LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

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\82N011425W.M
Title : SW846 8260

Signal : TIC: VN085731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.330	902	914	932	rBV2	187184	567347	7.78%	1.039%
2	8.000	1020	1028	1037	rVB	70852	164669	2.26%	0.302%
3	8.165	1046	1056	1060	rBV2	208538	488841	6.71%	0.895%
4	8.253	1060	1071	1080	rVV2	464043	1874081	25.71%	3.432%
5	8.577	1119	1126	1137	rVV3	231275	595667	8.17%	1.091%
6	8.735	1140	1153	1158	rVV3	145518	427765	5.87%	0.783%
7	8.788	1158	1162	1168	rVV2	71039	171162	2.35%	0.313%
8	8.853	1168	1173	1181	rVV2	80284	186677	2.56%	0.342%
9	9.100	1206	1215	1222	rBV	581899	1231404	16.89%	2.255%
10	9.376	1258	1262	1271	rVB2	34405	75006	1.03%	0.137%
11	9.600	1280	1300	1308	rBV	510933	1212195	16.63%	2.220%
12	9.776	1322	1330	1337	rBV3	48291	93390	1.28%	0.171%
13	9.965	1350	1362	1366	rBV3	96277	309716	4.25%	0.567%
14	10.006	1366	1369	1378	rVB4	54400	116448	1.60%	0.213%
15	10.100	1378	1385	1390	rBV	79626	155329	2.13%	0.284%
16	10.447	1437	1444	1456	rVB	254360	511243	7.01%	0.936%
17	10.565	1456	1464	1470	rBV	913074	1725020	23.66%	3.159%
18	10.629	1470	1475	1483	rVB	310720	602113	8.26%	1.103%
19	10.759	1488	1497	1503	rVV4	146812	335255	4.60%	0.614%
20	10.829	1503	1509	1517	rVV2	113558	207548	2.85%	0.380%
21	10.906	1517	1522	1529	rVB	63689	113126	1.55%	0.207%
22	11.000	1529	1538	1546	rBV6	57804	164610	2.26%	0.301%
23	11.418	1605	1609	1614	rVB2	54808	88761	1.22%	0.163%
24	11.865	1677	1685	1692	rVV	723428	1300614	17.84%	2.382%
25	11.959	1692	1701	1711	rVV	1941474	3327511	45.65%	6.094%
26	12.070	1711	1720	1739	rVB	3919348	7287622	99.97%	13.347%
27	12.394	1763	1775	1794	rVB	1974597	3285080	45.06%	6.016%
28	12.576	1795	1806	1811	rBV3	40685	103351	1.42%	0.189%
29	12.694	1819	1826	1832	rBV	376727	613362	8.41%	1.123%
30	12.847	1845	1852	1862	rBV	596282	1026168	14.08%	1.879%
31	13.029	1877	1883	1889	rBV	345024	588864	8.08%	1.078%
32	13.094	1889	1894	1897	rVV	819140	1397185	19.17%	2.559%
33	13.129	1897	1900	1904	rVV	920201	1366306	18.74%	2.502%
34	13.170	1904	1907	1913	rVB	182654	275838	3.78%	0.505%
35	13.335	1927	1935	1944	rVB	1361242	2293490	31.46%	4.200%
36	13.476	1952	1959	1966	rVV	4521583	7289685	100.00%	13.350%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

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\82N011425W.M
Title : SW846 8260

37	13.611	1972	1982	1987	rVB3	45380	120689	1.66%	0.221%
38	13.670	1987	1992	1996	rBV	104462	159659	2.19%	0.292%
39	13.729	1996	2002	2006	rBV2	126124	216942	2.98%	0.397%
40	13.817	2006	2017	2033	rVB2	1558543	3832912	52.58%	7.020%
41	13.947	2033	2039	2041	rBV	139018	208840	2.86%	0.382%
42	13.994	2041	2047	2052	rBV	662934	1114873	15.29%	2.042%
43	14.111	2062	2067	2072	rBV	61370	99581	1.37%	0.182%
44	14.176	2072	2078	2084	rVV2	168338	276670	3.80%	0.507%
45	14.241	2084	2089	2091	rBV	232287	352664	4.84%	0.646%
46	14.270	2091	2094	2099	rVV	247233	374149	5.13%	0.685%
47	14.329	2099	2104	2110	rVB	341150	526527	7.22%	0.964%
48	14.394	2110	2115	2118	rBV	90925	153829	2.11%	0.282%
49	14.441	2118	2123	2132	rVB2	438225	762820	10.46%	1.397%
50	14.570	2139	2145	2151	rVB2	129566	207555	2.85%	0.380%
51	14.653	2151	2159	2161	rVV	180344	299151	4.10%	0.548%
52	14.688	2161	2165	2170	rVV	341066	556775	7.64%	1.020%
53	14.923	2200	2205	2211	rBV	226611	389106	5.34%	0.713%
54	15.047	2217	2226	2232	rBV2	491409	1141069	15.65%	2.090%
55	15.111	2232	2237	2246	rVB3	88581	179824	2.47%	0.329%
56	15.206	2246	2253	2261	rBV2	165777	304542	4.18%	0.558%
57	15.311	2261	2271	2276	rBV3	82368	219290	3.01%	0.402%
58	15.435	2284	2292	2299	rVB3	71675	179452	2.46%	0.329%
59	15.635	2319	2326	2334	rVB	631288	1178429	16.17%	2.158%
60	15.741	2337	2344	2350	rBV	90375	175177	2.40%	0.321%

