LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

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: VN073346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	238	245	253	rVB6	8583	21018	1.22%	0.094%
2	3.769	311	320	327	rBV3	8344	21960	1.28%	0.098%
3	4.769	478	490	509	rBV	49411	158909	9.26%	0.710%
4	5.210	552	565	579	rBV2	23705	95575	5.57%	0.427%
5	7.281	907	917	930	rBV3	24097	74032	4.31%	0.331%
6	7.945	1021	1030	1034	rBV	191224	450251	26.24%	2.011%
7	8.004	1034	1040	1051	rVV	374610	889251	51.82%	3.972%
8	8.210	1066	1075	1079	rBV3	9537	22177	1.29%	0.099%
9	8.363	1092	1101	1113	rBV	209202	499260	29.09%	2.230%
10	8.486	1113	1122	1126	rBV7	6926	18307	1.07%	0.082%
11	8.628	1140	1146	1155	rVB4	14210	33663	1.96%	0.150%
12	8.745	1159	1166	1176	rBV4	18237	47781	2.78%	0.213%
13	8.898	1183	1192	1202	rBV	522874	1105291	64.41%	4.937%
14	9.386	1261	1275	1281	rBV	92925	238897	13.92%	1.067%
15	9.569	1300	1306	1310	rBV8	10431	19261	1.12%	0.086%
16	9.669	1314	1323	1326	rVV5	16172	36477	2.13%	0.163%
17	9.810	1342	1347	1353	rVB5	22790	40778	2.38%	0.182%
18	9.951	1365	1371	1376	rBV3	28753	53806	3.14%	0.240%
19	10.010	1376	1381	1385	rBV3	26806	45926	2.68%	0.205%
20	10.139	1396	1403	1410	rBV4	26255	76464	4.46%	0.342%
21	10.333	1426	1436	1438	rBV	84808	198641	11.58%	0.887%
22	10.374	1438	1443	1449	rVV	816451	1536243	89.52%	6.861%
23	10.439	1449	1454	1462	rVB	865064	1575231	91.79%	7.035%
24	10.557	1468	1474	1483	rVB4	67735	157621	9.18%	0.704%
25	10.716	1496	1501	1509	rVB2	70944	128894	7.51%	0.576%
26	10.810	1511	1517	1522	rBV5	53936	113344	6.60%	0.506%
27	10.898	1528	1532	1537	rBV2	28232	48347	2.82%	0.216%
28	10.986	1543	1547	1553	rVB	59815	100062	5.83%	0.447%
29	11.092	1561	1565	1573	rVB2	36013	68272	3.98%	0.305%
30	11.163	1573	1577	1579	rBV3	23835	31729	1.85%	0.142%
31	11.227	1584	1588	1593	rVV	94148	151722	8.84%	0.678%
32	11.280	1593	1597	1603	rVB2	96872	169720	9.89%	0.758%
33	11.333	1603	1606	1610	rVB5	28087	34837	2.03%	0.156%
34	11.392	1611	1616	1620	rBV3	67535	113727	6.63%	0.508%
35	11.480	1625	1631	1638	rVV6	63316	178396	10.40%	0.797%
36	11.569	1641	1646	1651	rVV	63493	108418	6.32%	0.484%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

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	11.686	1659	1666	1676	rVB	811188	1466050	85.43%	6.548%
38	11.780	1679	1682	1685	rBV2	18443	29575	1.72%	0.132%
39	11.898	1693	1702	1705	rBV3	110195	275593	16.06%	1.231%
40	12.192	1745	1752	1761	rBV5	140723	396496	23.10%	1.771%
41	12.310	1768	1772	1776	rVB	123887	167826	9.78%	0.750%
42	12.392	1782	1786	1788	rBV4	81461	121336	7.07%	0.542%
43	12.674	1828	1834	1843	rBV	723833	1346389	78.46%	6.013%
44	12.839	1857	1862	1869	rBV3	119163	207002	12.06%	0.925%
45	12.992	1882	1888	1894	rBV5	220744	475289	27.70%	2.123%
46	13.133	1909	1912	1917	rVB6	101879	153786	8.96%	0.687%
47	13.221	1923	1927	1934	rVB	224547	349745	20.38%	1.562%
48	13.351	1946	1949	1953	rBV2	61422	78088	4.55%	0.349%
49	13.404	1955	1958	1961	rBV2	56774	82307	4.80%	0.368%
50	13.504	1968	1975	1979	rBV6	220383	511011	29.78%	2.282%
51	13.610	1988	1993	2003	rVB	979142	1716110	100.00%	7.665%
52	13.757	2015	2018	2020	rBV3	66818	95113	5.54%	0.425%
53	13.933	2043	2048	2053	rBV3	393426	633790	36.93%	2.831%
54	14.257	2100	2103	2109	rVB5	180305	313479	18.27%	1.400%
55	14.327	2111	2115	2121	rVB5	124129	241799	14.09%	1.080%
56	14.445	2131	2135	2139	rBV4	289864	483255	28.16%	2.158%
57	14.557	2151	2154	2157	rBV3	143926	184129	10.73%	0.822%
58	14.609	2159	2163	2168	rVV4	165253	266269	15.52%	1.189%
59	14.857	2200	2205	2210	rBV3	338714	749291	43.66%	3.347%
60	14.909	2210	2214	2221	rVB5	287085	616566	35.93%	2.754%
61	15.127	2247	2251	2255	rVB4	241567	388127	22.62%	1.733%
62	15.239	2265	2270	2277	rVB5	291030	582428	33.94%	2.601%
63	15.398	2293	2297	2305	rVB6	281268	555051	32.34%	2.479%
64	16.727	2517	2523	2533	rBV4	477718	1239648	72.24%	5.537%

