LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 441

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\82X040225W.M
Title : SW846 8260

Signal : TIC: VX045834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.069	154	161	167	rBV	7151	12828	1.58%	0.260%
2	2.288	192	197	202	rBV	5310	8295	1.02%	0.168%
3	2.380	206	212	222	rVB	37980	60931	7.51%	1.236%
4	2.544	233	239	250	rVB2	5544	11359	1.40%	0.230%
5	2.971	302	309	320	rVB4	3163	8287	1.02%	0.168%
6	4.562	560	570	587	rBV	11489	35438	4.37%	0.719%
7	5.385	692	705	719	rBV	57587	173728	21.41%	3.524%
8	5.544	719	731	746	rVV2	84291	241691	29.79%	4.902%
9	5.952	788	798	817	rBV	70516	182273	22.46%	3.697%
10	6.629	900	909	921	rBV	65799	177691	21.90%	3.604%
11	6.757	921	930	943	rVB	148184	361188	44.51%	7.326%
12	7.464	1040	1046	1063	rBV	15363	40430	4.98%	0.820%
13	7.903	1111	1118	1133	rVB3	3819	10231	1.26%	0.208%
14	8.574	1223	1228	1233	rBV2	6839	11541	1.42%	0.234%
15	8.647	1233	1240	1247	rVV	321597	504310	62.15%	10.229%
16	8.714	1247	1251	1260	rVV2	16376	33884	4.18%	0.687%
17	8.805	1261	1266	1280	rVB	18023	32891	4.05%	0.667%
18	9.244	1331	1338	1344	rBV	8333	16429	2.02%	0.333%
19	9.427	1363	1368	1382	rBV	171475	261232	32.19%	5.299%
20	9.641	1398	1403	1408	rBV	7198	12836	1.58%	0.260%
21	9.945	1447	1453	1460	rBV	11866	19250	2.37%	0.390%
22	10.049	1464	1470	1490	rVV	334835	472876	58.28%	9.592%
23	10.214	1490	1497	1505	rVV	35758	57999	7.15%	1.176%
24	10.372	1517	1523	1535	rVB	14174	23635	2.91%	0.479%
25	10.768	1582	1588	1600	rBV	84155	122812	15.14%	2.491%
26	10.878	1600	1606	1613	rVV4	10289	21780	2.68%	0.442%
27	11.079	1634	1639	1651	rVB	262949	356082	43.88%	7.223%
28	11.366	1681	1686	1692	rBV4	4430	9570	1.18%	0.194%
29	11.476	1699	1704	1710	rVB4	8275	16414	2.02%	0.333%
30	11.750	1746	1749	1759	rVB3	9866	15036	1.85%	0.305%
31	11.969	1781	1785	1789	rBV	15842	22365	2.76%	0.454%
32	12.018	1789	1793	1801	rVV	333770	418874	51.62%	8.496%
33	12.097	1801	1806	1813	rVB	69406	98441	12.13%	1.997%
34	12.213	1820	1825	1838	rBV	573314	811410	100.00%	16.459%
35	12.421	1855	1859	1864	rVB	12902	14351	1.77%	0.291%
36	12.768	1911	1916	1918	rBV3	18153	27053	3.33%	0.549%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

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\82X040225W.M
Title : SW846 8260

37	12.859	1927	1931	1937	rBV3	17749	30197	3.72%	0.613%
38	12.969	1945	1949	1955	rBV6	11172	20212	2.49%	0.410%
39	13.103	1967	1971	1973	rBV3	12584	16722	2.06%	0.339%
40	13.262	1994	1997	2000	rBV	15913	18374	2.26%	0.373%
41	13.420	2019	2023	2033	rVV6	10762	20208	2.49%	0.410%
42	13.512	2033	2038	2045	rVB4	13763	25886	3.19%	0.525%
43	13.841	2088	2092	2097	rBV6	7394	13904	1.71%	0.282%
44	14.036	2120	2124	2128	rVB	17796	17984	2.22%	0.365%
45	14.609	2215	2218	2226	rBV8	9758	24424	3.01%	0.495%
46	14.755	2238	2242	2245	rBV	11897	12965	1.60%	0.263%
47	15.487	2358	2362	2369	rBV7	6281	12214	1.51%	0.248%
48	16.078	2455	2459	2466	rVB8	5690	11463	1.41%	0.233%