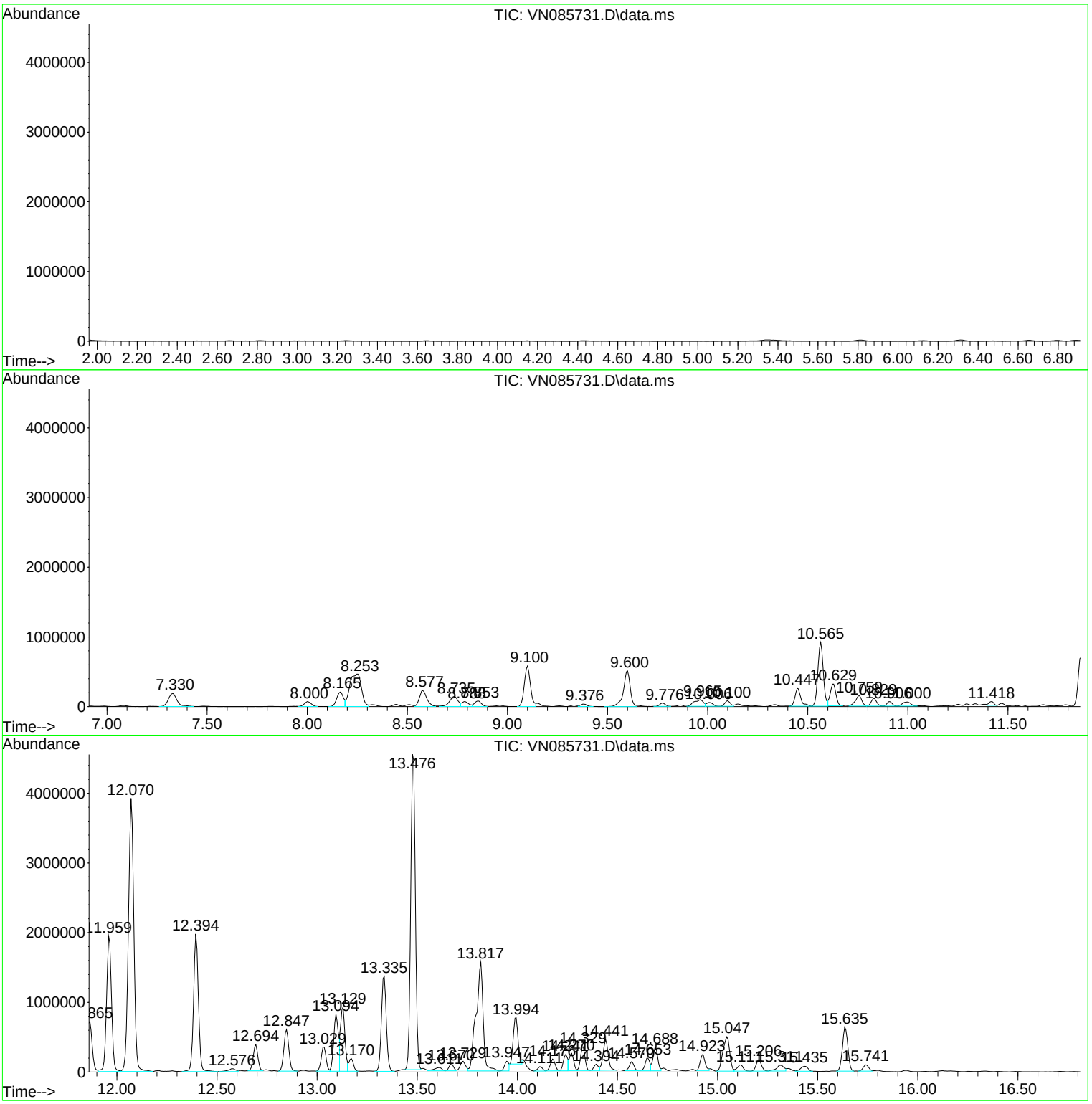
Sum of corrected areas: 54602974

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

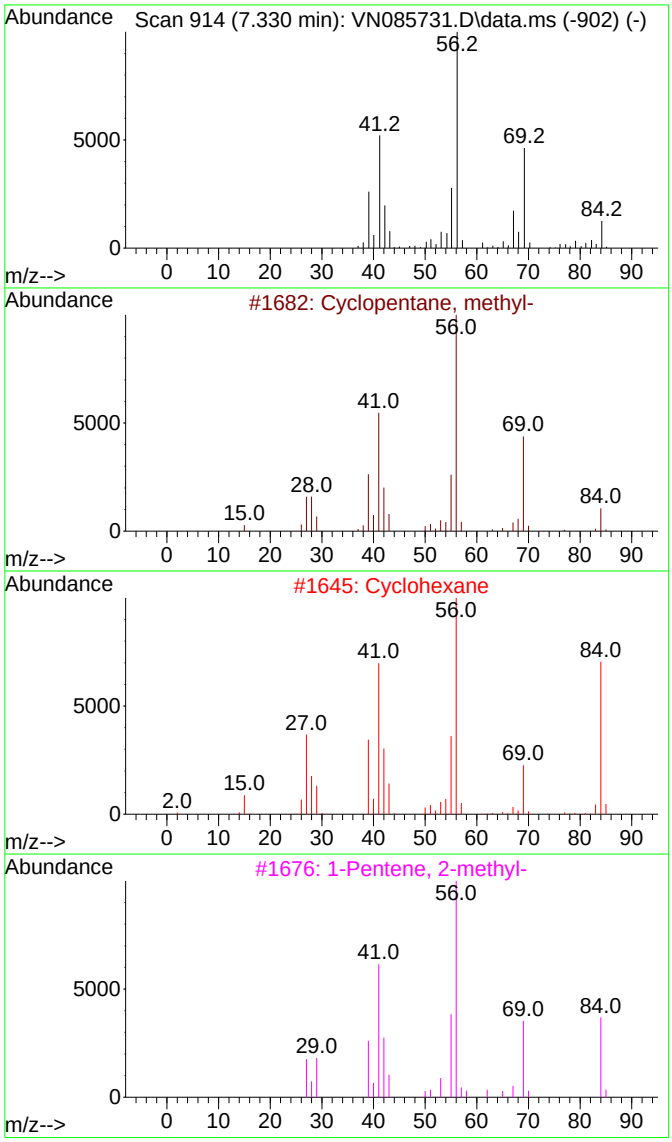
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

