LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

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\82X090722W.M
Title : SW846 8260

Signal : TIC: VX031224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	205	212	230	rBV	552662	903898	43.64%	11.211%
2	2.550	232	240	252	rVB	17002	41194	1.99%	0.511%
3	4.562	561	570	585	rBV	24157	68674	3.32%	0.852%
4	5.385	695	705	718	rBV3	69339	208049	10.04%	2.580%
5	5.556	721	733	746	rVB	82326	227193	10.97%	2.818%
6	5.958	789	799	807	rBV2	81014	206732	9.98%	2.564%
7	6.044	807	813	823	rVB3	17151	45483	2.20%	0.564%
8	6.763	922	931	942	rBV	118062	286585	13.84%	3.555%
9	8.220	1163	1170	1177	rBV	25368	40124	1.94%	0.498%
10	8.653	1234	1241	1246	rBV	357223	555973	26.84%	6.896%
11	8.720	1246	1252	1261	rVB	1366405	2071273	100.00%	25.691%
12	9.445	1366	1371	1377	rBV	68092	107680	5.20%	1.336%
13	10.000	1455	1462	1466	rBV3	9713	21129	1.02%	0.262%
14	10.055	1466	1471	1480	rVB	248403	332214	16.04%	4.121%
15	10.195	1488	1494	1502	rBV	47382	66774	3.22%	0.828%
16	10.299	1507	1511	1518	rVB	251770	350182	16.91%	4.343%
17	10.415	1524	1530	1534	rBV4	15730	24021	1.16%	0.298%
18	10.640	1563	1567	1573	rVV	137067	195571	9.44%	2.426%
19	10.768	1582	1588	1597	rVB2	26791	46102	2.23%	0.572%
20	11.085	1634	1640	1645	rBV	308190	402240	19.42%	4.989%
21	11.146	1645	1650	1659	rVB4	13290	29404	1.42%	0.365%
22	11.311	1672	1677	1682	rVB	23413	28648	1.38%	0.355%
23	11.610	1723	1726	1733	rVB5	11707	23501	1.13%	0.291%
24	11.756	1744	1750	1755	rVB	61811	81697	3.94%	1.013%
25	11.847	1762	1765	1775	rVB5	14334	24616	1.19%	0.305%
26	12.024	1789	1794	1800	rVB	266424	320389	15.47%	3.974%
27	12.085	1800	1804	1808	rBV	24328	31821	1.54%	0.395%
28	12.225	1818	1827	1829	rBV	52075	87110	4.21%	1.080%
29	12.414	1853	1858	1863	rBV	61813	75784	3.66%	0.940%
30	12.799	1912	1921	1928	rBV	178722	232903	11.24%	2.889%
31	12.945	1940	1945	1951	rBV5	11494	25892	1.25%	0.321%
32	13.140	1972	1977	1986	rVB2	21688	32348	1.56%	0.401%
33	13.347	2006	2011	2015	rBV2	20028	27353	1.32%	0.339%
34	13.713	2066	2071	2076	rBV	52135	77781	3.76%	0.965%
35	13.774	2076	2081	2087	rVV	427835	557117	26.90%	6.910%
36	13.829	2087	2090	2094	rVV	29578	43348	2.09%	0.538%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

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\82X090722W.M
Title : SW846 8260

37	13.872	2094	2097	2104	rVB2	40349	61195	2.95%	0.759%
38	14.640	2218	2223	2230	rVB	48636	64538	3.12%	0.800%
39	14.780	2242	2246	2252	rVV3	25438	35863	1.73%	0.445%

Sum of corrected areas: 8062399

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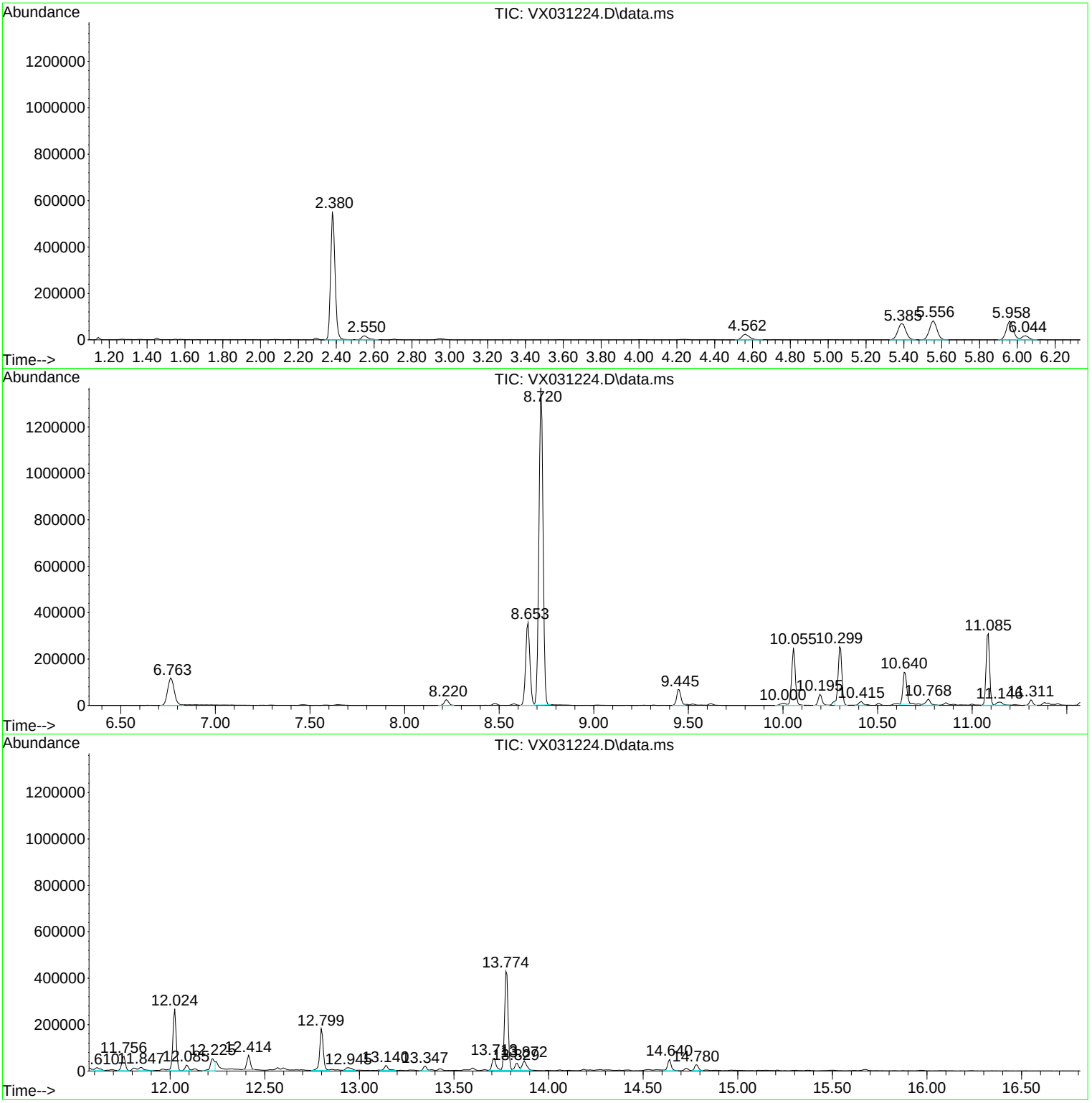
Instrument :
MSVOA_X
ClientSampleId :
CLI-108

