LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

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\82N062822W.M
Title : SW846 8260

Signal : TIC: VN073542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	48	53	61	rBV	28476	59101	1.30%	0.239%
2	3.634	289	297	311	rBV	31007	83734	1.85%	0.339%
3	4.222	388	397	407	rBV	77995	228408	5.04%	0.924%
4	7.745	986	996	1010	rBV3	19476	55390	1.22%	0.224%
5	7.951	1021	1031	1036	rBV	199298	466015	10.29%	1.886%
6	8.016	1036	1042	1054	rVB	361673	830463	18.33%	3.361%
7	8.375	1093	1103	1120	rBV2	250971	689942	15.23%	2.792%
8	8.904	1184	1193	1212	rVB	506779	1063953	23.49%	4.306%
9	10.275	1418	1426	1436	rBV2	35774	67852	1.50%	0.275%
10	10.381	1436	1444	1450	rBV	726972	1307480	28.86%	5.291%
11	10.445	1450	1455	1466	rVB	306942	572790	12.64%	2.318%
12	10.698	1491	1498	1510	rVB2	27444	53052	1.17%	0.215%
13	11.092	1558	1565	1570	rBV2	41331	85986	1.90%	0.348%
14	11.163	1570	1577	1587	rVV	578863	1071604	23.66%	4.337%
15	11.686	1658	1666	1670	rBV	767422	1375703	30.37%	5.567%
16	11.728	1670	1673	1679	rVV	288789	523104	11.55%	2.117%
17	11.786	1679	1683	1690	rVV	104641	224731	4.96%	0.909%
18	11.892	1690	1701	1711	rVV	540690	1176715	25.98%	4.762%
19	12.027	1714	1724	1736	rVB4	188669	440643	9.73%	1.783%
20	12.175	1745	1749	1751	rVV2	34497	55486	1.22%	0.225%
21	12.222	1751	1757	1766	rVB3	372960	716960	15.83%	2.901%
22	12.398	1782	1787	1792	rBV4	31735	53207	1.17%	0.215%
23	12.463	1792	1798	1802	rVV2	112308	206474	4.56%	0.836%
24	12.510	1802	1806	1814	rVB3	59799	116536	2.57%	0.472%
25	12.675	1827	1834	1845	rBV	648698	1184024	26.14%	4.791%
26	12.951	1869	1881	1886	rBV2	176893	378819	8.36%	1.533%
27	13.098	1893	1906	1908	rBV8	63546	231665	5.11%	0.937%
28	13.245	1925	1931	1934	rBV2	52094	93717	2.07%	0.379%
29	13.298	1934	1940	1946	rVV2	169177	451168	9.96%	1.826%
30	13.357	1946	1950	1955	rVV	75926	131823	2.91%	0.533%
31	13.410	1955	1959	1963	rVV2	60339	121022	2.67%	0.490%
32	13.498	1965	1974	1985	rVV5	166469	745636	16.46%	3.017%
33	13.616	1987	1994	2007	rVV	882847	1833456	40.48%	7.420%
34	13.710	2007	2010	2016	rVB4	28863	48299	1.07%	0.195%
35	13.810	2023	2027	2032	rBV2	40554	70520	1.56%	0.285%
36	13.945	2045	2050	2053	rBV2	41239	74633	1.65%	0.302%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

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\82N062822W.M
Title : SW846 8260

37	13.998	2053	2059	2066	rVV	359510	678456	14.98%	2.746%
38	14.080	2066	2073	2074	rVV5	47562	115514	2.55%	0.467%
39	14.098	2074	2076	2086	rVB4	56330	119577	2.64%	0.484%
40	14.369	2117	2122	2125	rBV2	28277	51166	1.13%	0.207%
41	14.663	2164	2172	2182	rVB2	33236	121713	2.69%	0.493%
42	14.857	2196	2205	2214	rBV2	33095	125085	2.76%	0.506%
43	15.016	2227	2232	2236	rVV4	28517	57438	1.27%	0.232%
44	15.080	2236	2243	2257	rVB8	41856	176865	3.90%	0.716%
45	15.433	2291	2303	2314	rBV	2256798	4529821	100.00%	18.331%
46	15.533	2314	2320	2328	rVB	86468	168962	3.73%	0.684%
47	16.457	2471	2477	2481	rBV3	21296	46594	1.03%	0.189%
48	16.527	2481	2489	2502	rVB	370736	860499	19.00%	3.482%
49	16.739	2516	2525	2533	rVB	337120	769399	16.99%	3.114%