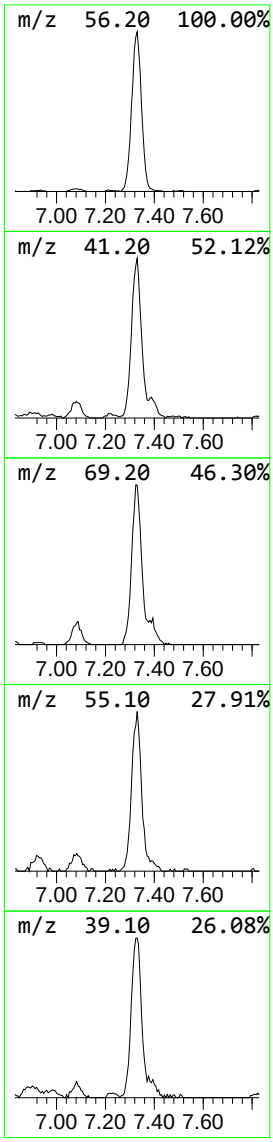
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.330	15.14 ug/l	567347	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclohexane	84	C6H12	000110-82-7	74
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	58
5	Cyclobutane	56	C4H8	000287-23-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

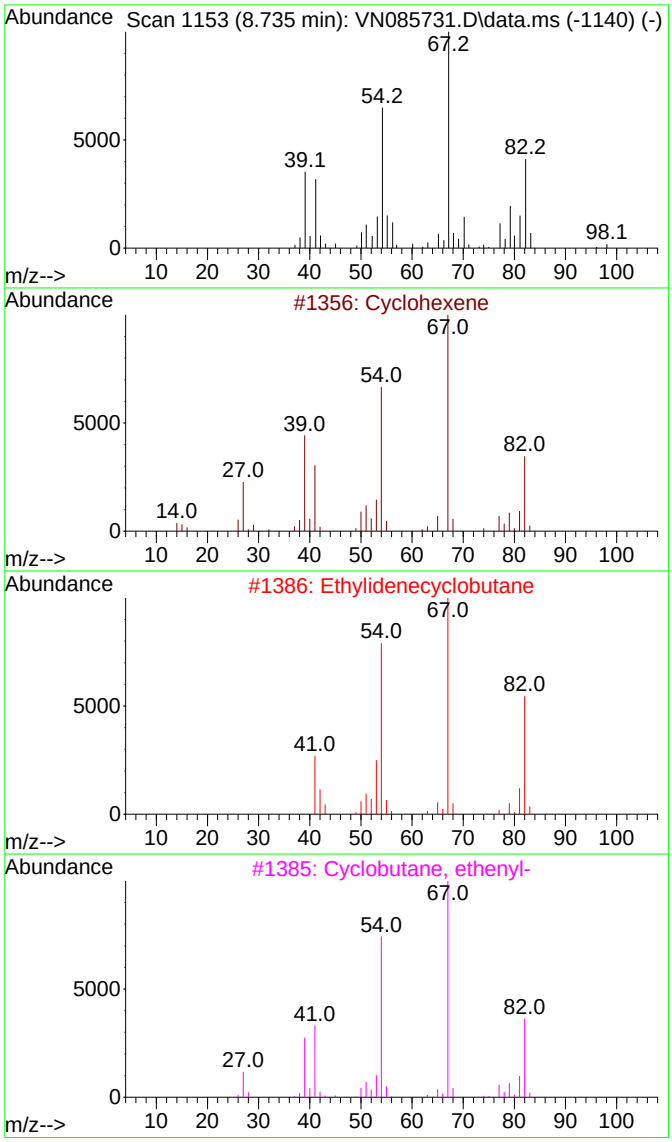
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

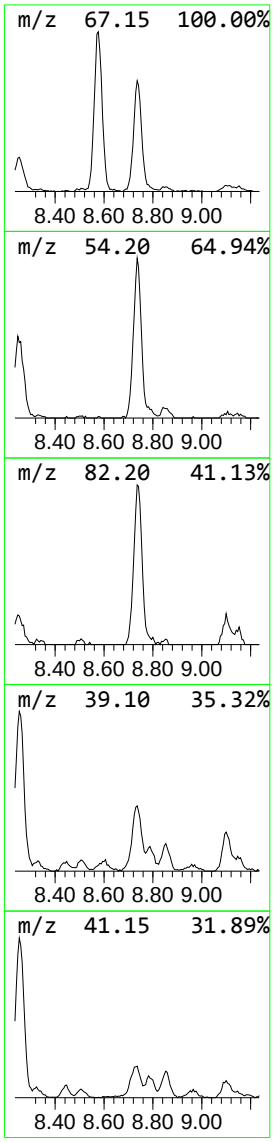
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.735	17.37 ug/l	427765	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	93
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	76
3	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	76
4	Cyclopentane, methylene-	82	C6H10	001528-30-9	64
5	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