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
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Instrument :
MSVOA_X
ClientSampleId :
CLI-108

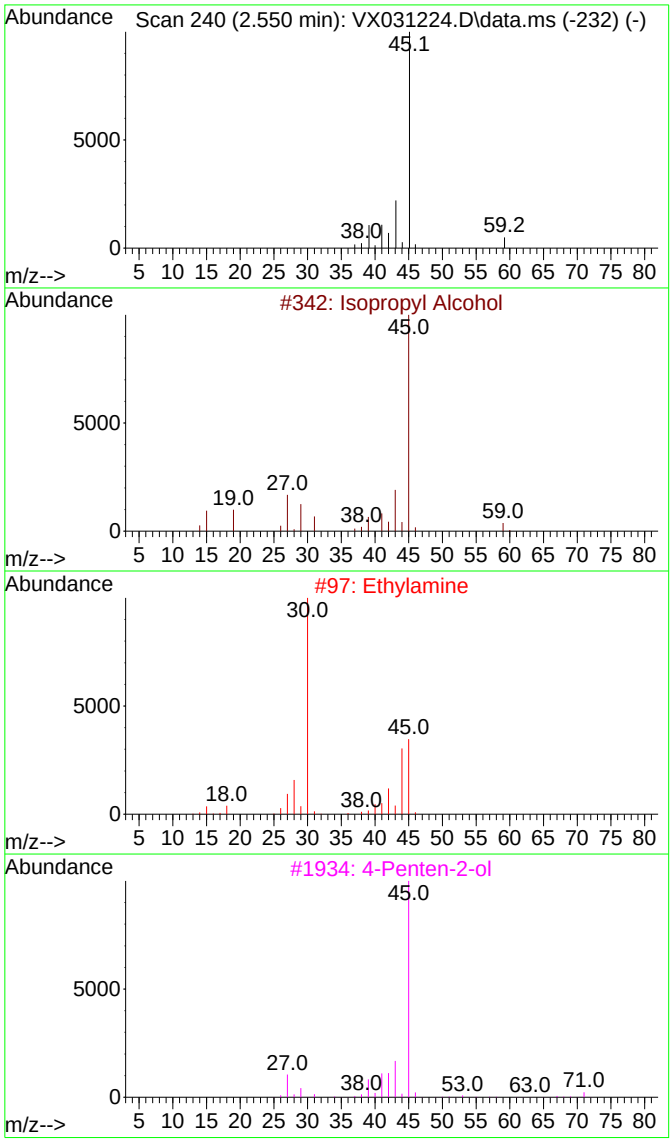
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

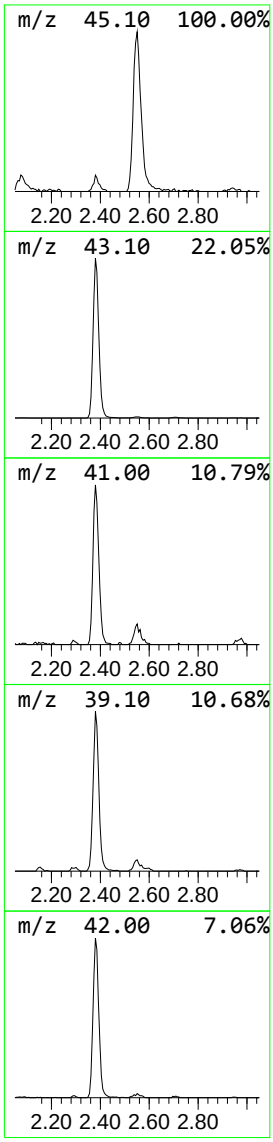
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.550	9.07 ug/l	41194	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2	Ethylamine	45	C2H7N	000075-04-7	5
3	4-Penten-2-ol	86	C5H10O	000625-31-0	4
4	Formamide	45	CH3NO	000075-12-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