Sum of corrected areas: 22389836

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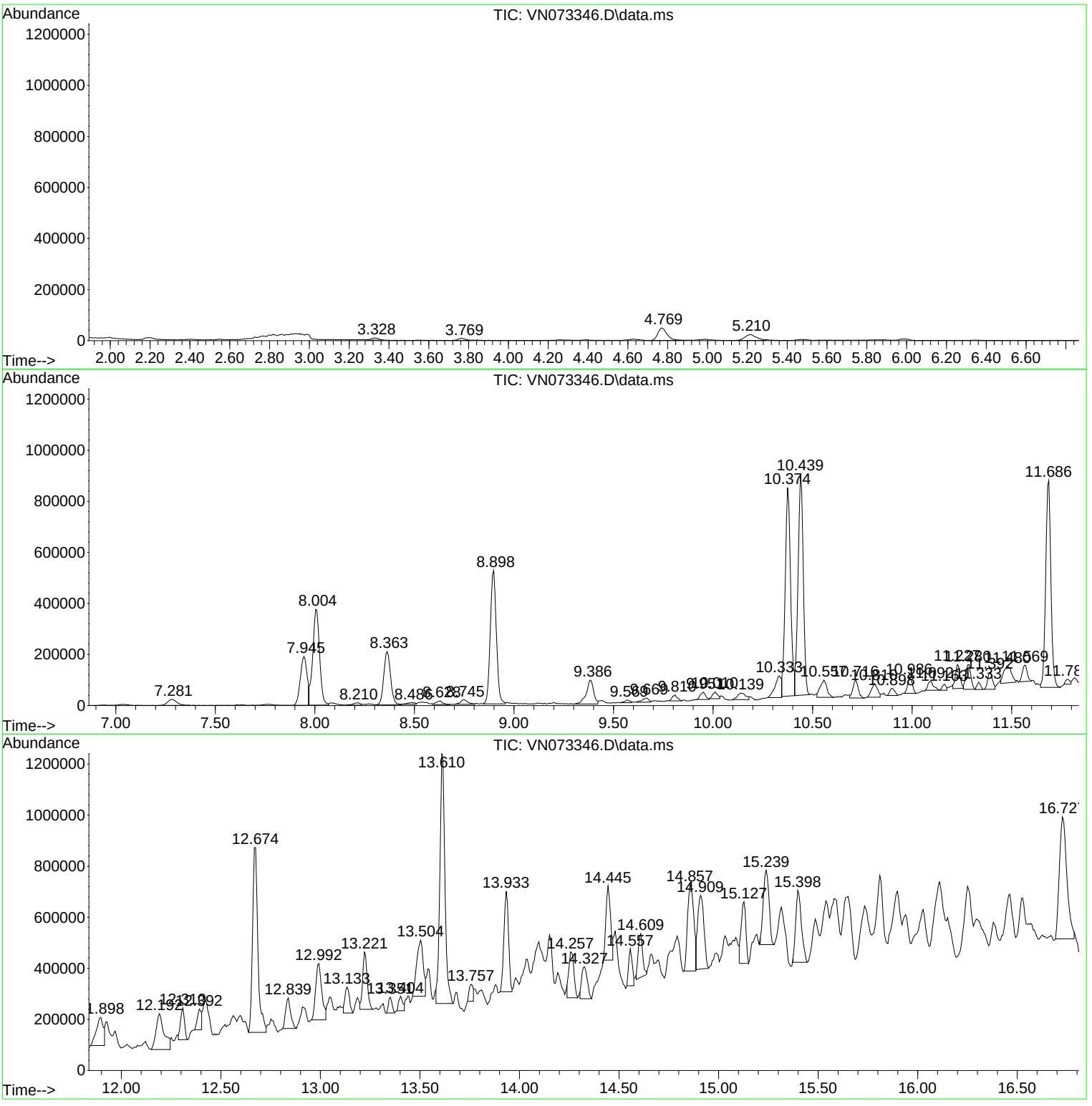
MSVOA_N
ClientSampleId :
WC-16-2-6

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\VN070622\
Data File : VN073346.D
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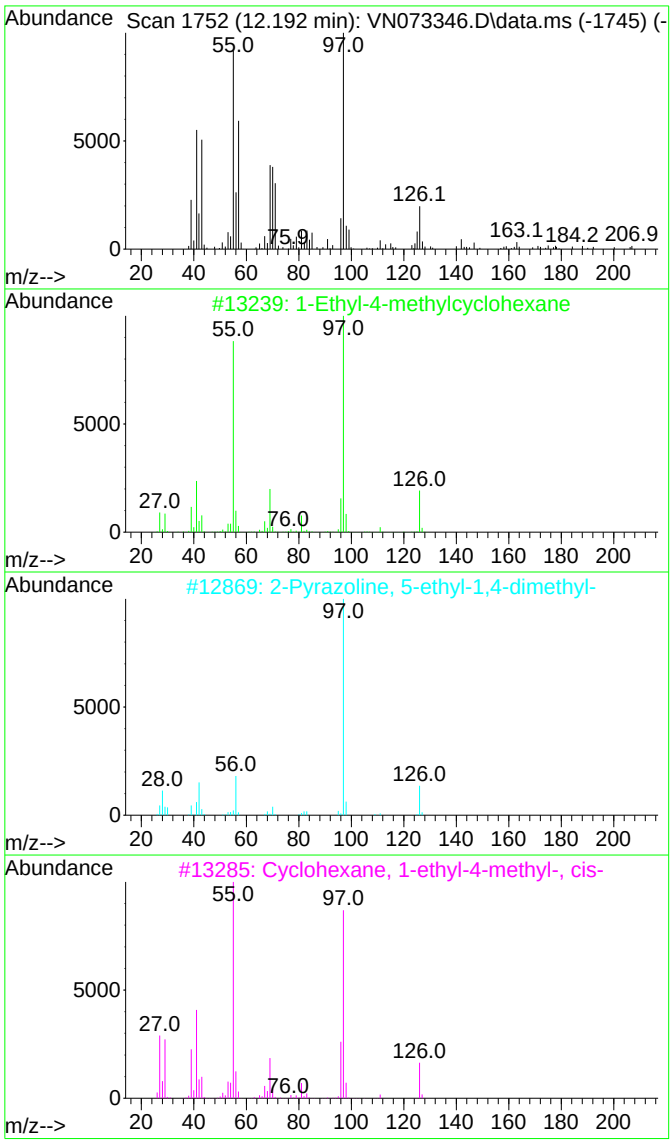
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