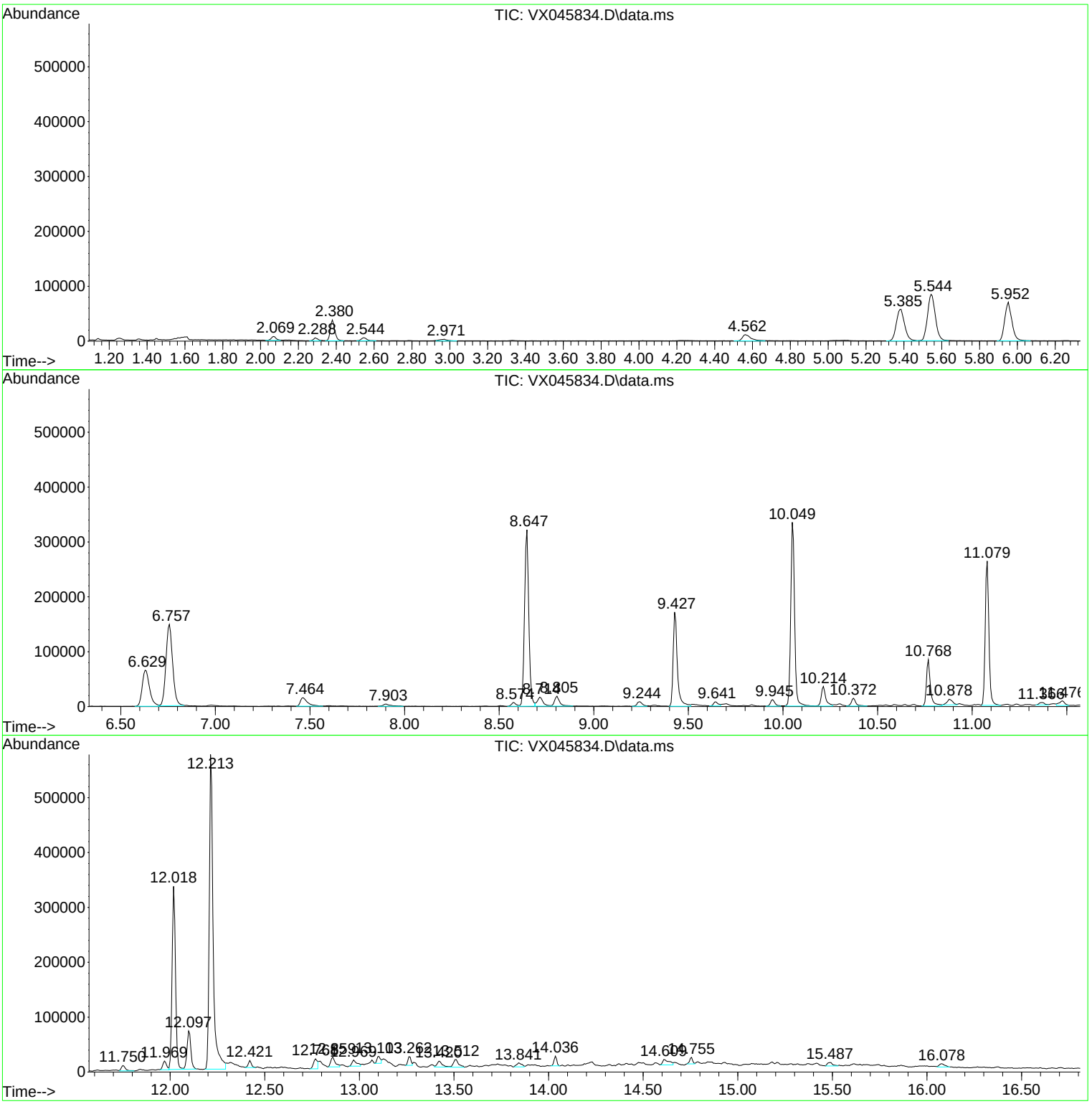
Sum of corrected areas: 4929994

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

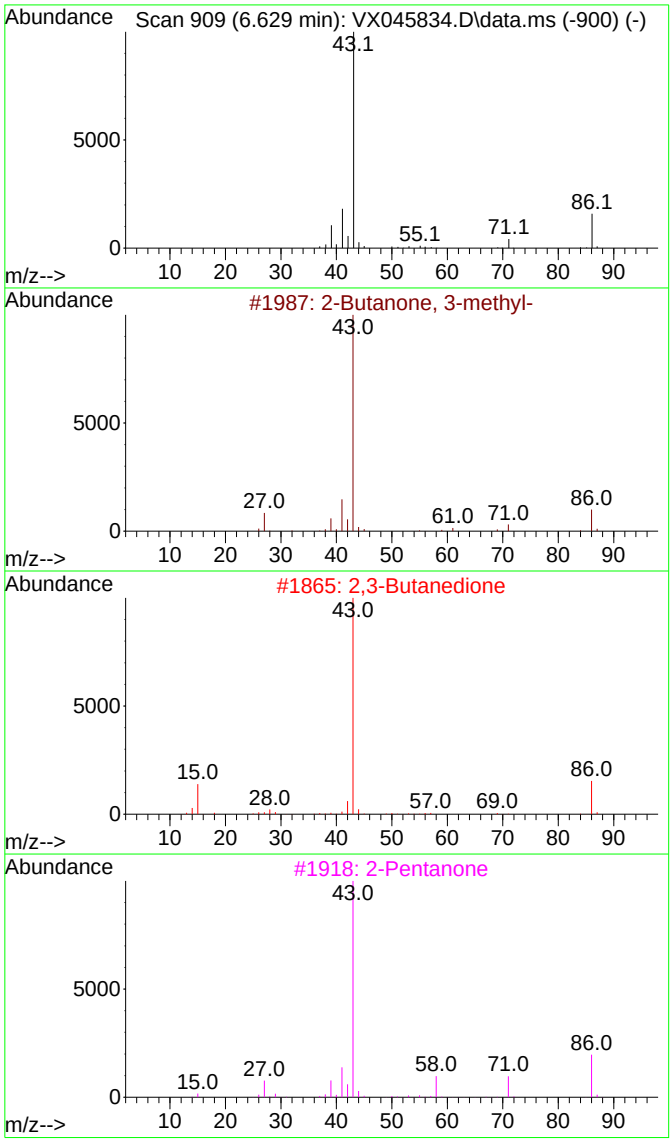
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

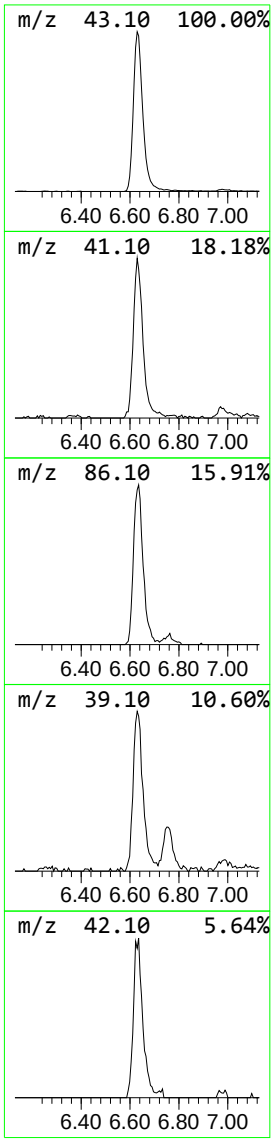
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Butanone, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.629	24.60 ug/l	177691	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
2	2,3-Butanedione	86	C4H6O2	000431-03-8	53
3	2-Pentanone	86	C5H10O	000107-87-9	45
4	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	36
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