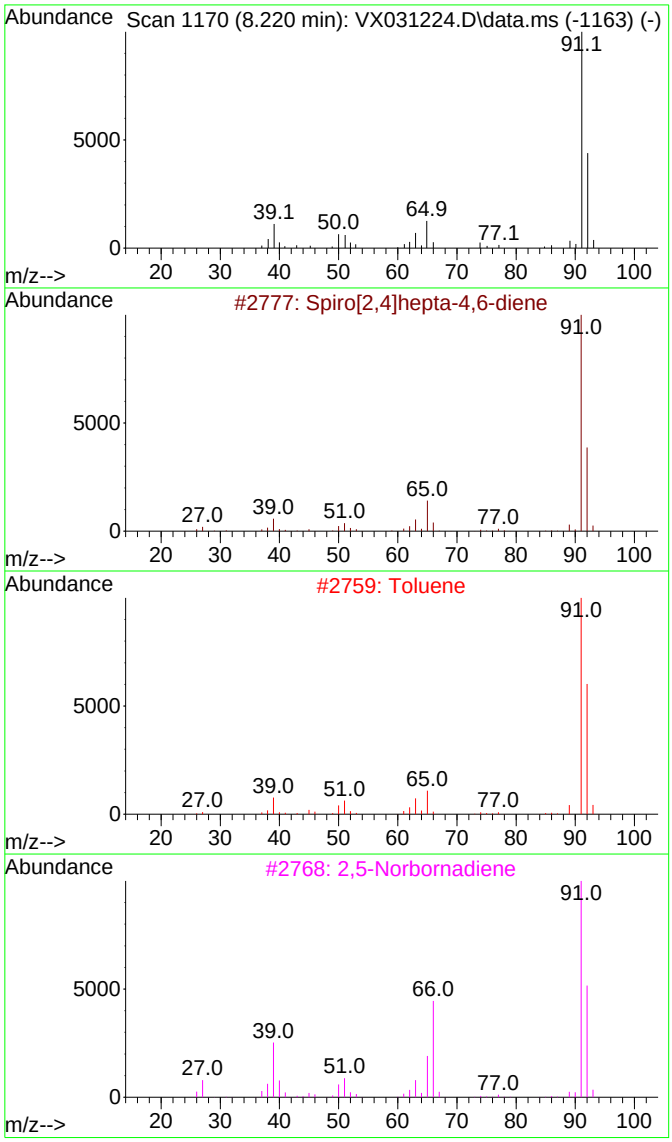
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

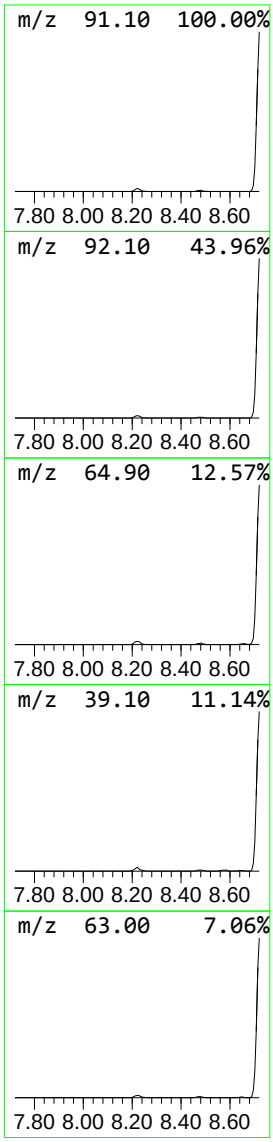
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Spiro[2,4]hepta-4,6-diene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.220	7.00 ug/l	40124	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
2	Toluene	92	C7H8	000108-88-3	90
3	2,5-Norbornadiene	92	C7H8	000121-46-0	87
4	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
5	Spiro[3.3]hepta-1,5-diene	92	C7H8	022635-78-5	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

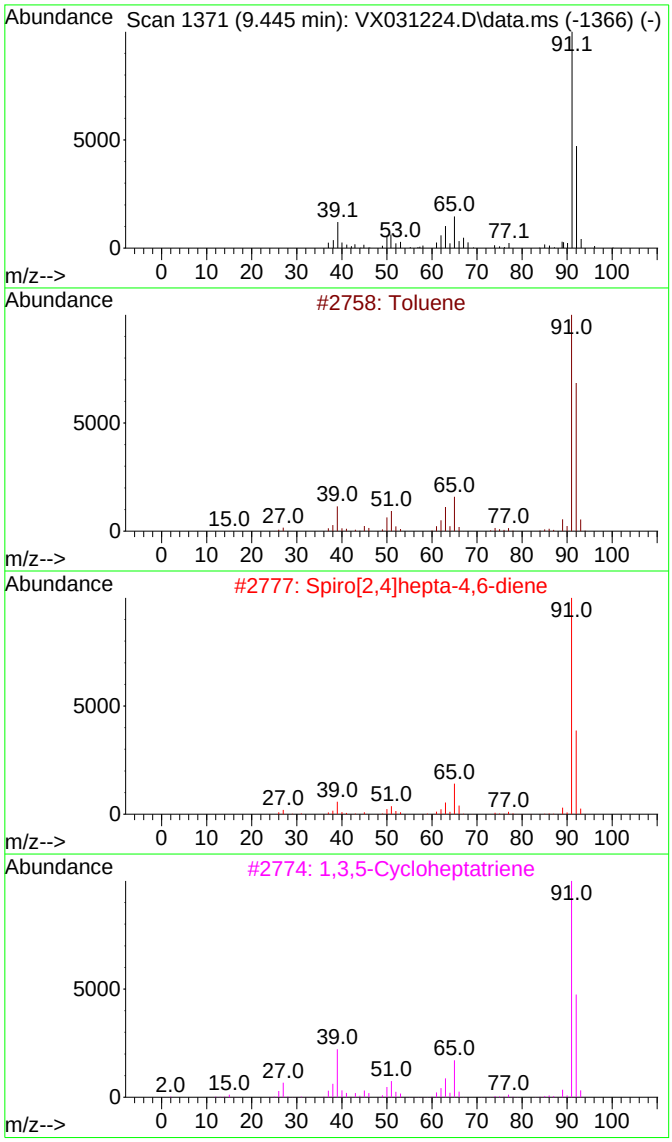
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