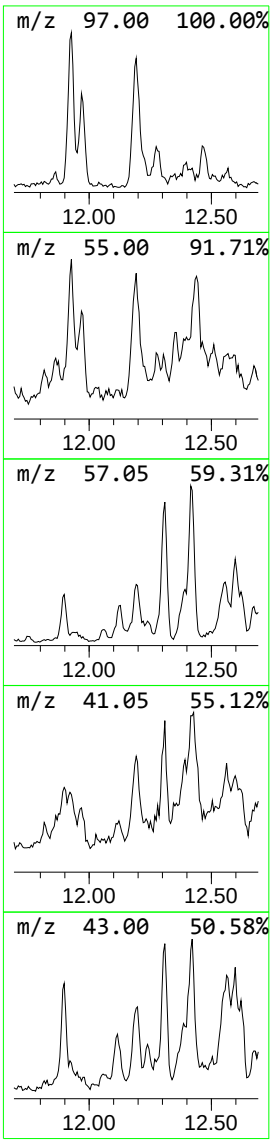
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Ethyl-4-methylcyclohexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.192	13.52 ug/l	396496	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	70
2	2-Pyrazoline, 5-ethyl-1,4-dimethyl-	126	C7H14N2	014339-23-2	52
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	52
4	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	52
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	52





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

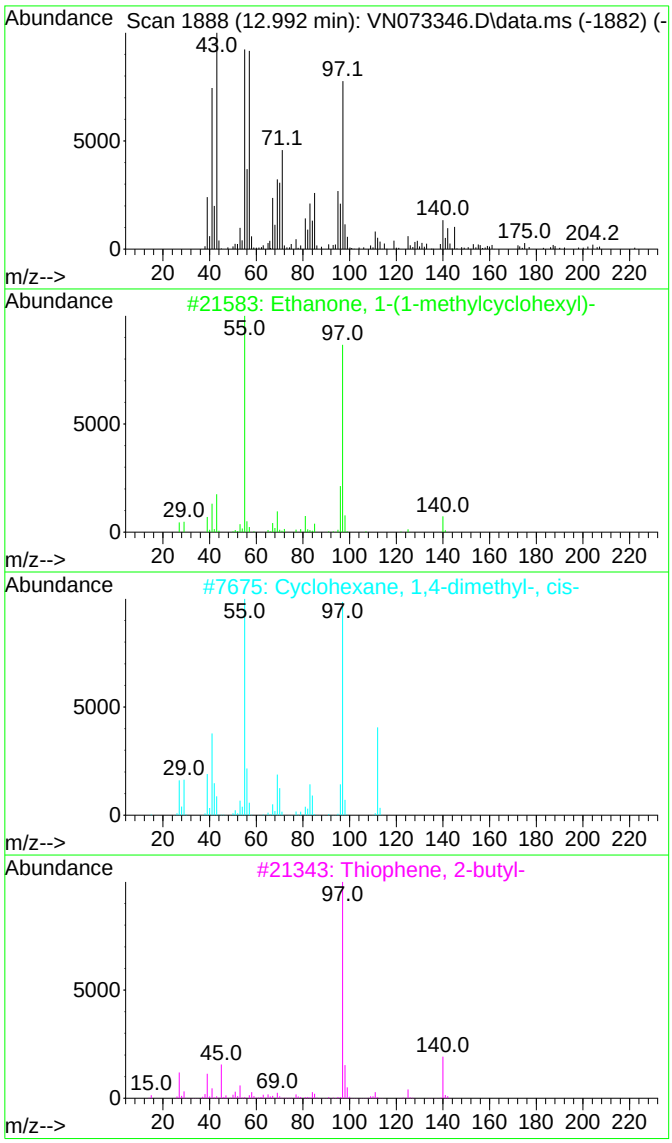
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

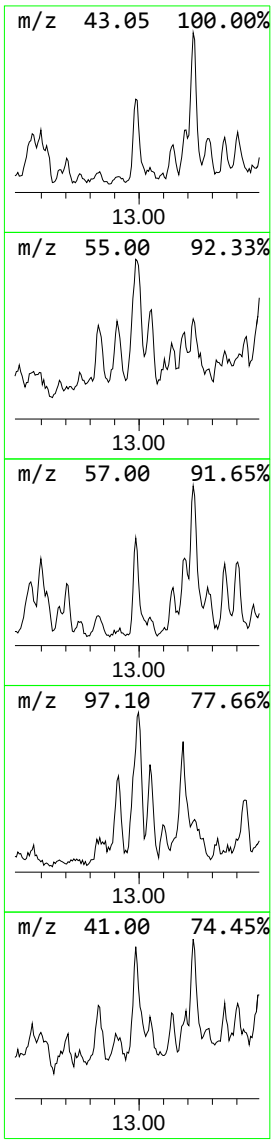
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown12.992 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.992	13.85 ug/l	475289	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	46
2	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	38
3	Thiophene, 2-butyl-	140	C8H12S	001455-20-5	38
4	Decane	142	C10H22	000124-18-5	38
5	2-Thiopheneacetic acid	142	C6H6O2S	001918-77-0	30





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Operator : JC\MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