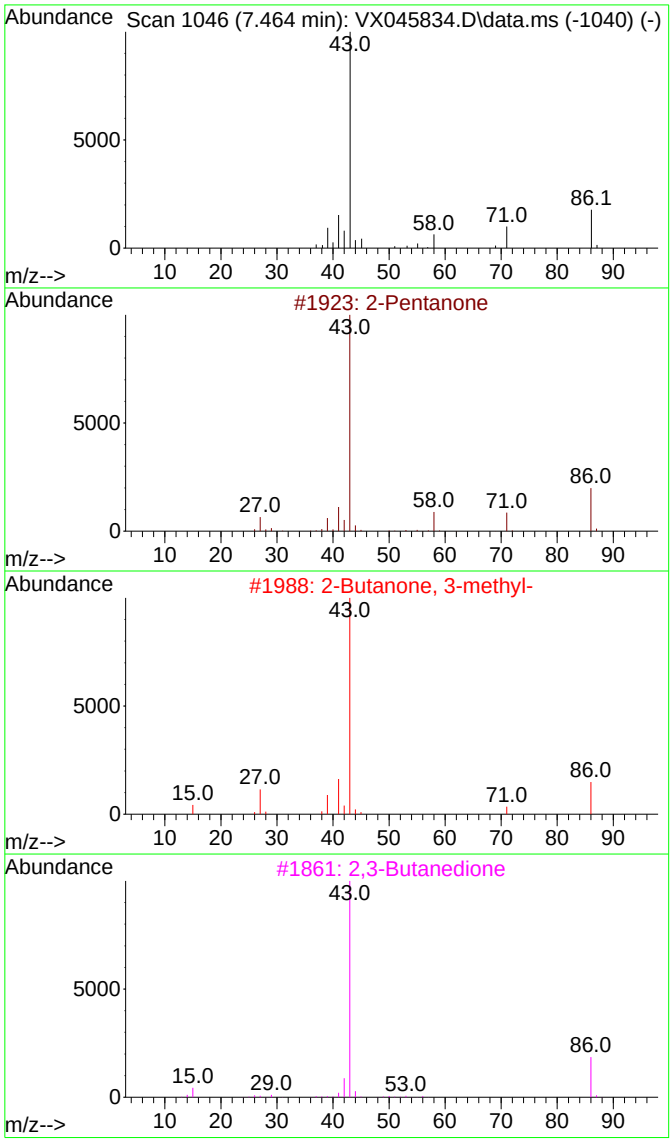
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

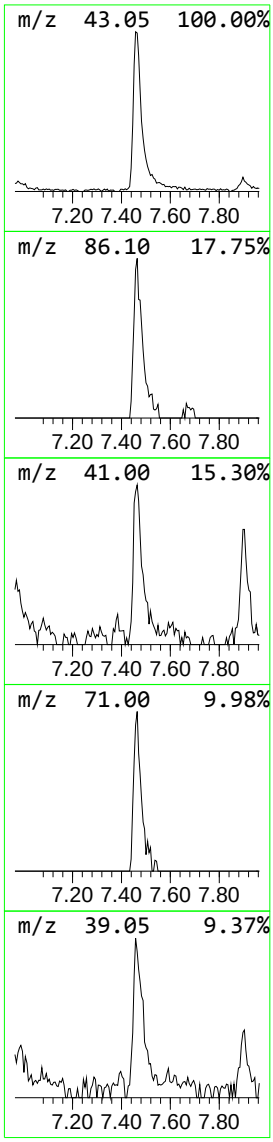
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.464	5.60 ug/l	40430	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	80
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	47
3	2,3-Butanedione	86	C4H6O2	000431-03-8	38
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9
5	3-Aminopyrrolidine	86	C4H10N2	079286-79-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