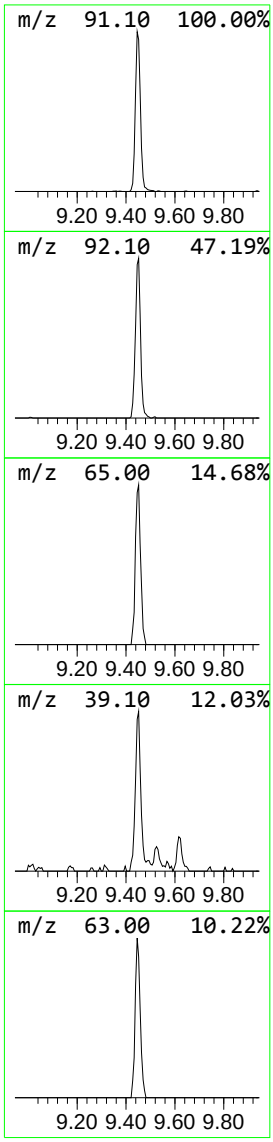
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3,5-Cycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.445	16.21 ug/l	107680	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	91
2	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
3	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
4	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	72
5	1,6-Heptadien-3-yne	92	C7H8	005150-80-1	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

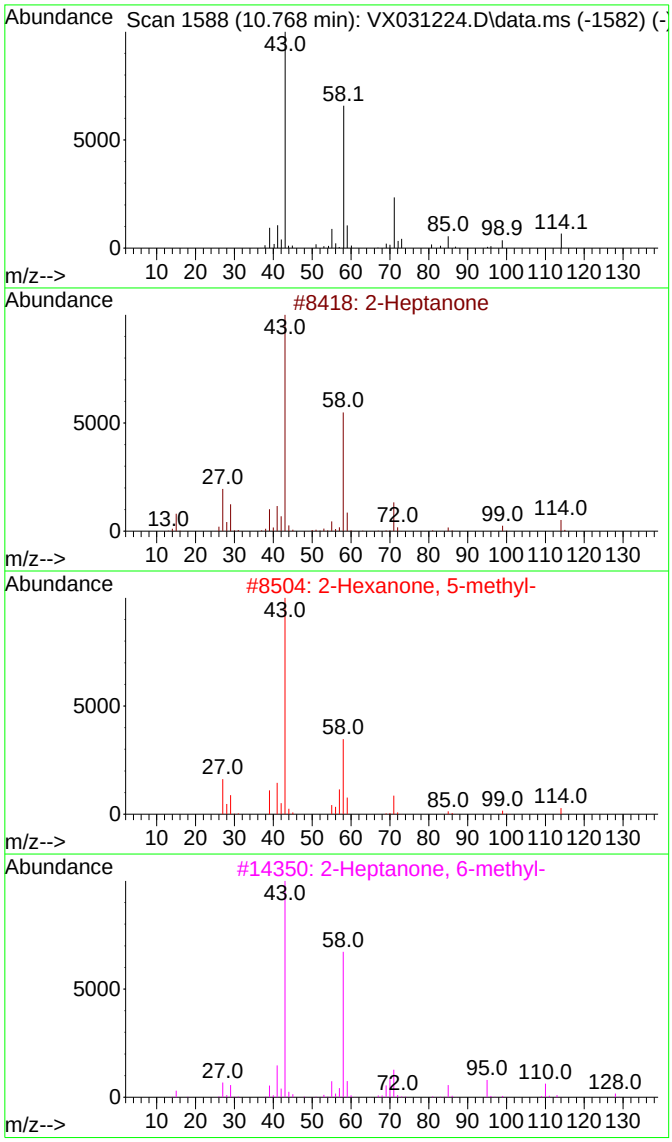
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

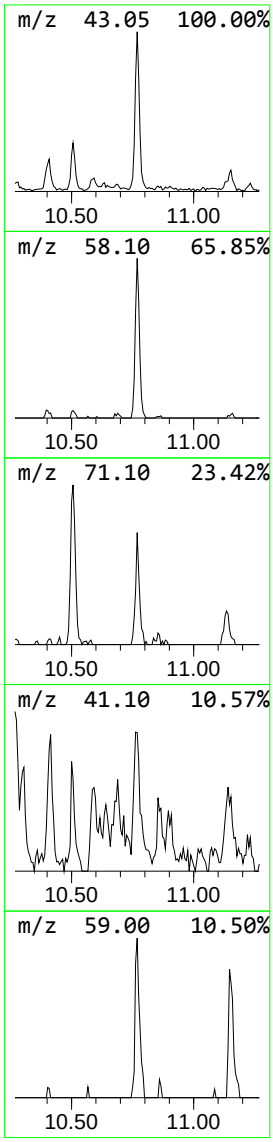
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Heptanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	6.94 ug/l	46102	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	78
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64
3	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	42
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	42
5	Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