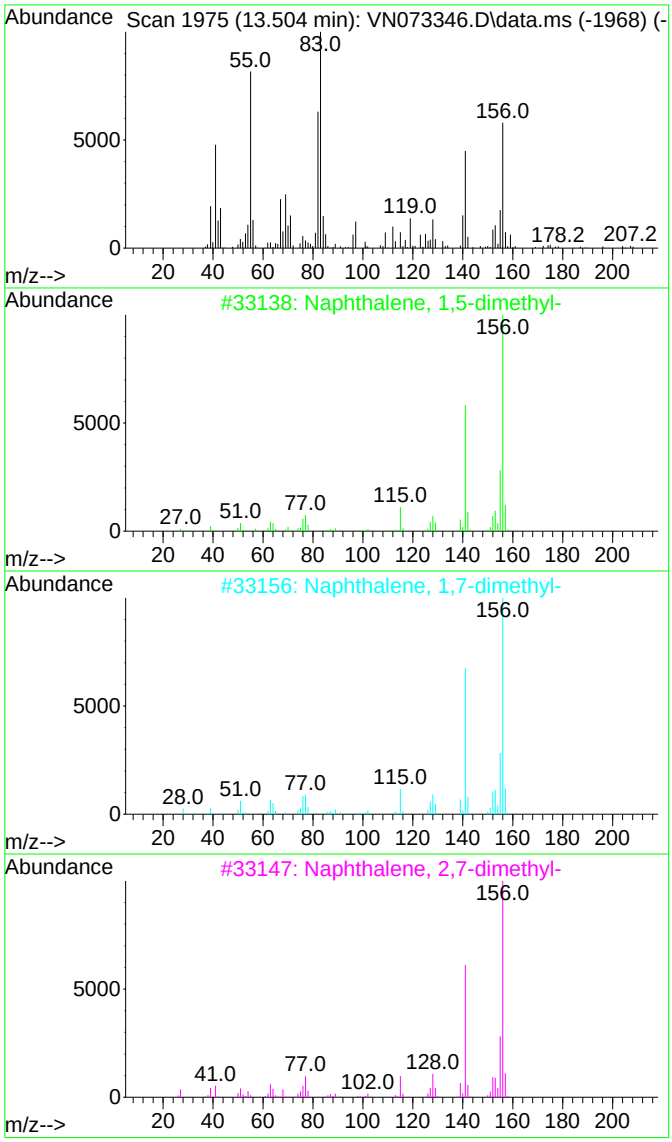
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

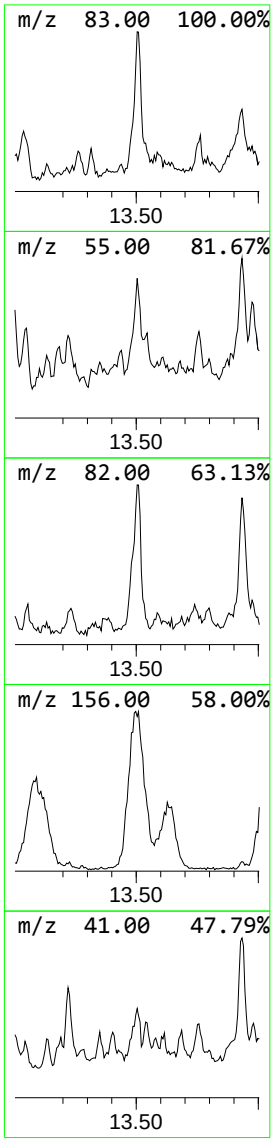
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	14.89 ug/l	511011	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	55
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	55
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	55
4	Cyclohexane, isothiocyanato-	141	C7H11NS	001122-82-3	53
5	Cyclohexane, butyl-	140	C10H20	001678-93-9	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
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Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

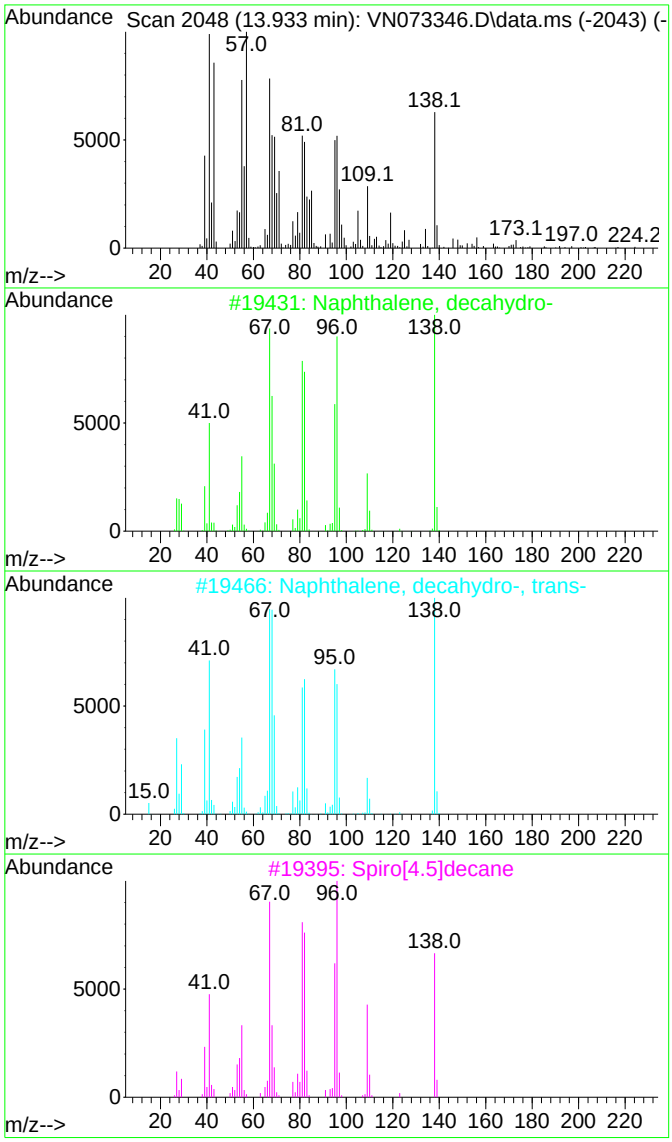
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

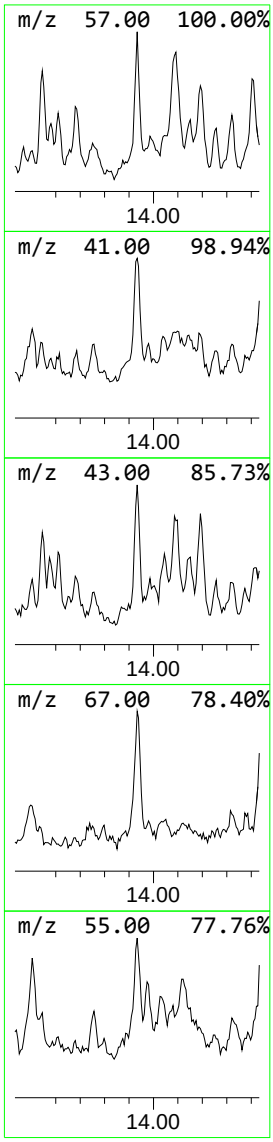
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, decahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	18.47 ug/l	633790	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
3	Spiro[4.5]decane	138	C10H18	000176-63-6	70
4	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	70
5	Spiro[4.4]nonan-2-one	138	C9H14O	034177-18-9	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
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Sample : N3564-16
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ALS Vial : 16 Sample Multiplier: 1