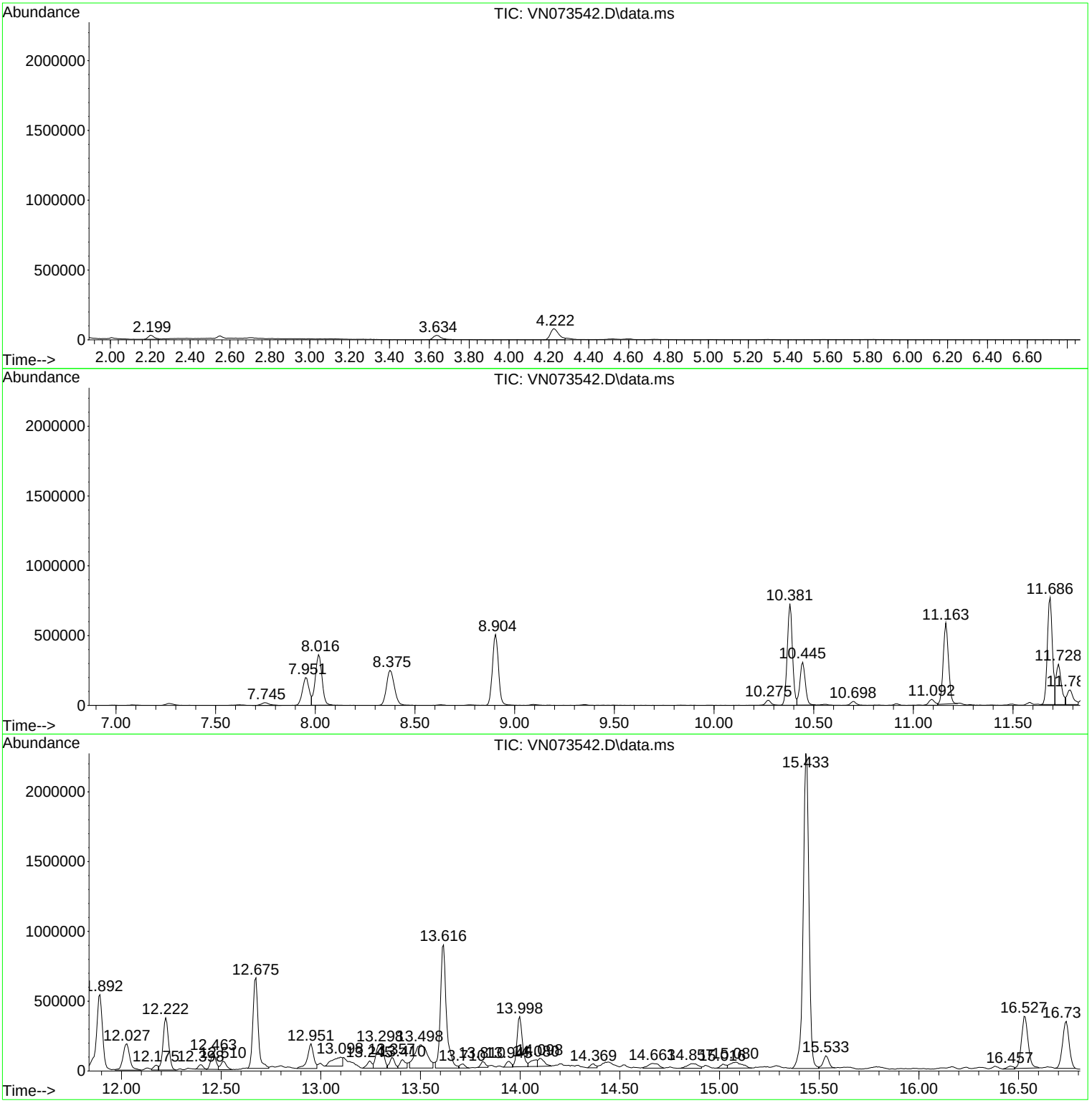
Sum of corrected areas: 24711200

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

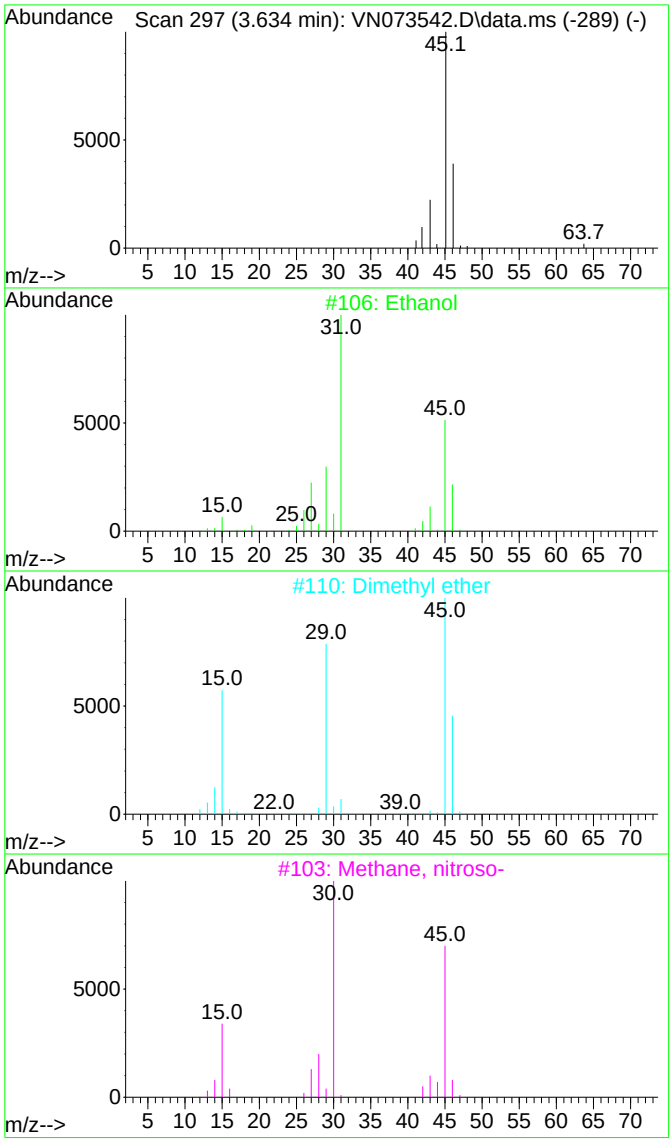
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