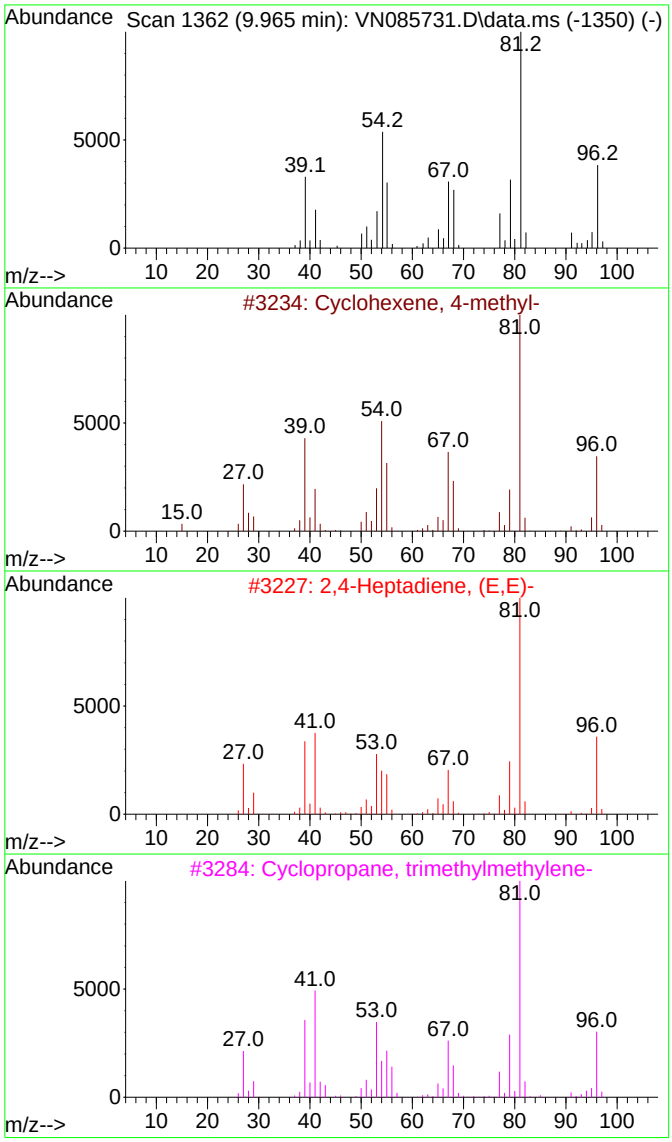
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

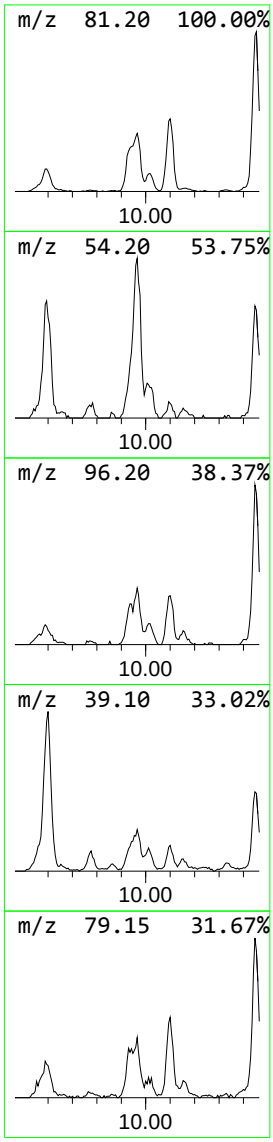
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexene, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.965	12.58 ug/l	309716	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	87
2	2,4-Heptadiene, (E,E)-	96	C7H12	002384-94-3	81
3	Cyclopropane, trimethylmethylene-	96	C7H12	034462-28-7	81
4	2,4-Hexadiene, 2-methyl-	96	C7H12	028823-41-8	76
5	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

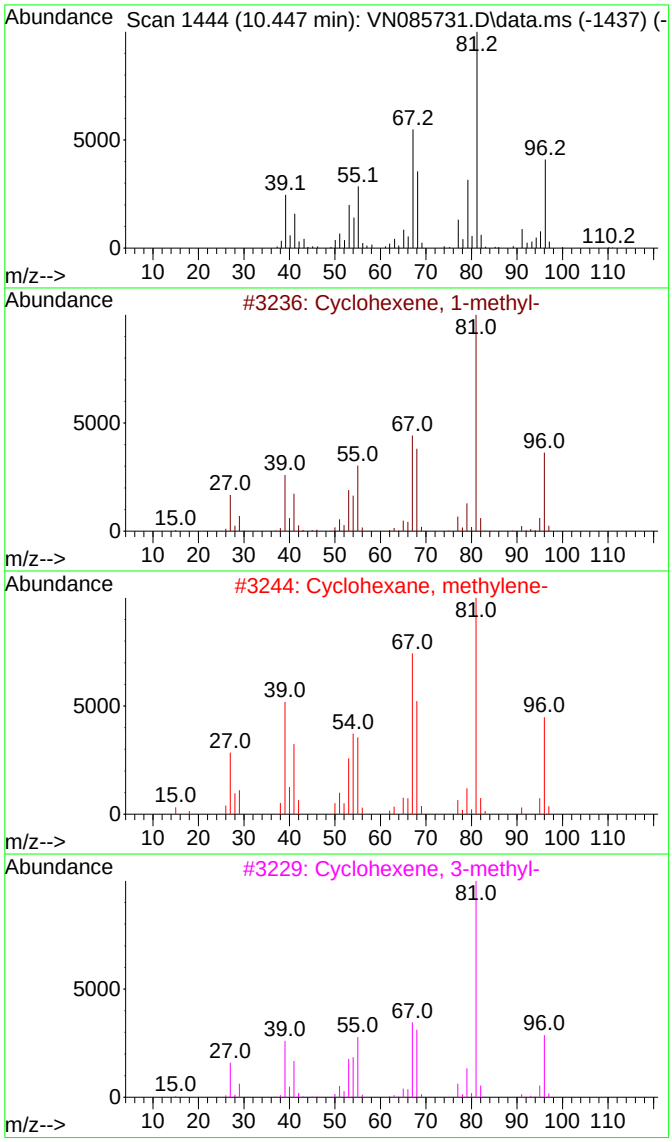
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