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

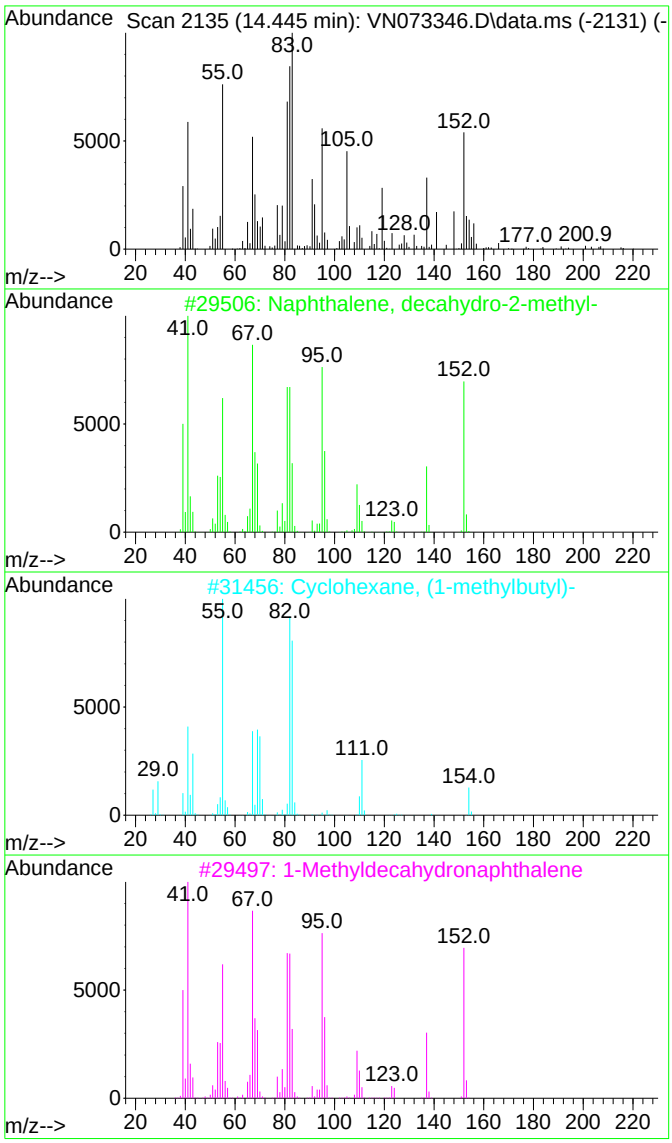
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

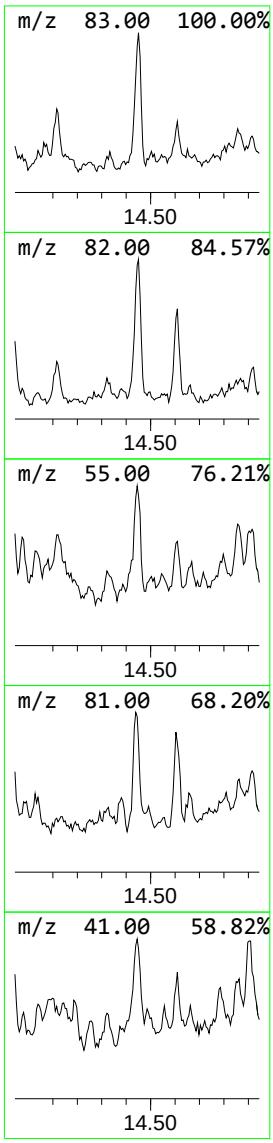
****

Peak Number 5 unknown14.445 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	14.08 ug/l	483255	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	46
2	Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	46
3	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	46
4	Cyclohexane, pentyl-	154	C11H22	004292-92-6	43
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

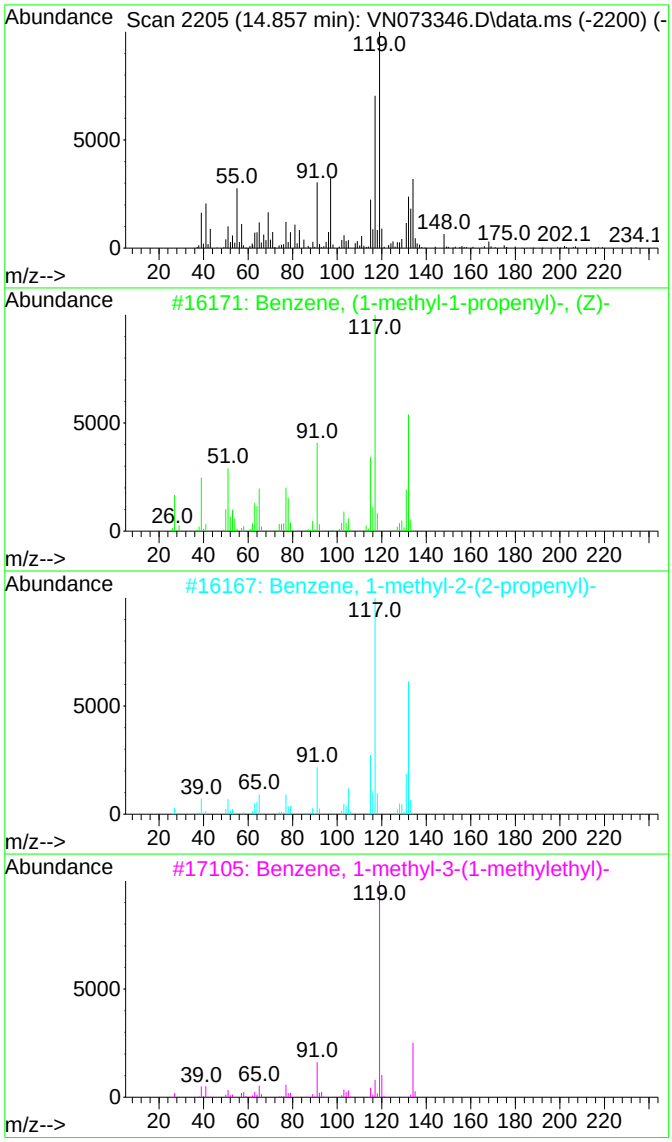
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