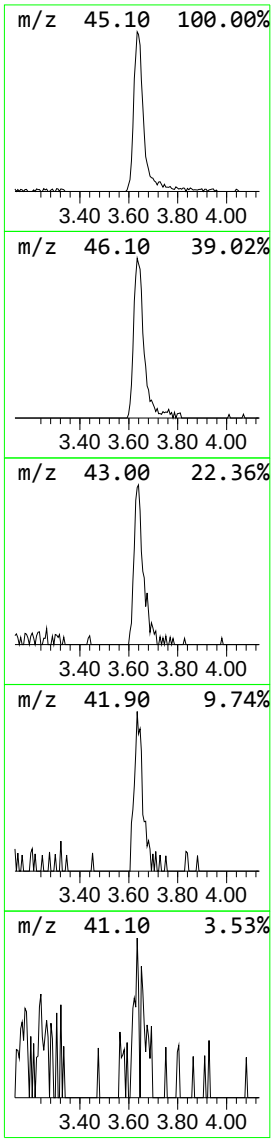
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	5.04 ug/l	83734	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Methoxyacetyl chloride	108	C3H5ClO2	038870-89-2	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

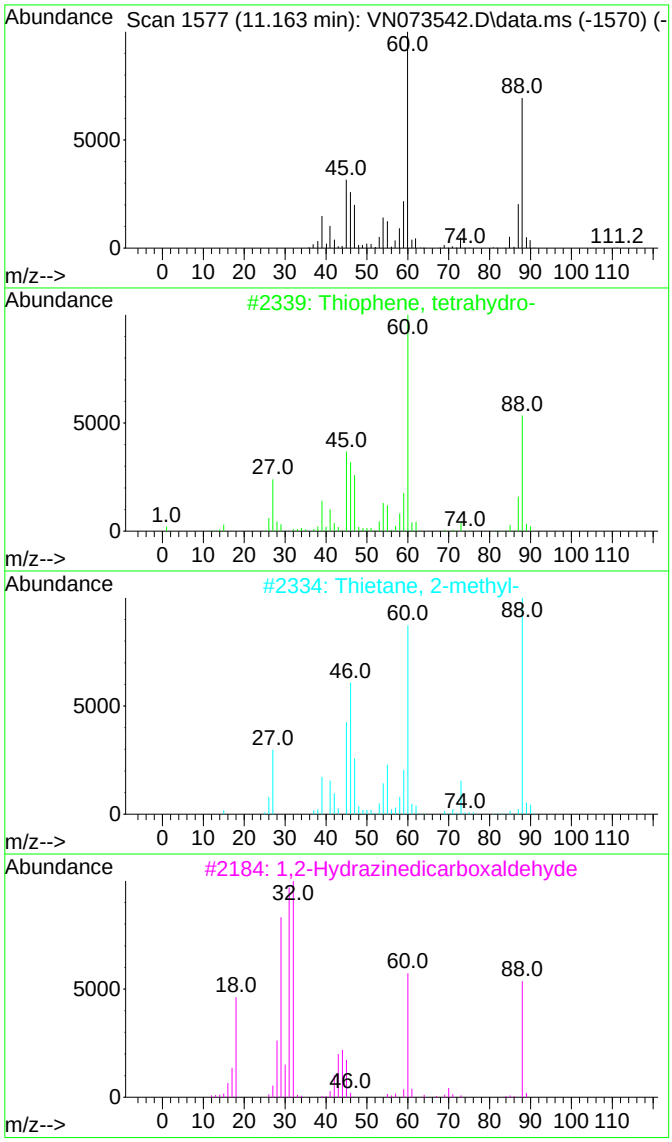
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

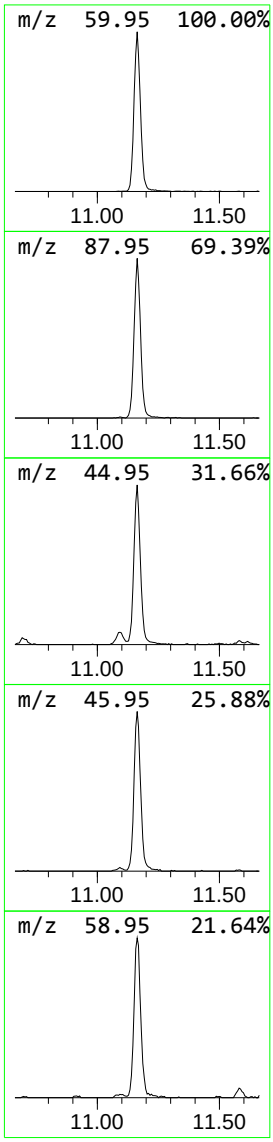
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Thiophene, tetrahydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	38.95 ug/l	1071600	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
4	Sulfide, allyl methyl	88	C4H8S	010152-76-8	25
5	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

