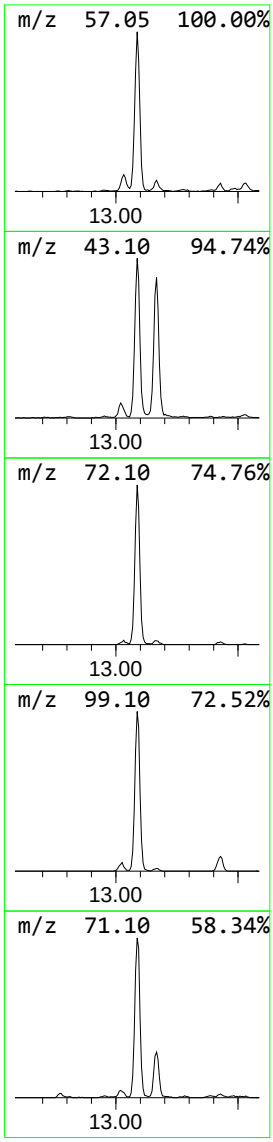
Peak Number 7 3-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	14.44 ug/l	246649	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	96
2	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	53
3	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	52
4	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	46
5	1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	43





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Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

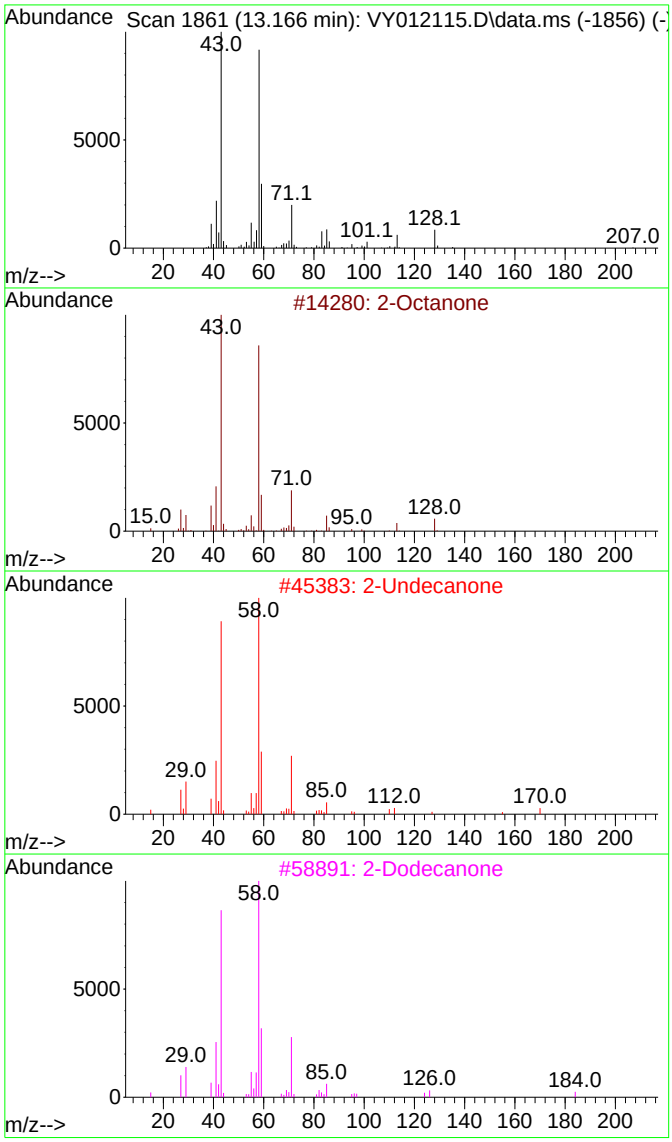
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.M
Quant Title : SW846 8260

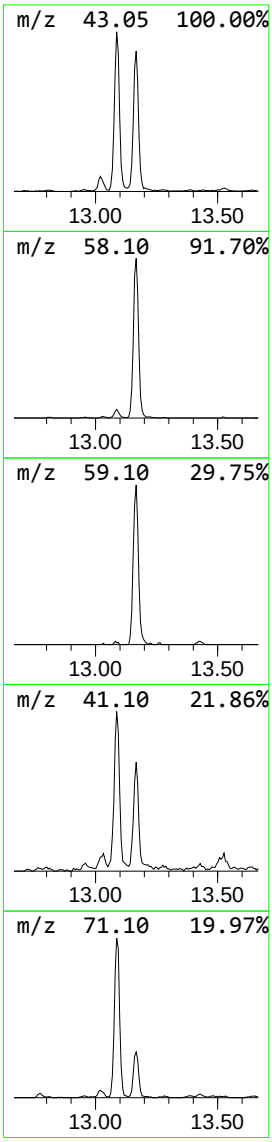
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Octanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.166	7.68 ug/l	131194	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	90
2	2-Undecanone	170	C11H22O	000112-12-9	72
3	2-Dodecanone	184	C12H24O	006175-49-1	64
4	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	64
5	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010923\
Data File : VY012115.D
Acq On : 09 Jan 2023 16:57
Operator : KP/MD
Sample : 01064-07
Misc : 1.24g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-14-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010623S.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
Pentane	3.253	21.7	ug/l	238433	1	7.789	548947	50.0
2-Pentanone	9.136	164.3	ug/l	2354480	2	8.691	716500	50.0
3-Pentanone	9.283	14.4	ug/l	205695	2	8.691	716500	50.0
2-Pentanol	9.447	10.4	ug/l	149657	2	8.691	716500	50.0
1-Hexanol	11.886	9.0	ug/l	159818	3	11.490	889127	50.0
2-Heptanone	12.105	22.0	ug/l	391049	3	11.490	889127	50.0
3-Octanone	13.087	14.4	ug/l	246649	4	13.428	854260	50.0
2-Octanone	13.166	7.7	ug/l	131194	4	13.428	854260	50.0