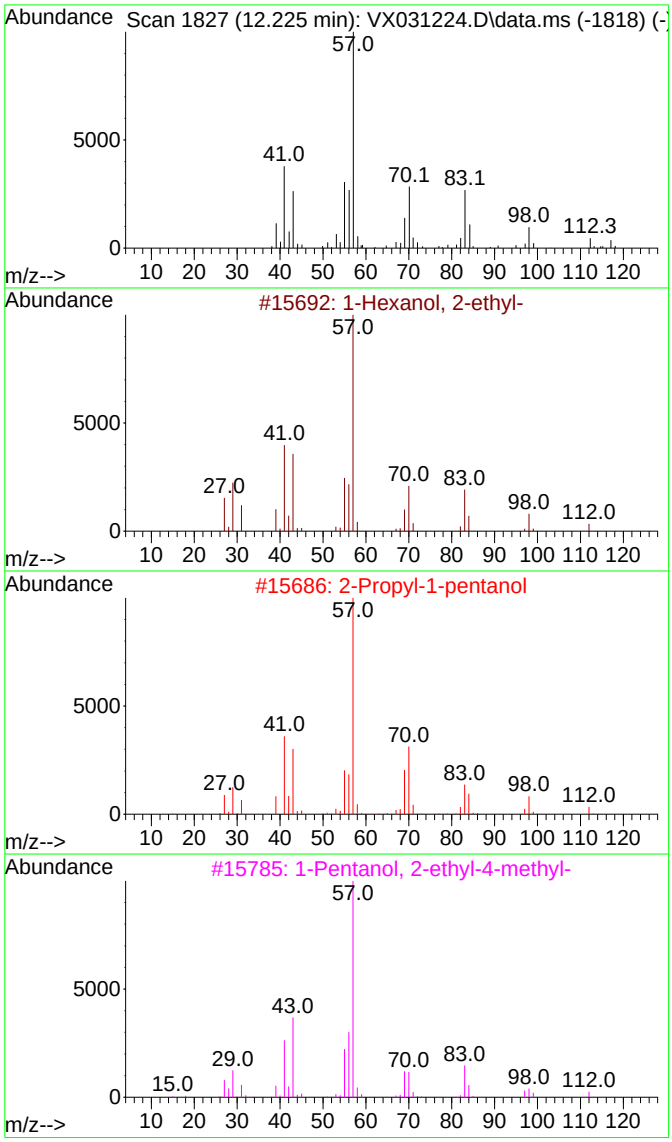
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

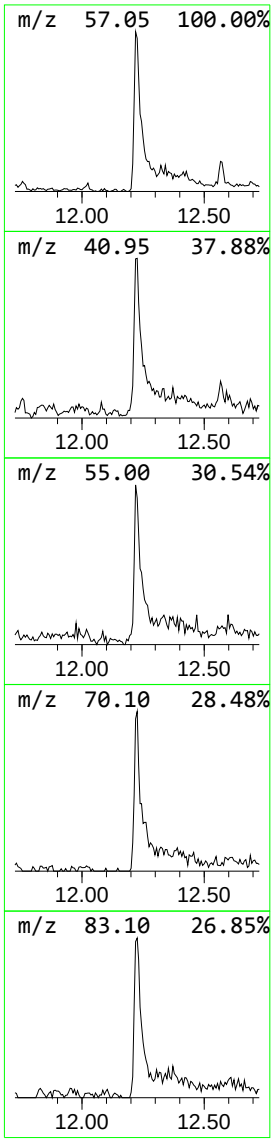
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.226	13.59 ug/l	87110	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Carbonic acid, butyl 2-ethylhexy...	230	C13H26O3	1000357-84-4	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47





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Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

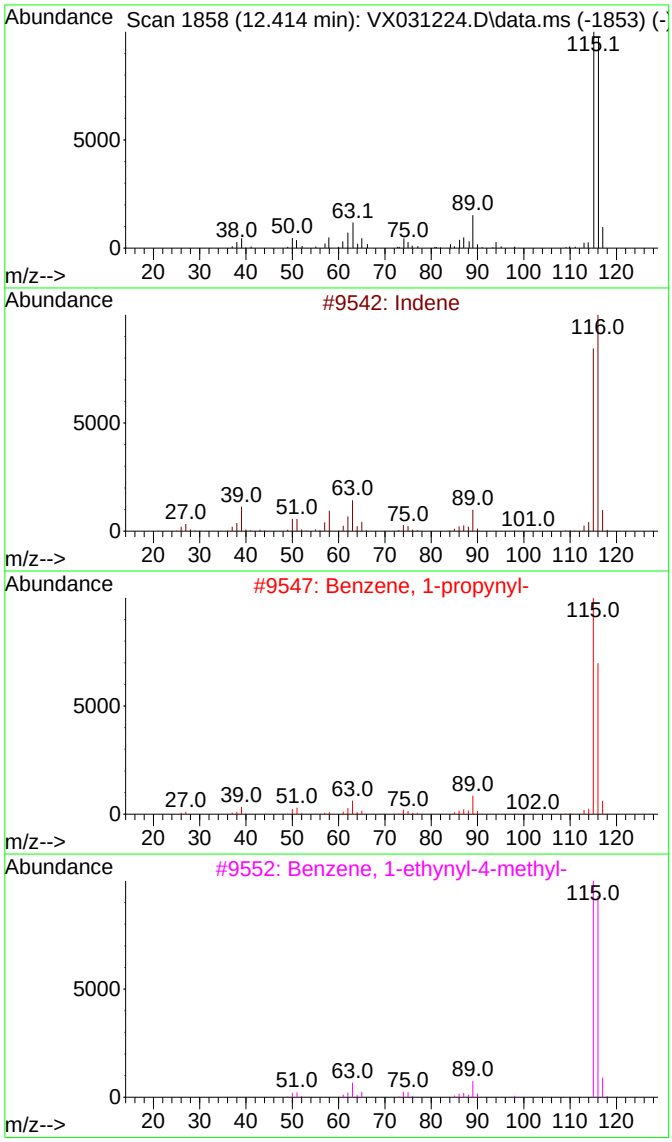
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