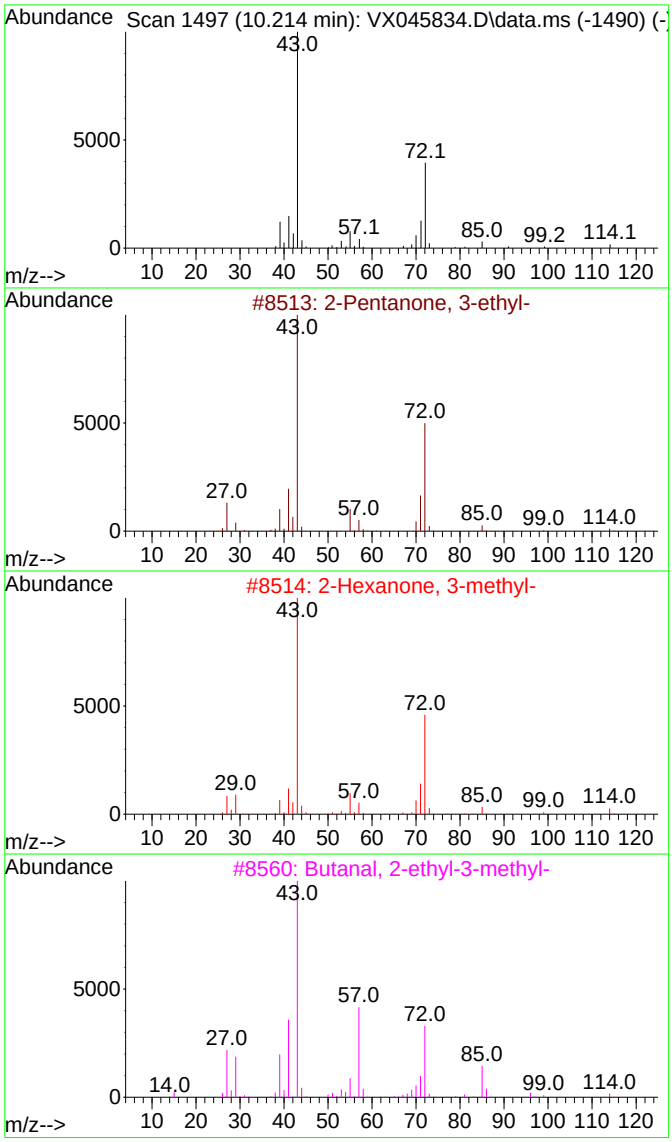
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

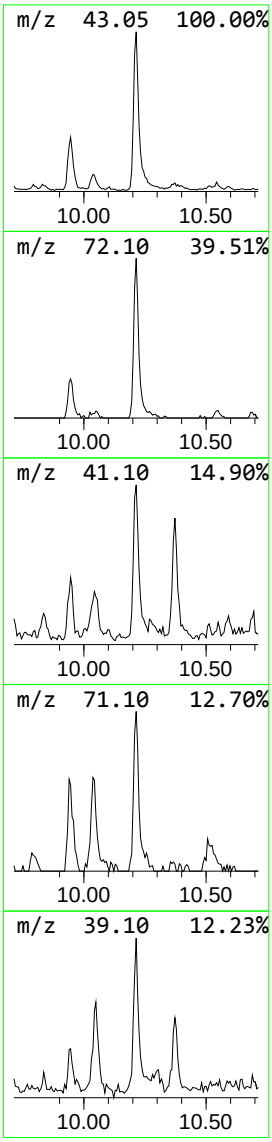
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.214	6.13 ug/l	57999	Chlorobenzene-d5	10.049

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	91
2	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	86
3	Butanal, 2-ethyl-3-methyl-	114	C7H14O	026254-92-2	80
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	59
5	1-Methylallyl acetate	114	C6H10O2	006737-11-7	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