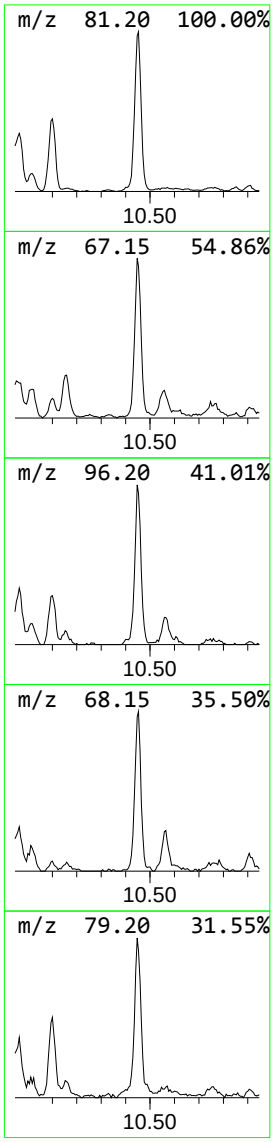
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.447	20.76 ug/l	511243	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	90
2	Cyclohexane, methylene-	96	C7H12	001192-37-6	87
3	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	87
4	1,4-Heptadiene	96	C7H12	005675-22-9	86
5	2,4-Hexadiene, 3-methyl-	96	C7H12	028823-42-9	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

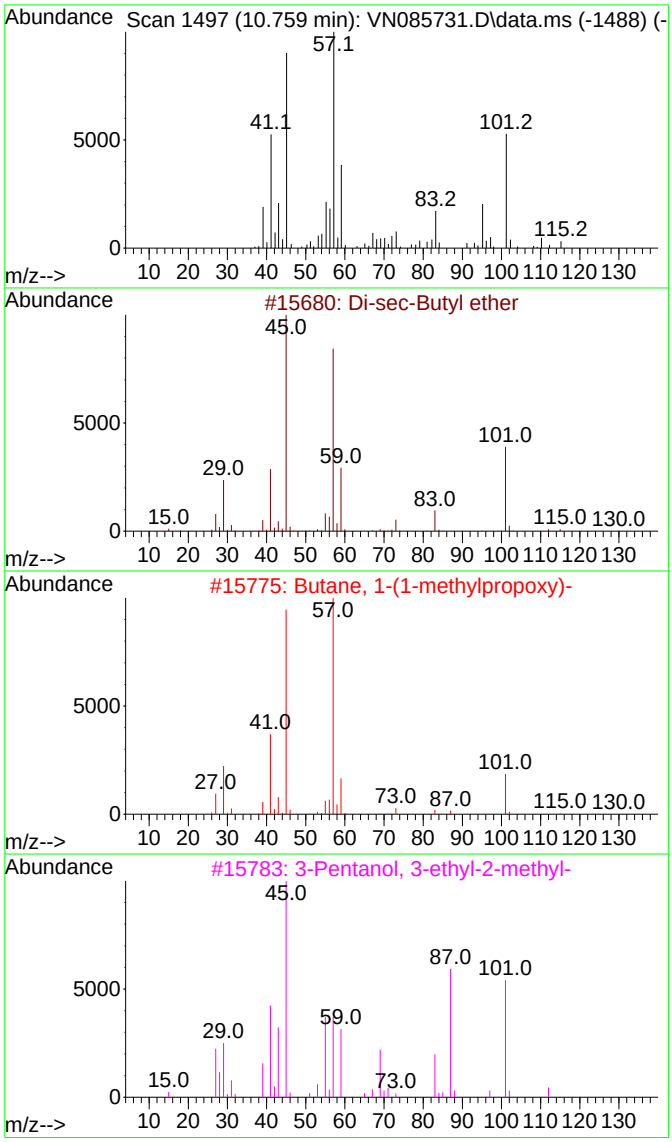
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

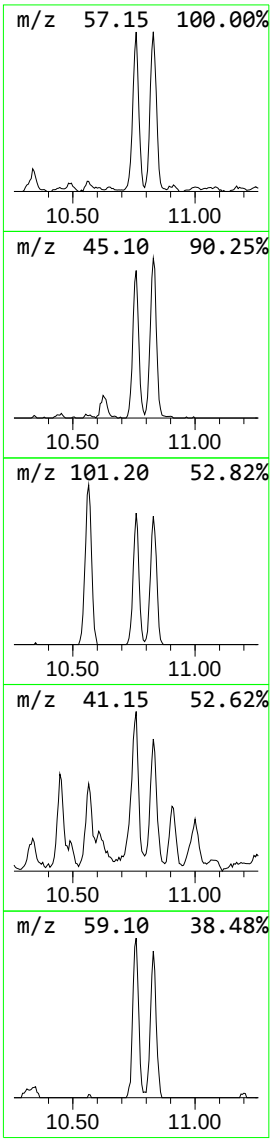
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Di-sec-Butyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.759	12.89 ug/l	335255	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	72
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	50
4	Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	43
5	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

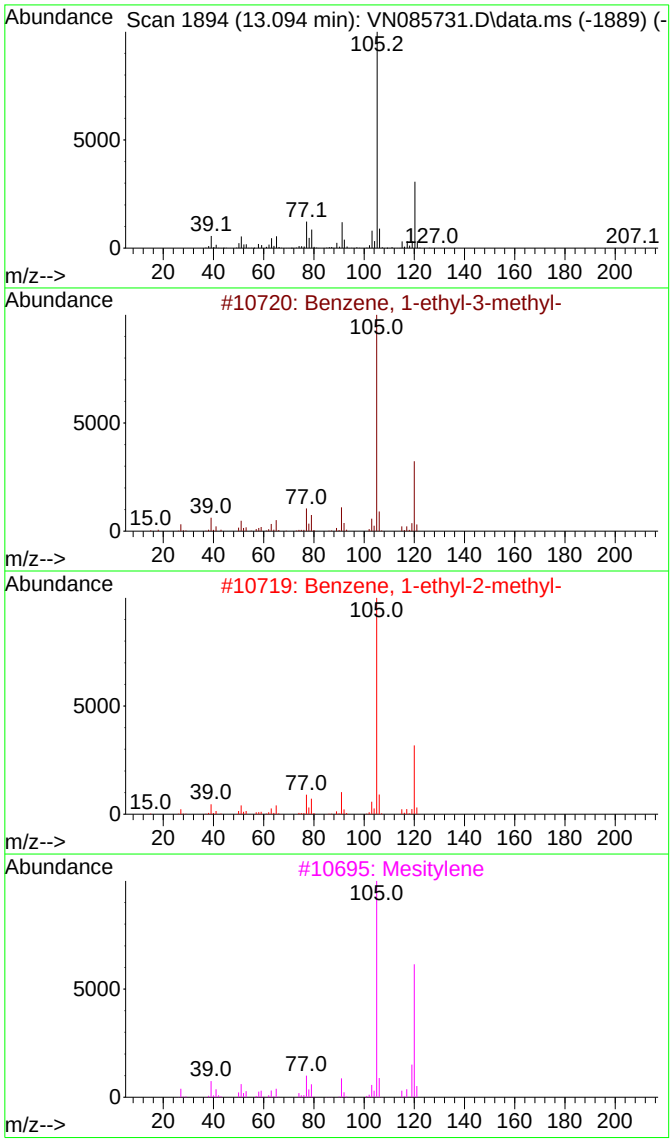
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