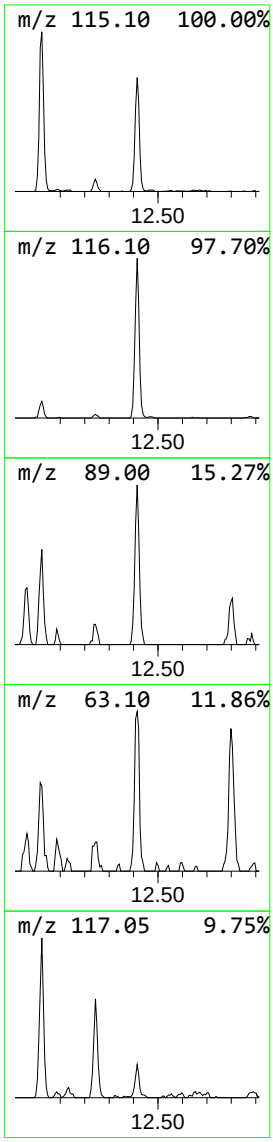
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	11.83 ug/l	75784	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	91
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90





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Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

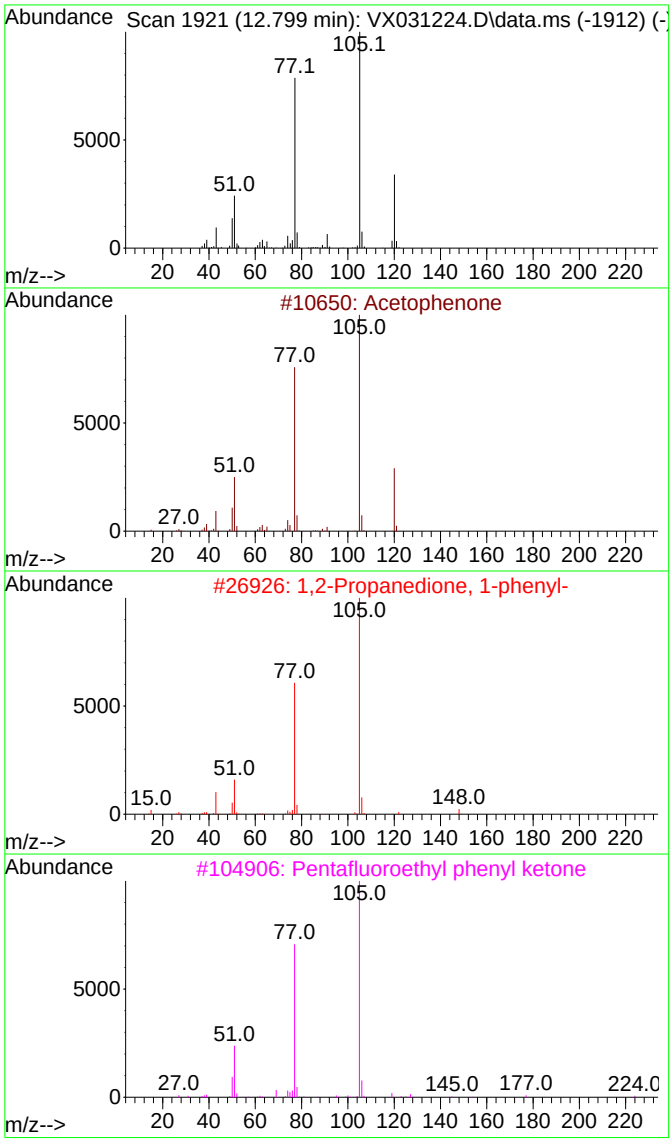
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

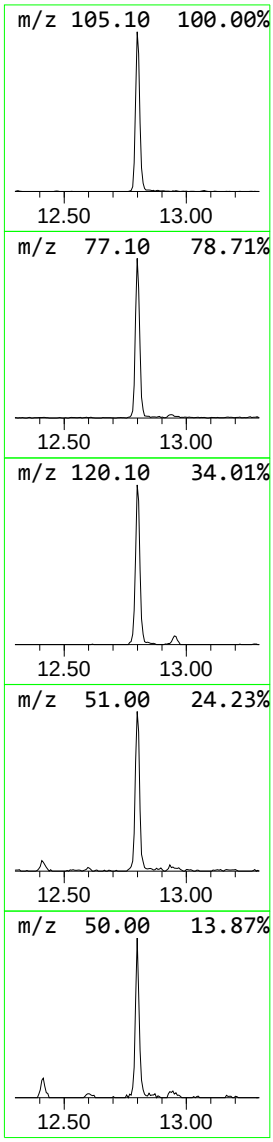
****

Peak Number 7 Acetophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.799	36.35 ug/l	232903	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	95
2	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	72
3	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	72
4	N-cyanobenzamide	146	C8H6N2O	015150-25-1	72
5	Benzoylformic acid	150	C8H6O3	000611-73-4	72





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Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