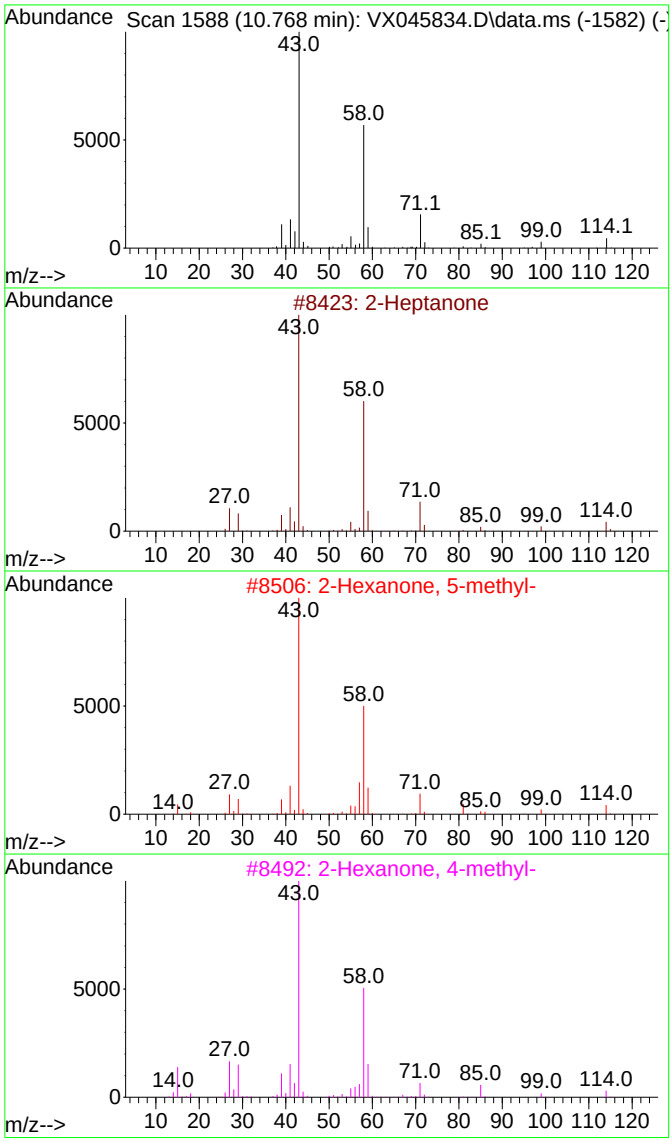
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

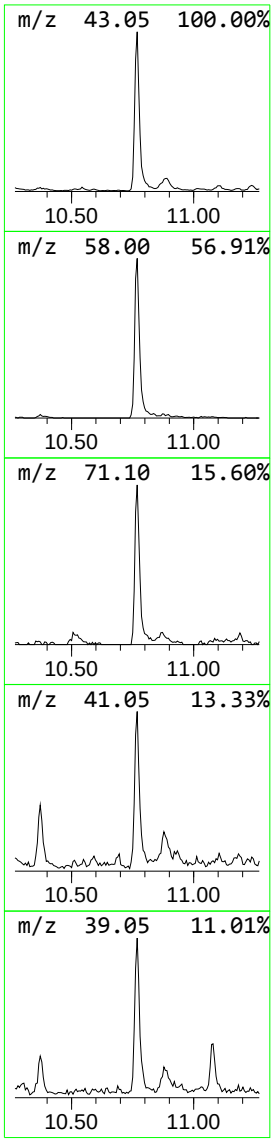
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	12.99 ug/l	122812	Chlorobenzene-d5	10.049

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	86
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4	2-Hexanone	100	C6H12O	000591-78-6	56
5	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