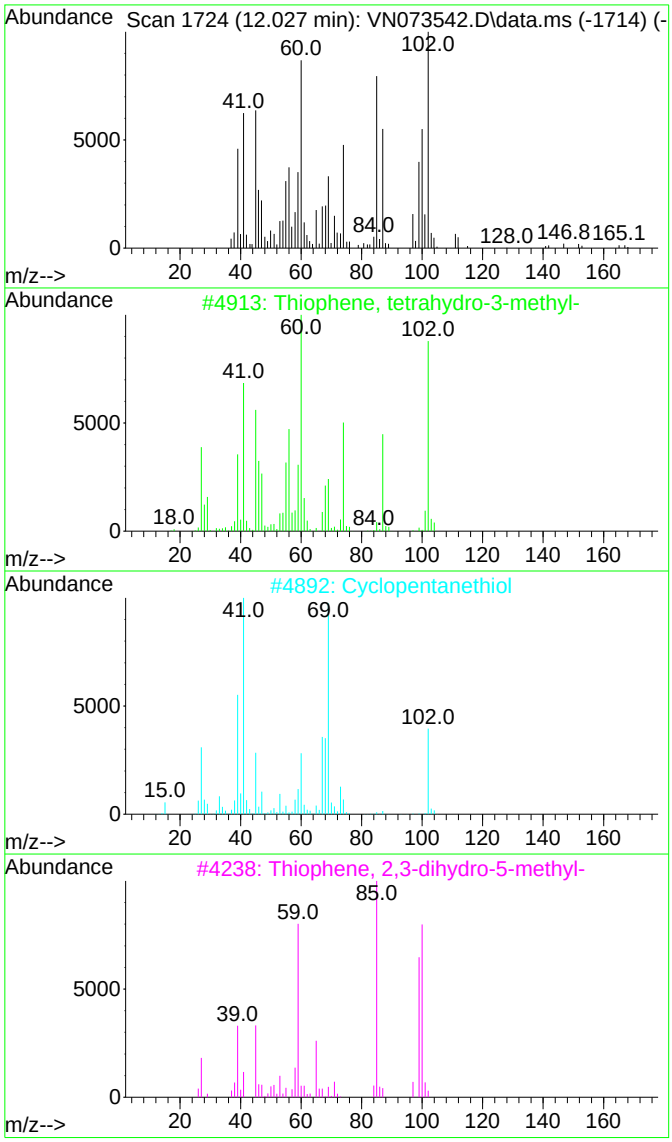
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

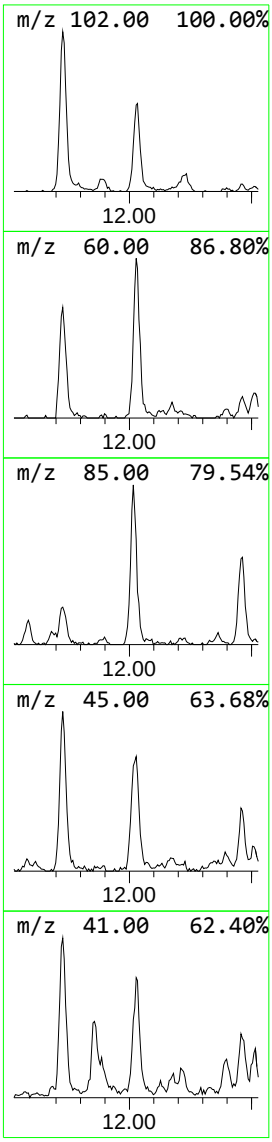
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	16.02 ug/l	440643	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	95
2	Cyclopentanethiol	102	C5H10S	001679-07-8	25
3	Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	16
4	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	14
5	1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

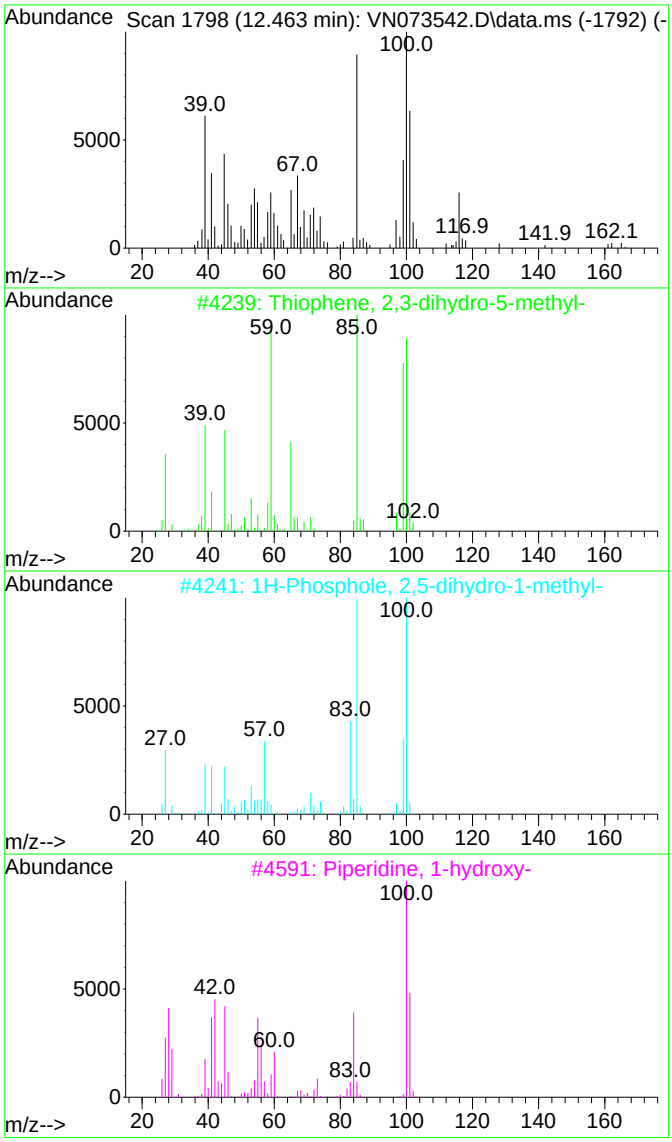
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