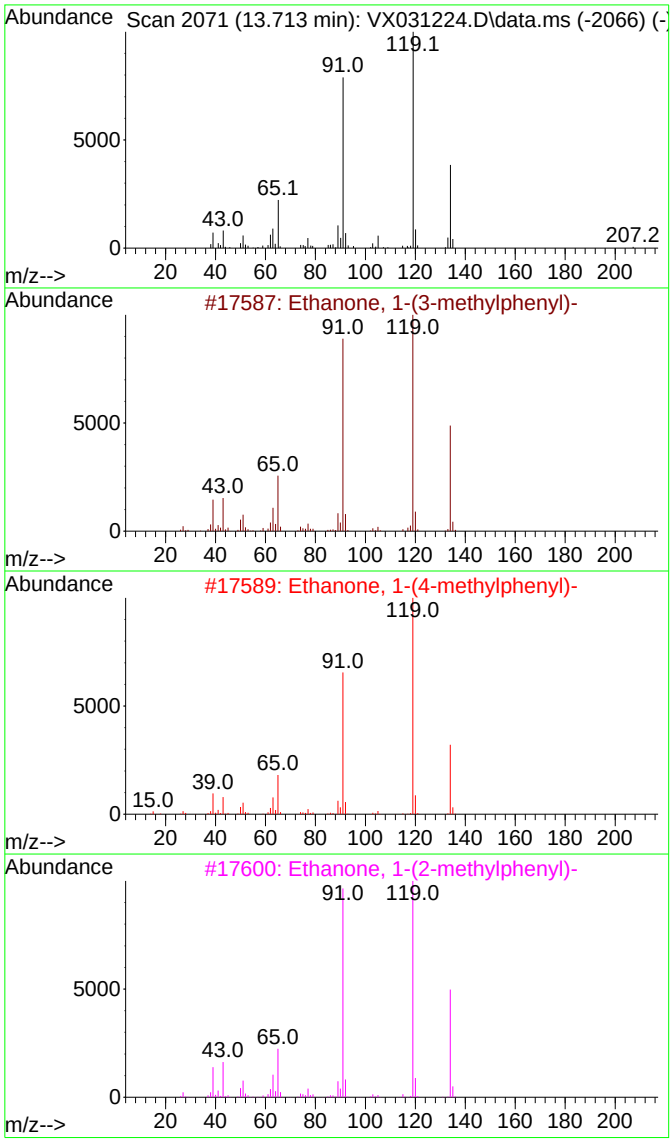
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

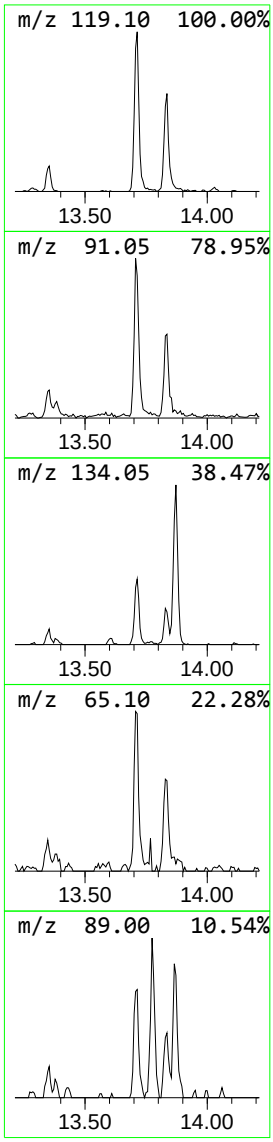
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Ethanone, 1-(3-methylphenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.713	12.14 ug/l	77781	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	97
2	Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	95
3	Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	94
4	3-Methyl-2,3-dihydro-benzofuran	134	C9H10O	013524-73-7	87
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

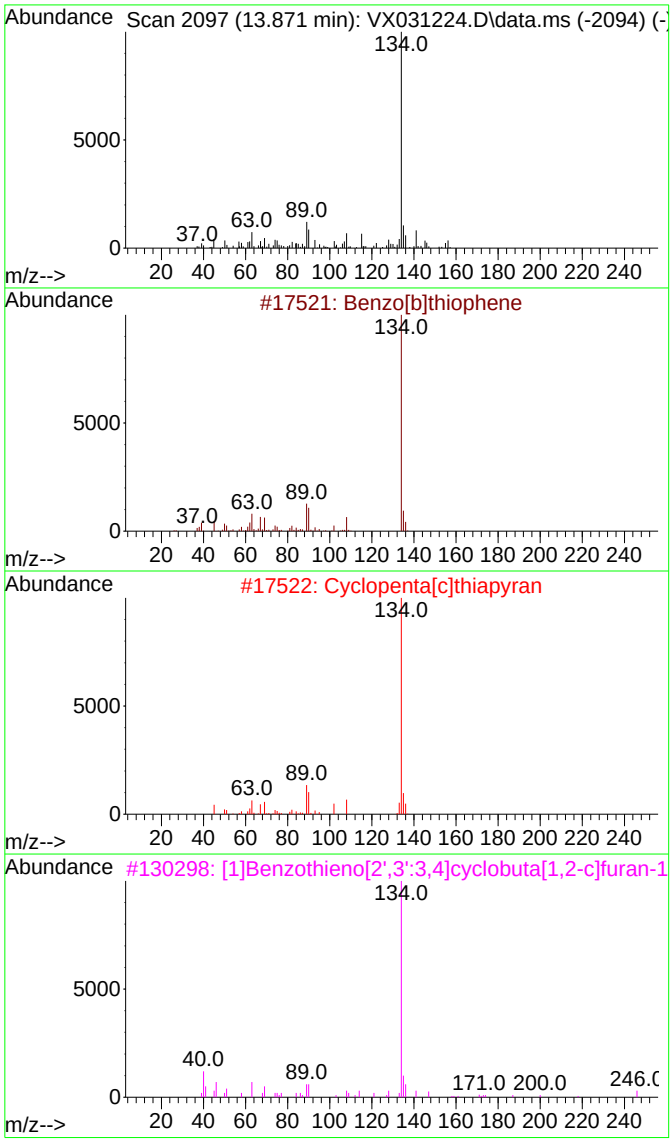
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