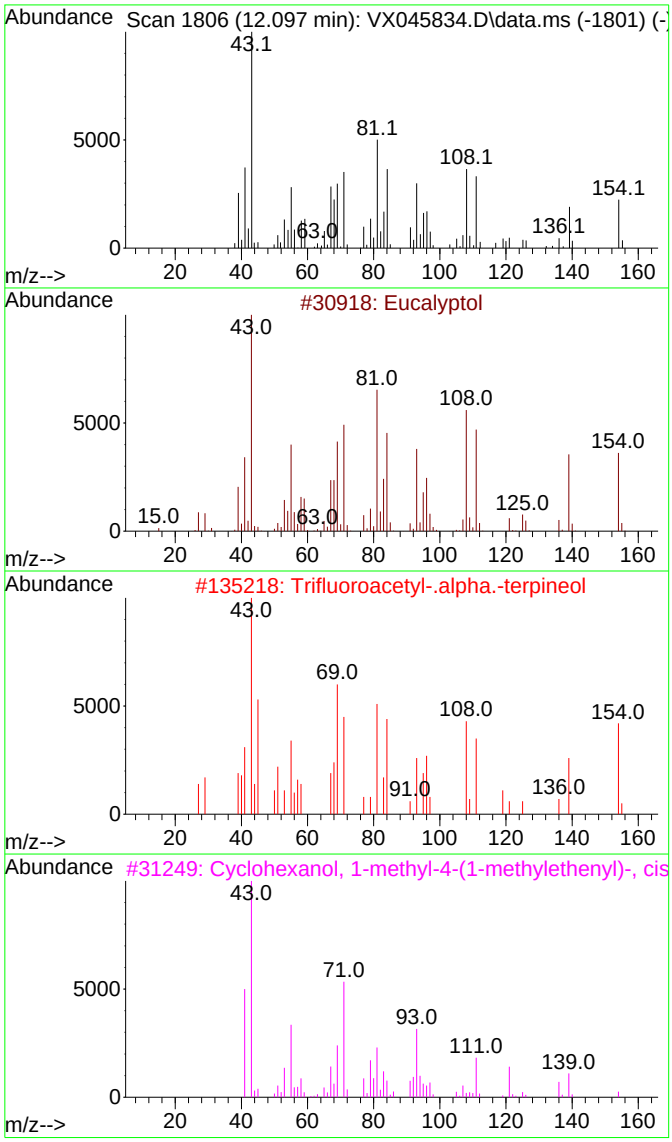
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

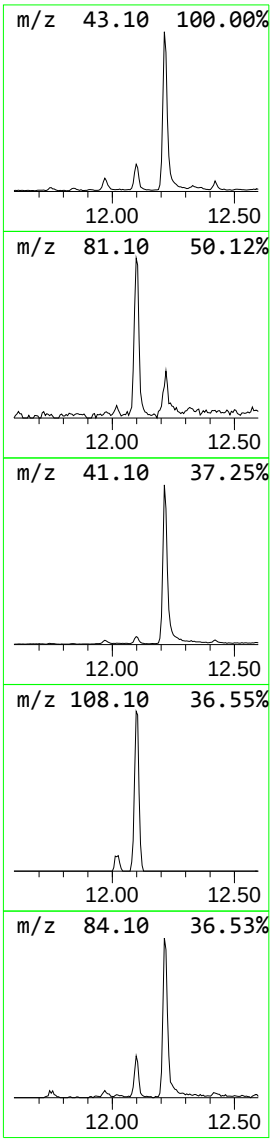
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.097	11.75 ug/l	98441	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	97
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	50
3	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-41-4	38
4	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	35
5	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