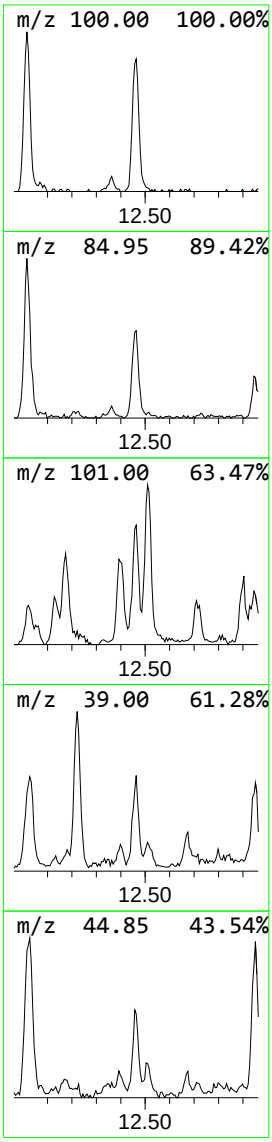
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown12.463 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	7.50 ug/l	206474	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	49
2	1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	43
3	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	38
4	Pentadecane-2,4-dione	240	C15H28O2	053759-23-2	35
5	D-Erythro-Tetrofuranose-3-ulose,...	198	C10H14O4	030645-00-2	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

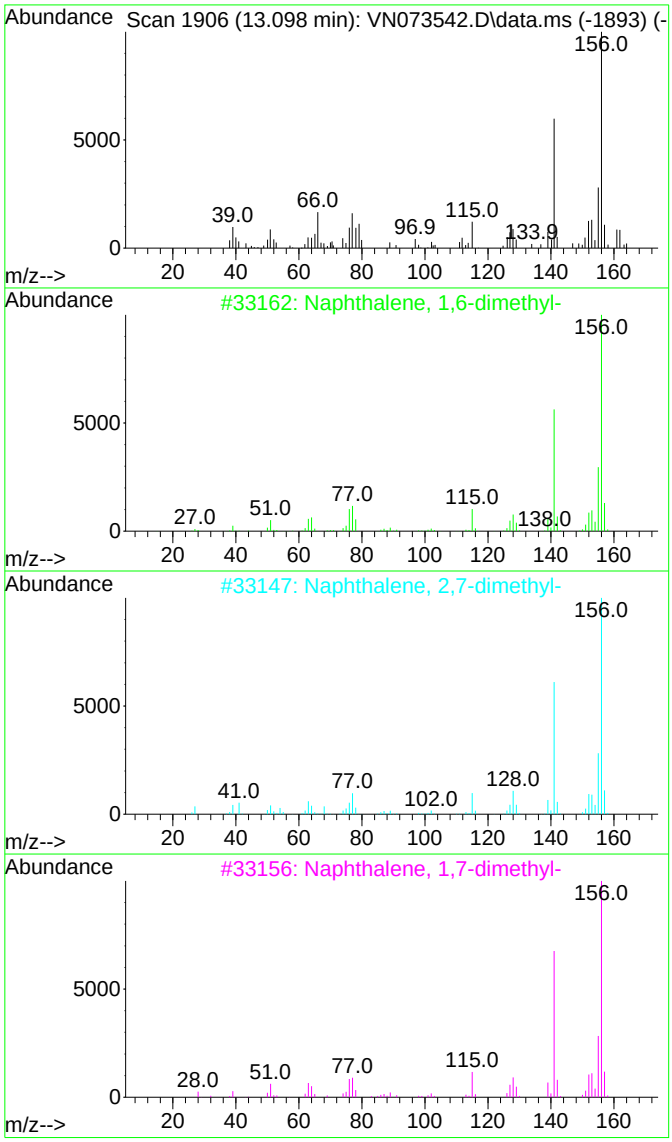
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

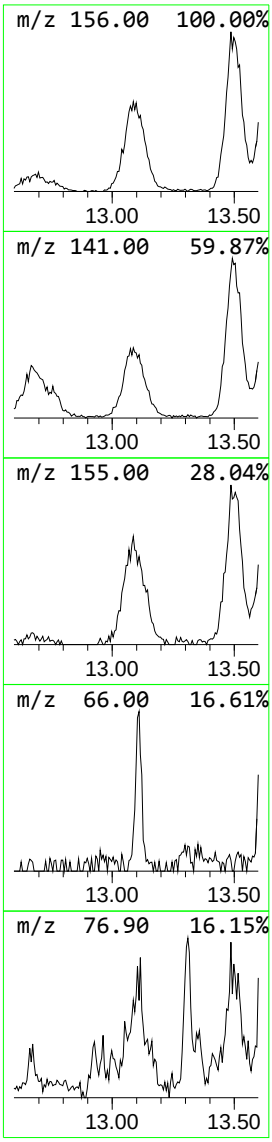
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	6.32 ug/l	231665	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