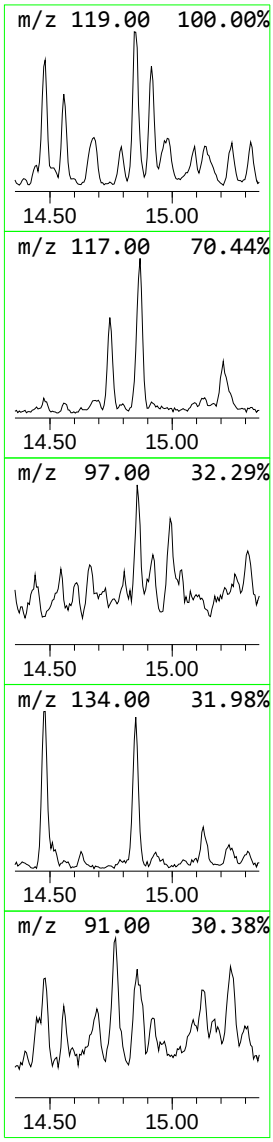
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (1-methyl-1-propen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	21.83 ug/l	749291	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	83
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	55
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	45
4	o-Cymene	134	C10H14	000527-84-4	43
5	p-Cymene	134	C10H14	000099-87-6	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

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

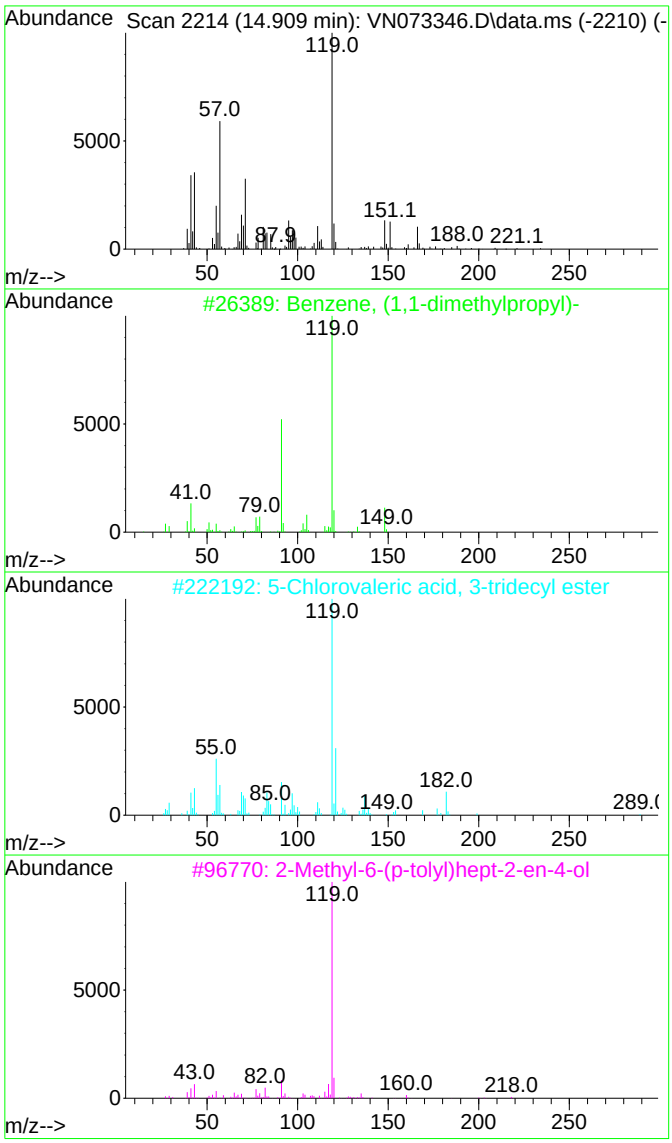
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

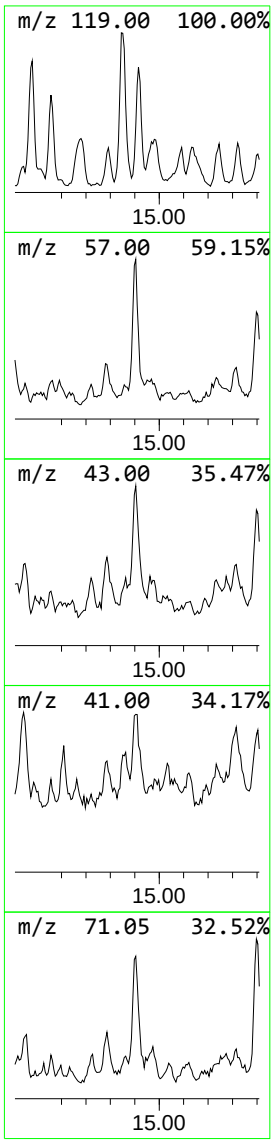
****

Peak Number 7 unknown14.910 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	17.96 ug/l	616566	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	47
2	5-Chlorovaleric acid, 3-tridecyl...	318	C18H35ClO2	1000299-91-3	43
3	2-Methyl-6-(p-tolyl)hept-2-en-4-ol	218	C15H22O	038142-57-3	43
4	p-Toluic acid, 5-tridecyl ester	318	C21H34O2	1000299-80-5	43
5	5-Chlorovaleric acid, 3-pentadec...	346	C20H39ClO2	1000299-92-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