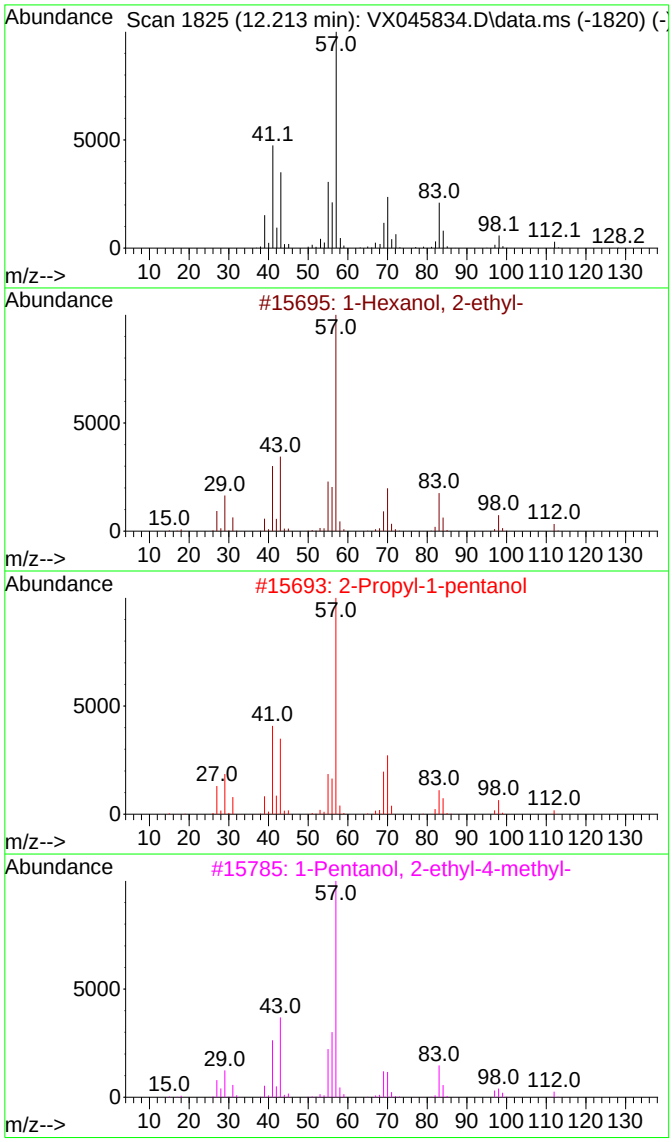
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

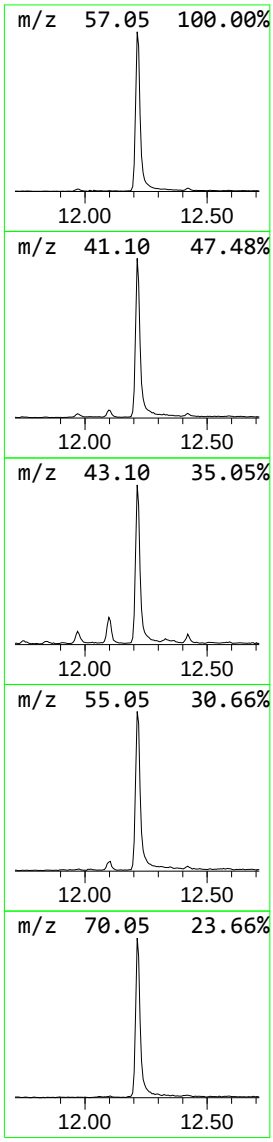
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	96.86 ug/l	811410	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045834.D
Acq On : 17 Apr 2025 17:28
Operator : JC/MD
Sample : Q1816-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
441

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.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
2-Butanone, 3-m...	6.629	24.6	ug/l	177691	2	6.757	361188	50.0
2-Pentanone	7.464	5.6	ug/l	40430	2	6.757	361188	50.0
2-Pentanone, 3-...	10.214	6.1	ug/l	57999	3	10.049	472876	50.0
2-Heptanone	10.768	13.0	ug/l	122812	3	10.049	472876	50.0
Eucalyptol	12.097	11.8	ug/l	98441	4	12.018	418874	50.0
1-Hexanol, 2-et...	12.213	96.9	ug/l	811410	4	12.018	418874	50.0