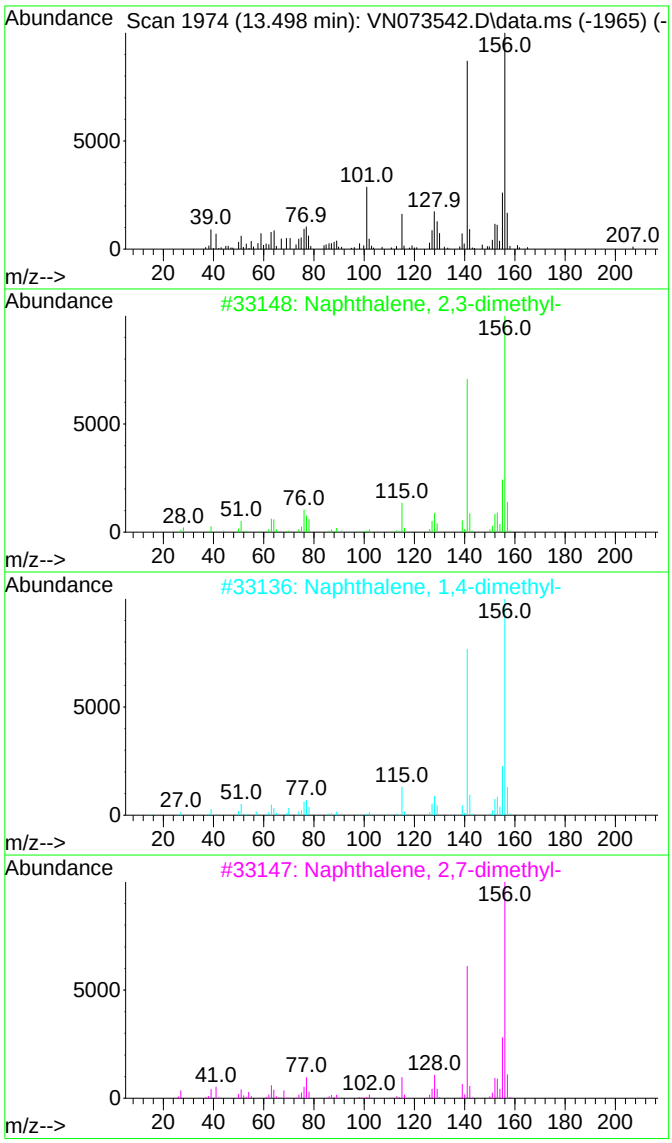
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

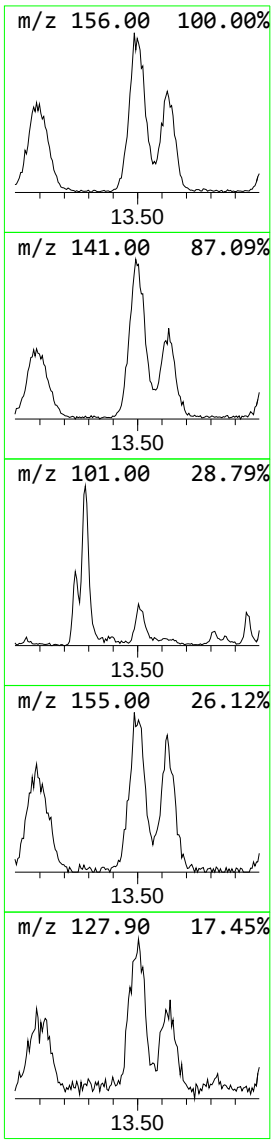
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	20.33 ug/l	745636	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