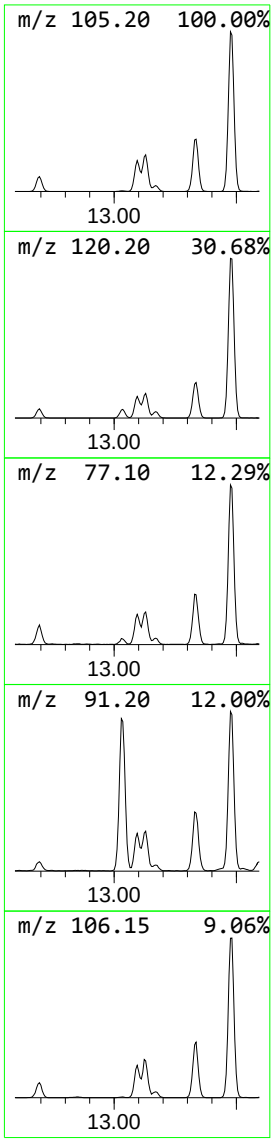
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	18.23 ug/l	1397190	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

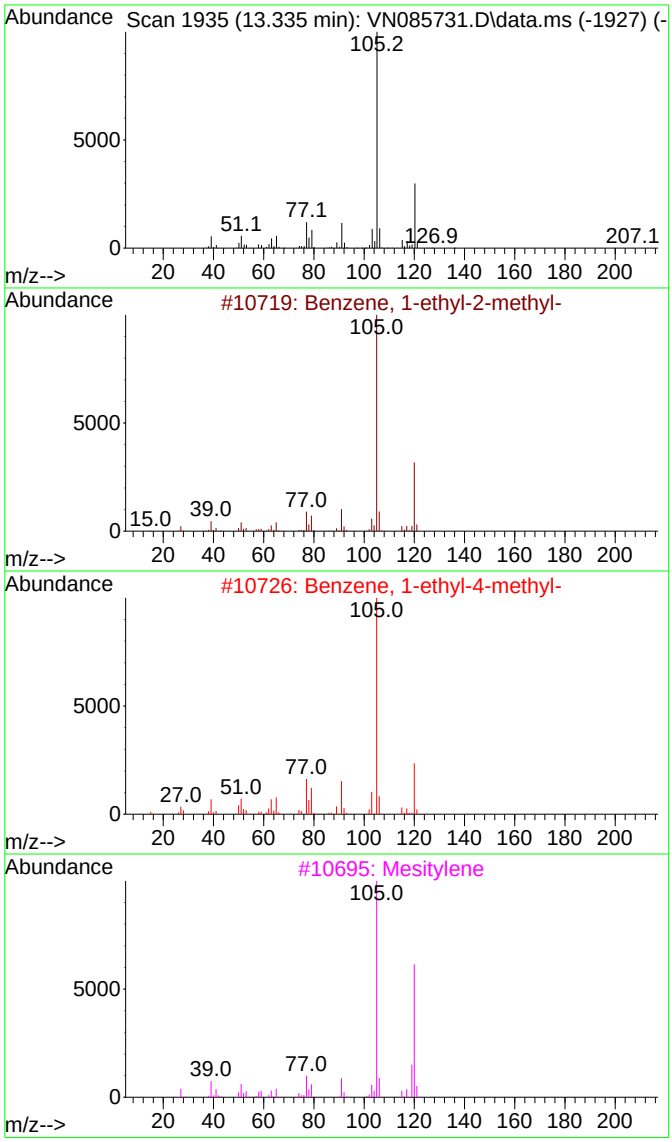
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

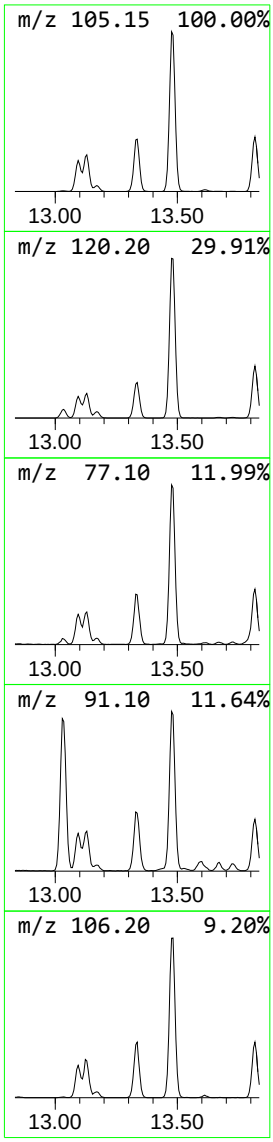
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	29.92 ug/l	2293490	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