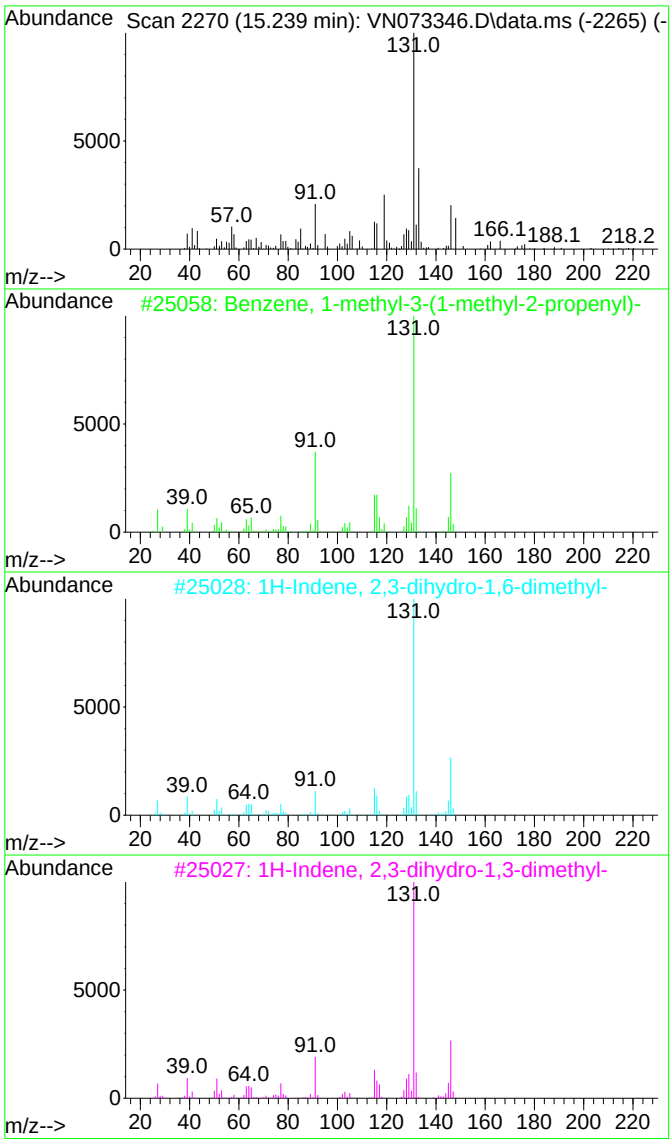
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

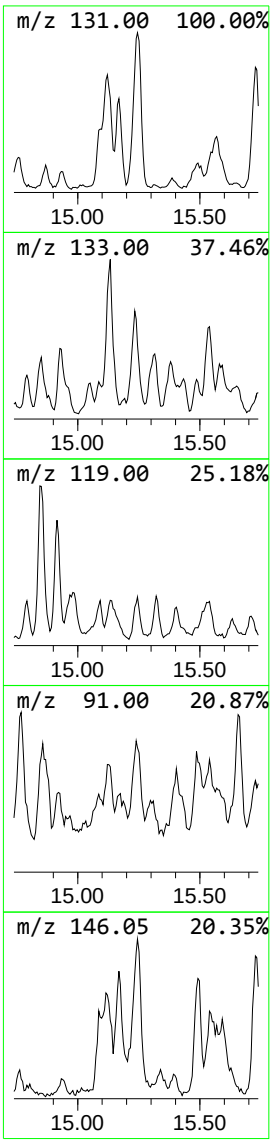
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-methyl-3-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	16.97 ug/l	582428	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	64
2	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	64
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	64
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	64
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

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

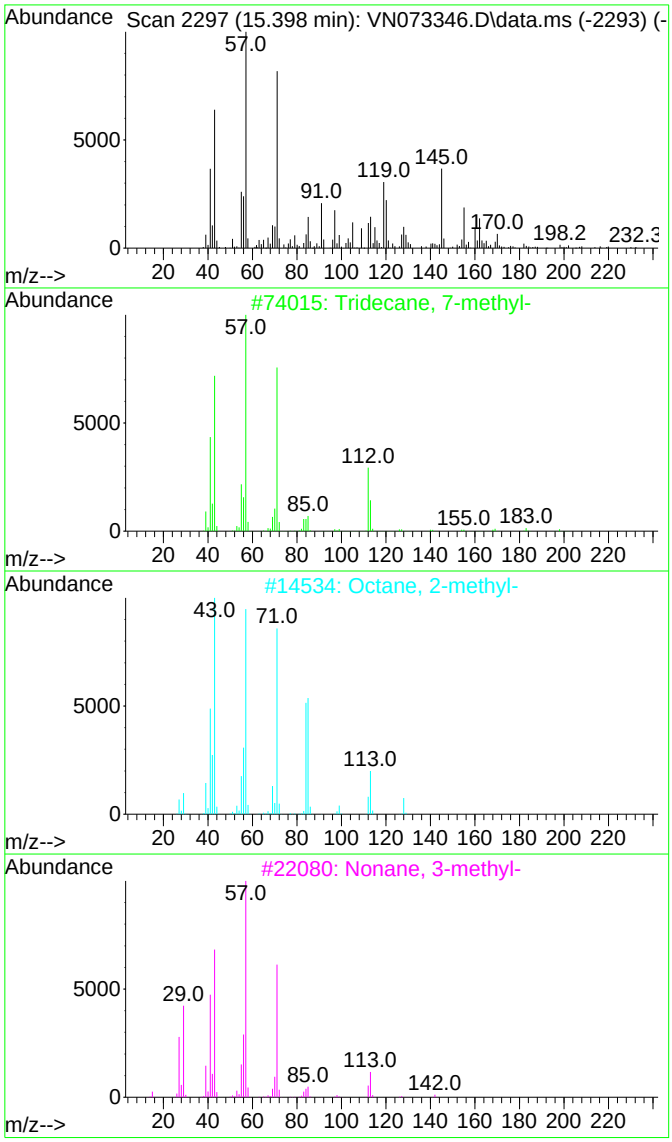
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