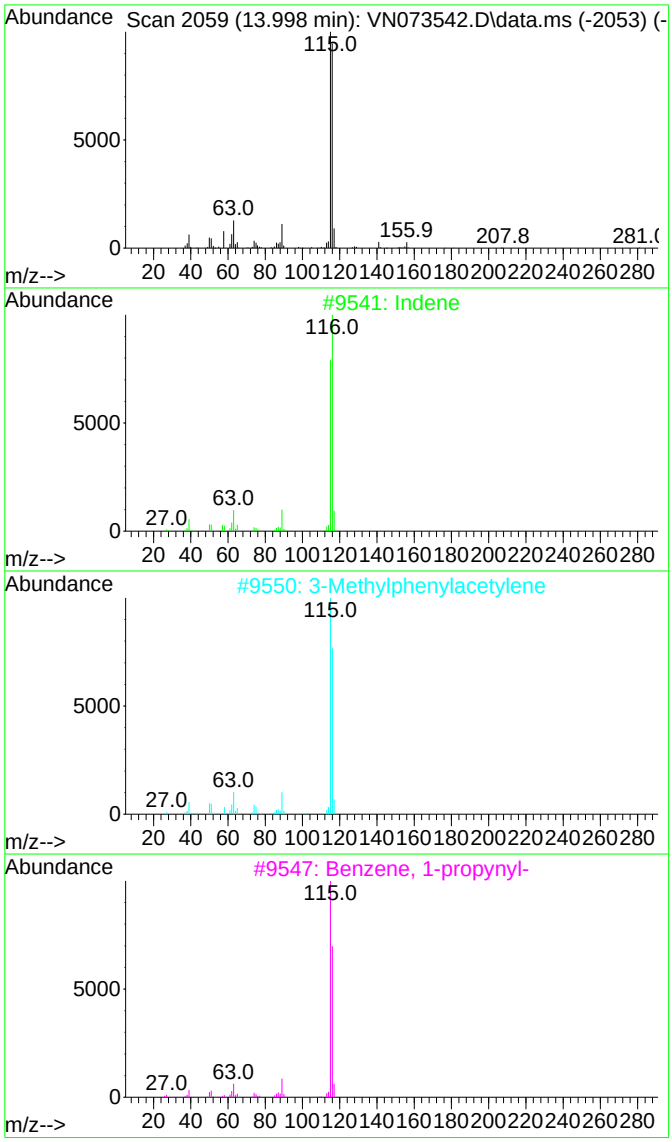
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

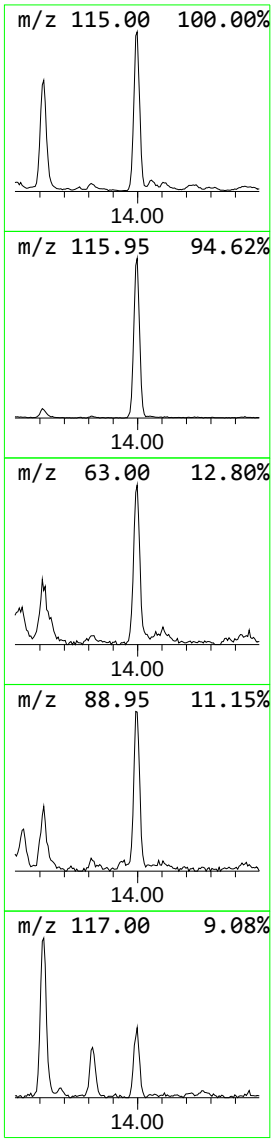
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	18.50 ug/l	678456	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

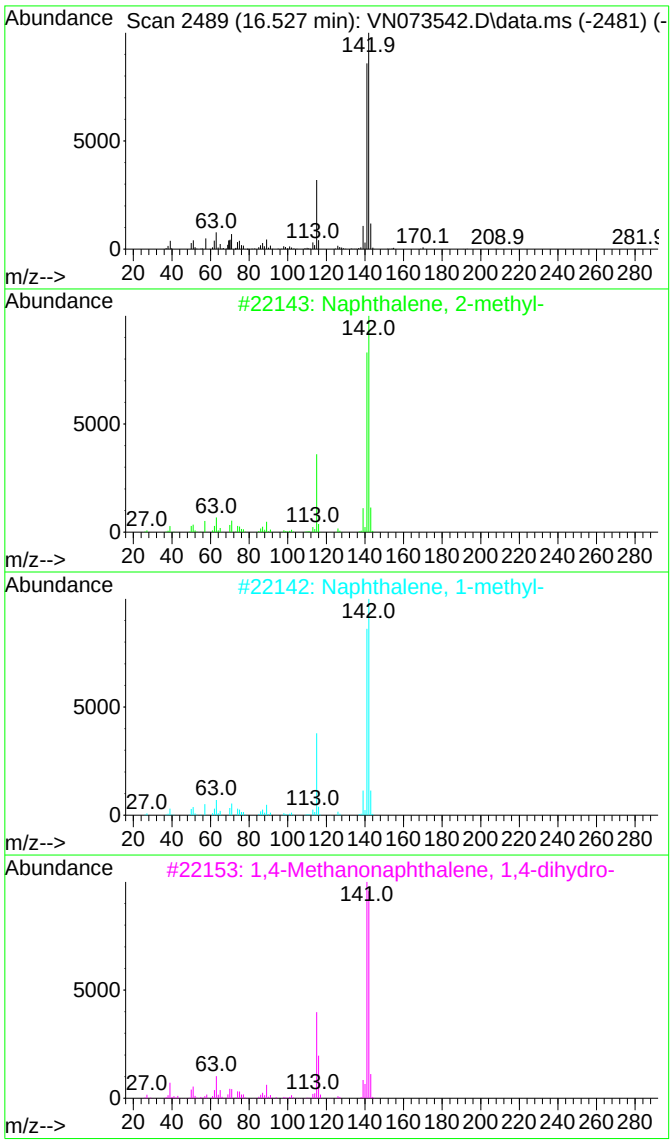
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