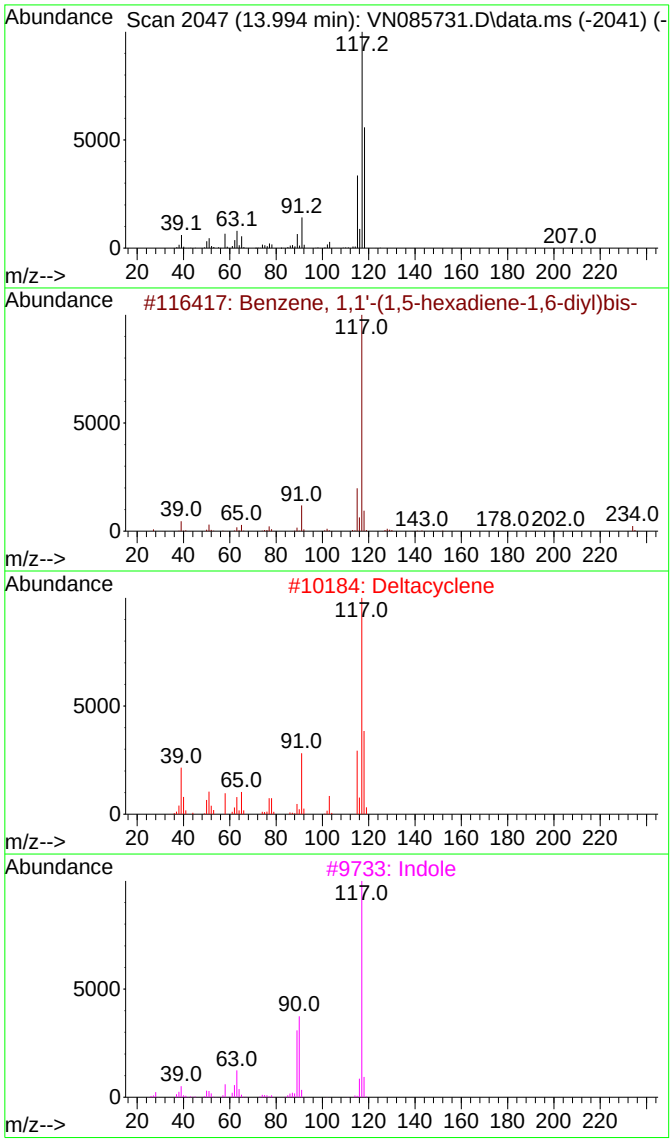
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

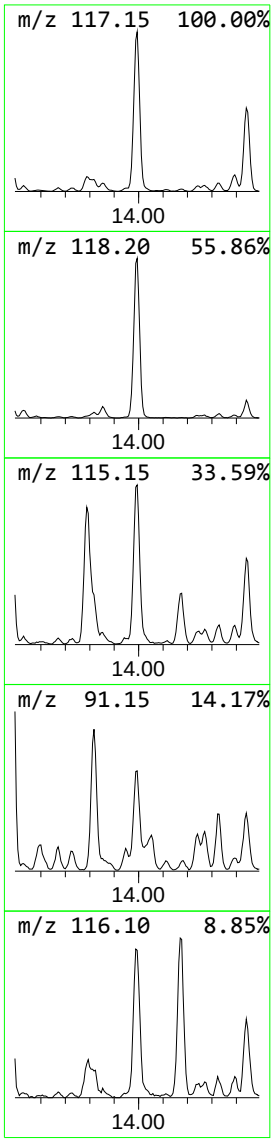
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	14.54 ug/l	1114870	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2	Deltacyclene	118	C9H10	007785-10-6	59
3	Indole	117	C8H7N	000120-72-9	47
4	4-Ethynylaniline	117	C8H7N	014235-81-5	43
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

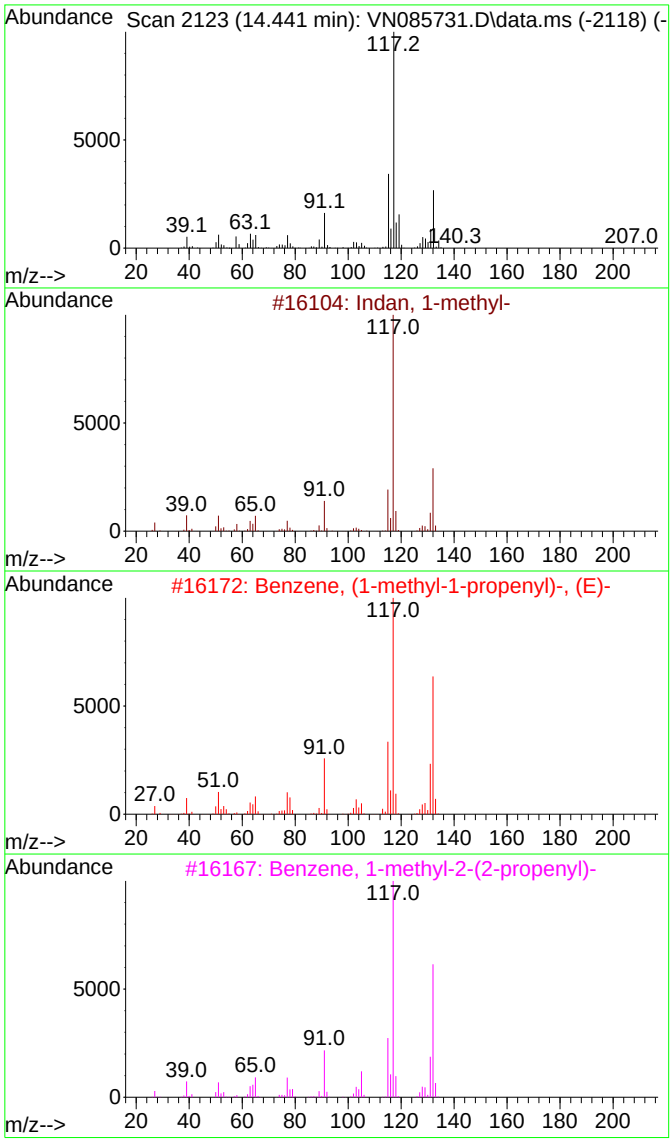
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