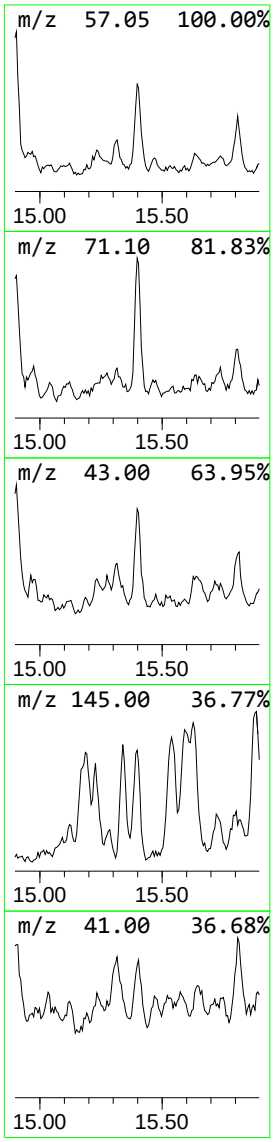
****

Peak Number 9 unknown15.398 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	16.17 ug/l	555051	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	46
2	Octane, 2-methyl-	128	C9H20	003221-61-2	43
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	41
4	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	41
5	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

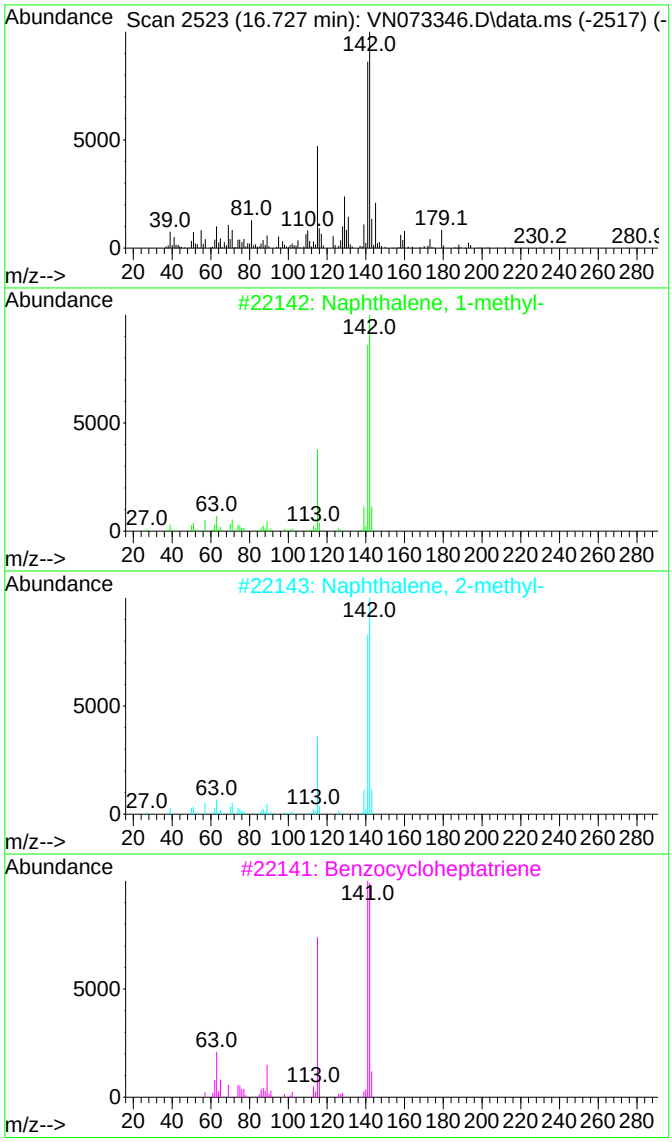
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

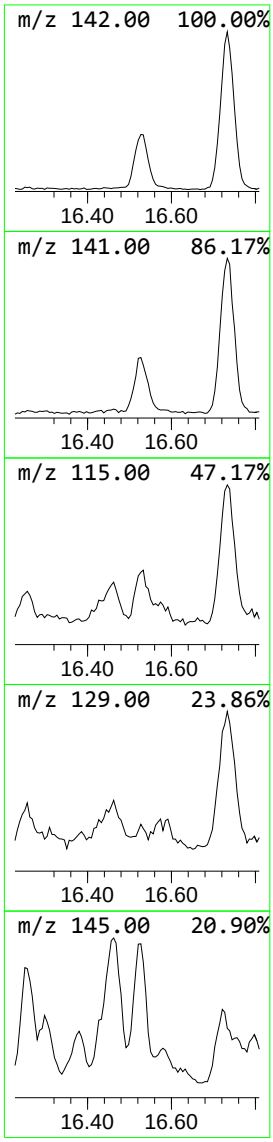
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.727	36.12 ug/l	1239650	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
3	Benzocycloheptatriene	142	C11H10	000264-09-5	76
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	76
5	Naphthalene, 1-(2-hydroxypropyl)	186	C13H14O	027653-13-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073346.D
Acq On : 06 Jul 2022 15:36
Operator : JC\MD
Sample : N3564-16
Misc : 4.87g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-6

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
1-Ethyl-4-methy...	12.192	13.5	ug/l	396496	3	11.686	1466050	50.0
unknown12.992	12.992	13.9	ug/l	475289	4	13.610	1716110	50.0
Naphthalene, 1,...	13.504	14.9	ug/l	511011	4	13.610	1716110	50.0
Naphthalene, de...	13.933	18.5	ug/l	633790	4	13.610	1716110	50.0
unknown14.445	14.445	14.1	ug/l	483255	4	13.610	1716110	50.0
Benzene, (1-met...	14.857	21.8	ug/l	749291	4	13.610	1716110	50.0
unknown14.910	14.910	18.0	ug/l	616566	4	13.610	1716110	50.0
Benzene, 1-meth...	15.239	17.0	ug/l	582428	4	13.610	1716110	50.0
unknown15.398	15.398	16.2	ug/l	555051	4	13.610	1716110	50.0
Naphthalene, 1-...	16.727	36.1	ug/l	1239650	4	13.610	1716110	50.0