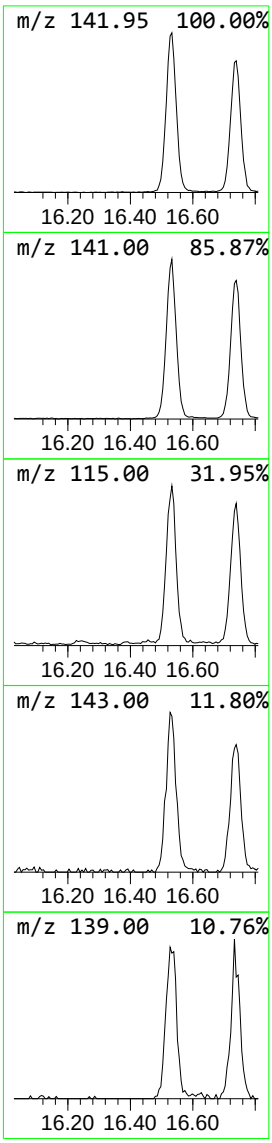
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	23.47 ug/l	860499	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

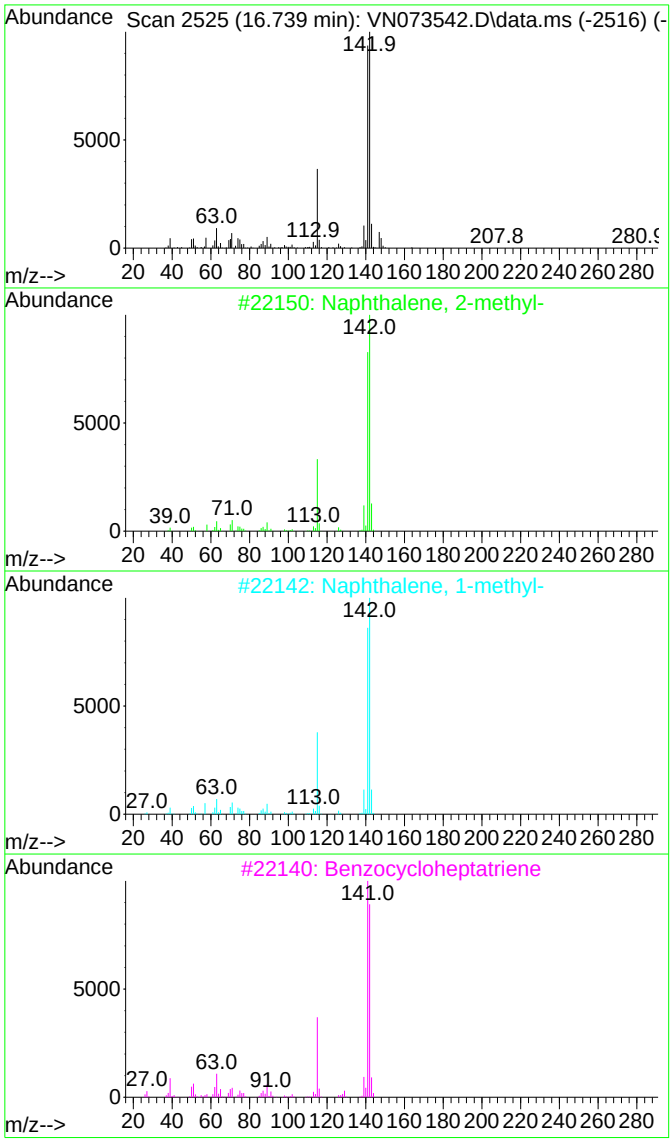
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

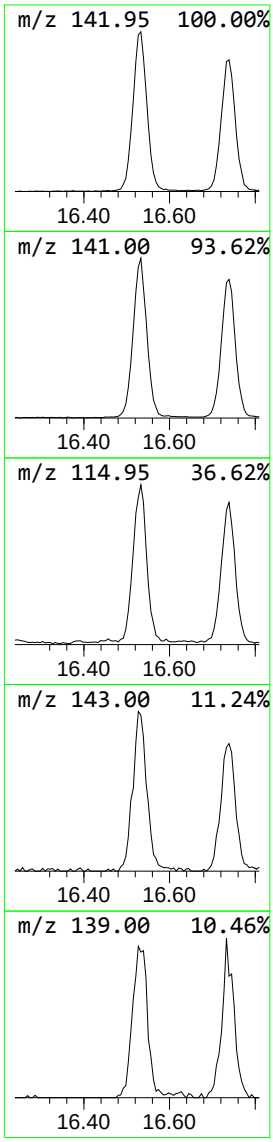
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	20.98 ug/l	769399	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	94
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073542.D
Acq On : 20 Jul 2022 23:27
Operator : JC\MD
Sample : N3779-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-H

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
Ethanol	3.634	5.0	ug/l	83734	1	8.016	830463	50.0
Thiophene, tetr...	11.163	39.0	ug/l	1071600	3	11.686	1375700	50.0
Thiophene, tetr...	12.028	16.0	ug/l	440643	3	11.686	1375700	50.0
unknown12.463	12.463	7.5	ug/l	206474	3	11.686	1375700	50.0
Naphthalene, 1,...	13.098	6.3	ug/l	231665	4	13.616	1833460	50.0
Naphthalene, 2,...	13.498	20.3	ug/l	745636	4	13.616	1833460	50.0
Indene	13.998	18.5	ug/l	678456	4	13.616	1833460	50.0
Naphthalene, 2-...	16.527	23.5	ug/l	860499	4	13.616	1833460	50.0
Naphthalene, 1-...	16.739	21.0	ug/l	769399	4	13.616	1833460	50.0