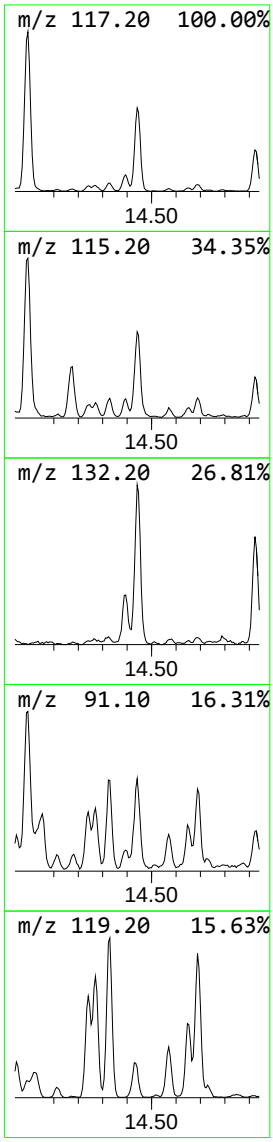
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.441	9.95 ug/l	762820	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	81
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	80
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	72
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	72
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

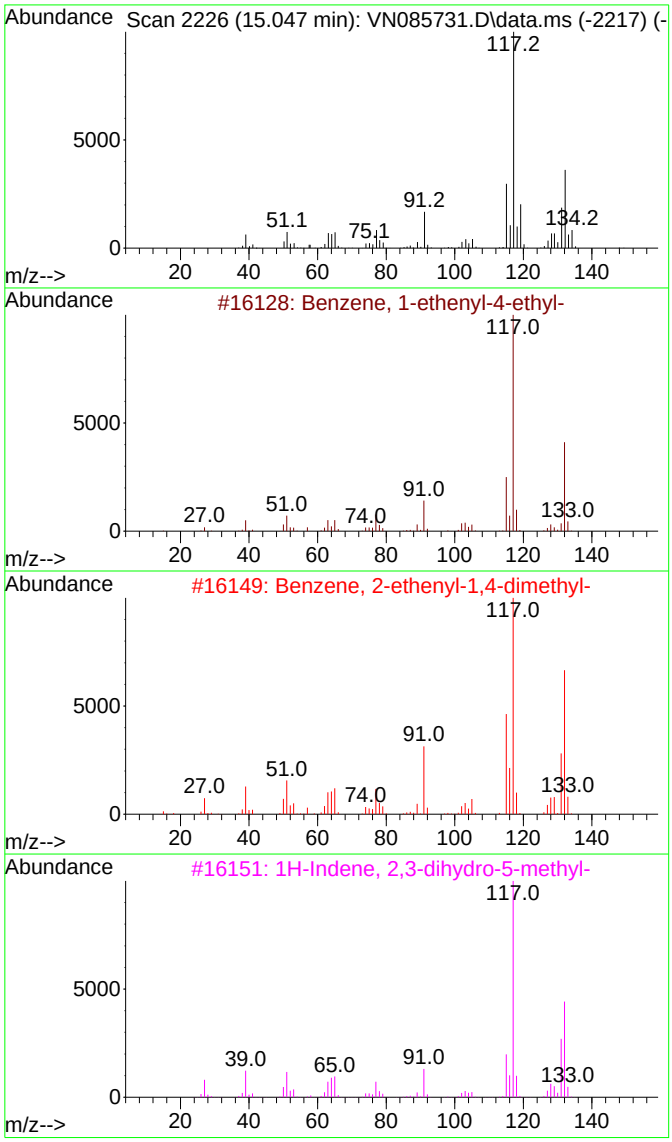
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

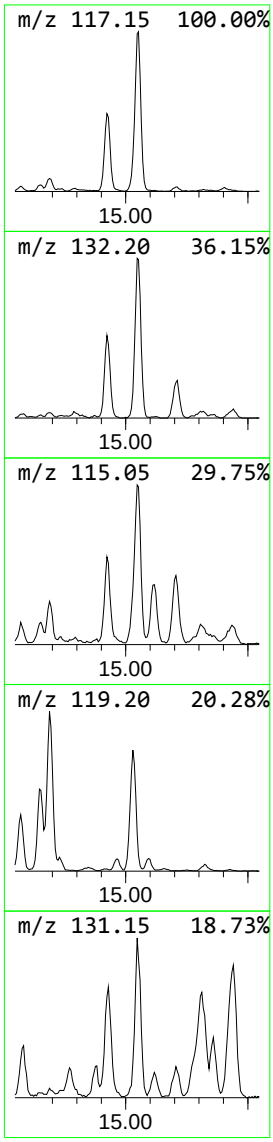
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	14.89 ug/l	1141070	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021025\
Data File : VN085731.D
Acq On : 10 Feb 2025 18:11
Operator : JC\MD
Sample : Q1332-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.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
Cyclopentane, m...	7.330	15.1	ug/l	567347	1	8.224	1874080	50.0
Cyclohexene	8.735	17.4	ug/l	427765	2	9.100	1231400	50.0
Cyclohexene, 4-...	9.965	12.6	ug/l	309716	2	9.100	1231400	50.0
Cyclohexene, 1-...	10.447	20.8	ug/l	511243	2	9.100	1231400	50.0
Di-sec-Butyl ether	10.759	12.9	ug/l	335255	3	11.865	1300610	50.0
Benzene, 1-ethy...	13.094	18.2	ug/l	1397190	4	13.788	3832910	50.0
Benzene, 1-ethy...	13.335	29.9	ug/l	2293490	4	13.788	3832910	50.0
Benzene, 1,1'-(...	13.994	14.5	ug/l	1114870	4	13.788	3832910	50.0
Indan, 1-methyl-	14.441	9.9	ug/l	762820	4	13.788	3832910	50.0
Benzene, 1-ethe...	15.047	14.9	ug/l	1141070	4	13.788	3832910	50.0