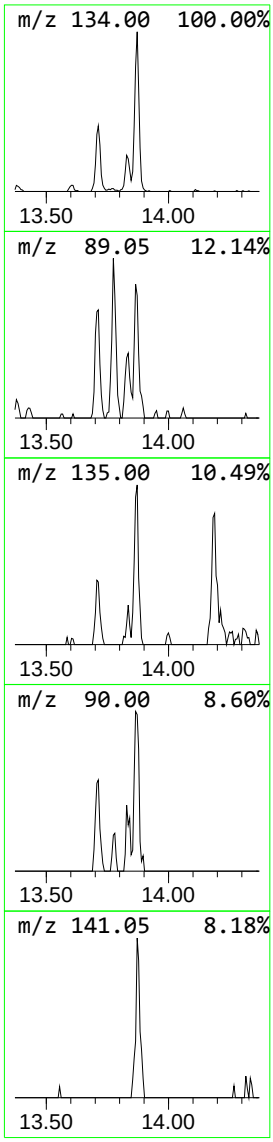
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzo[b]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	9.55 ug/l	61195	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene	134	C8H6S	000095-15-8	93
2	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	87
3	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	72
4	1H,1'H-2,2'-Biimidazole	134	C6H6N4	000492-98-8	53
5	3,4-Thiophenedicarbonitrile	134	C6H2N2S	018853-32-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

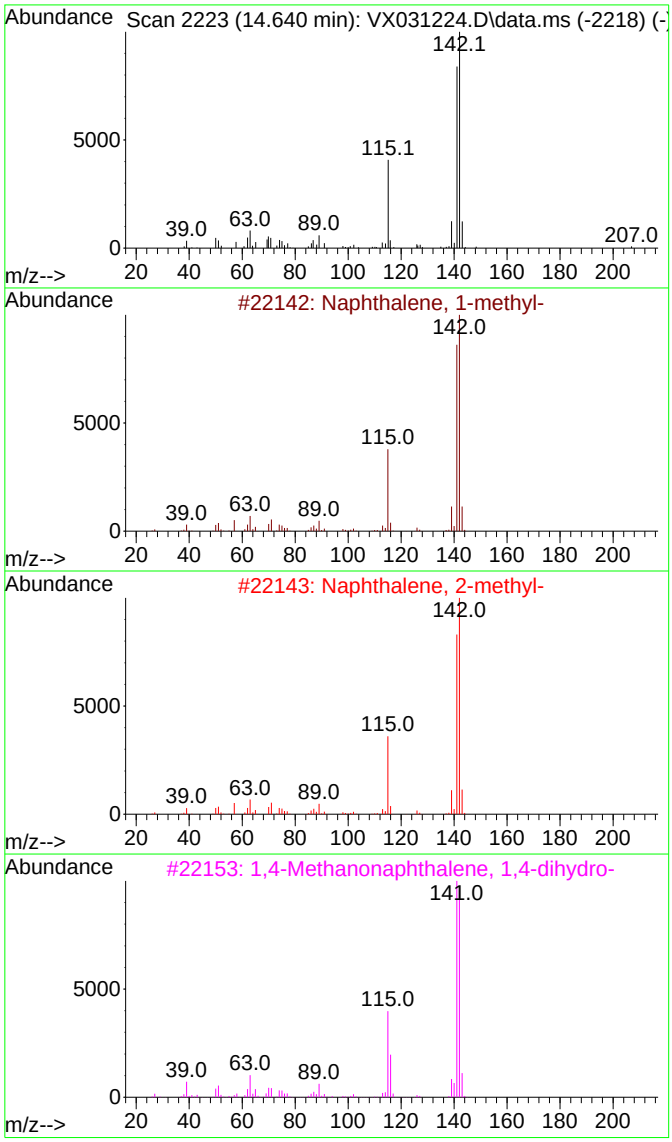
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

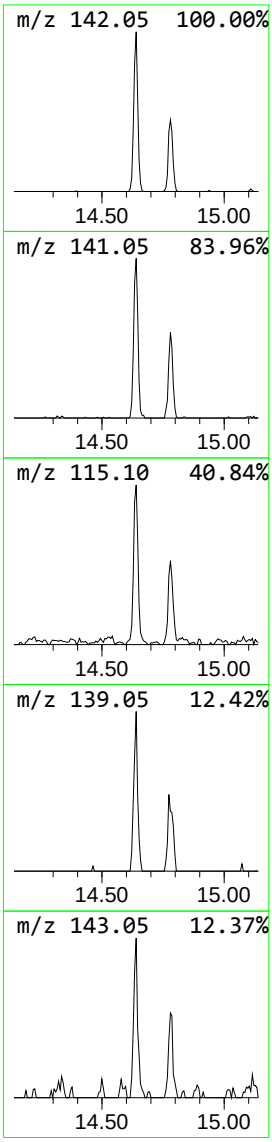
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	10.07 ug/l	64538	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Naphthalene, 1-(2-hydroxypropyl)	186	C13H14O	027653-13-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031224.D
Acq On : 08 Sep 2022 20:11
Operator : JC/MD
Sample : N4505-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-108

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.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
Isopropyl Alcohol	2.550	9.1	ug/l	41194	1	5.556	227193	50.0
Spiro[2,4]hepta...	8.220	7.0	ug/l	40124	2	6.763	286585	50.0
1,3,5-Cycloheptt...	9.445	16.2	ug/l	107680	3	10.055	332214	50.0
2-Heptanone	10.768	6.9	ug/l	46102	3	10.055	332214	50.0
1-Hexanol, 2-et...	12.226	13.6	ug/l	87110	4	12.024	320389	50.0
Indene	12.414	11.8	ug/l	75784	4	12.024	320389	50.0
Acetophenone	12.799	36.4	ug/l	232903	4	12.024	320389	50.0
Ethanone, 1-(3-...	13.713	12.1	ug/l	77781	4	12.024	320389	50.0
Benzo[b]thiophene	13.871	9.6	ug/l	61195	4	12.024	320389	50.0
Naphthalene, 1-...	14.640	10.1	ug/l	64538	4	12.024	320389	50.0