LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

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\82N110921W.M
Title : SW846 8260

Signal : TIC: VN069667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.024	2227	2250	2260	rBV	1199401	2858797	2.32%	0.482%
2	8.086	2261	2273	2296	rVB	2673319	6201800	5.03%	1.045%
3	8.440	2387	2405	2433	rVB2	1534935	3836223	3.11%	0.646%
4	8.968	2580	2602	2644	rBV	3547048	7498339	6.09%	1.263%
5	9.459	2753	2785	2803	rBV	1687442	3989807	3.24%	0.672%
6	10.440	3133	3151	3187	rBV	6622035	13181068	10.70%	2.221%
7	10.609	3202	3214	3238	rVB5	534698	1359415	1.10%	0.229%
8	10.781	3265	3278	3295	rVB2	1090707	2025430	1.64%	0.341%
9	10.878	3296	3314	3337	rBV3	618878	1366950	1.11%	0.230%
10	11.291	3449	3468	3479	rBV2	1263798	2573174	2.09%	0.434%
11	11.344	3479	3488	3501	rVB	1174804	1988004	1.61%	0.335%
12	11.744	3621	3637	3658	rBV	5406433	9999626	8.12%	1.685%
13	11.843	3659	3674	3695	rBV2	6119626	11232450	9.12%	1.892%
14	11.948	3696	3713	3725	rBV	7936385	16279521	13.21%	2.743%
15	12.154	3779	3790	3810	rVB4	642118	1474822	1.20%	0.248%
16	12.253	3810	3827	3833	rBV4	1728673	3549146	2.88%	0.598%
17	12.455	3892	3902	3911	rBV	2198658	3763272	3.05%	0.634%
18	12.578	3937	3948	3972	rVB	6623669	11285705	9.16%	1.901%
19	12.731	3992	4005	4022	rBV	4583768	7941143	6.44%	1.338%
20	12.809	4024	4034	4048	rBV3	1128373	2056080	1.67%	0.346%
21	12.919	4058	4075	4087	rBV	8869613	15814768	12.83%	2.664%
22	12.983	4087	4099	4106	rBV	5666735	9435403	7.66%	1.590%
23	13.058	4116	4127	4142	rVB2	28780863	47354483	38.43%	7.978%
24	13.219	4171	4187	4203	rBV	13696844	23747057	19.27%	4.001%
25	13.291	4204	4214	4218	rBV5	1134939	1781204	1.45%	0.300%
26	13.369	4230	4243	4268	rVB3	69634992	123223898	100.00%	20.761%
27	13.498	4274	4291	4302	rBV3	5002407	10893762	8.84%	1.835%
28	13.560	4303	4314	4326	rVB	4918295	7958203	6.46%	1.341%
29	13.610	4326	4333	4344	rVB2	955536	1497494	1.22%	0.252%
30	13.704	4345	4368	4383	rBV3	39525215	75819138	61.53%	12.774%
31	13.771	4384	4393	4404	rVB	1885358	2839089	2.30%	0.478%
32	13.838	4406	4418	4422	rBV	5203841	7823753	6.35%	1.318%
33	13.871	4423	4430	4437	rVV3	6170616	9406650	7.63%	1.585%
34	13.908	4438	4444	4467	rVB3	8543978	17289425	14.03%	2.913%
35	13.999	4467	4478	4490	rBV2	3905337	6406176	5.20%	1.079%
36	14.069	4492	4504	4515	rBV	3868638	6116824	4.96%	1.031%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

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\82N110921W.M
Title : SW846 8260

37	14.131	4516	4527	4532	rBV	4926168	7827708	6.35%	1.319%
38	14.217	4548	4559	4571	rVB	9260639	14285431	11.59%	2.407%
39	14.278	4572	4582	4588	rBV	1998473	3110064	2.52%	0.524%
40	14.324	4589	4599	4611	rVV3	7941264	13748578	11.16%	2.316%
41	14.394	4612	4625	4636	rVB10	974394	2421553	1.97%	0.408%
42	14.461	4637	4650	4661	rBV3	4665836	7758660	6.30%	1.307%
43	14.538	4661	4679	4687	rBV	5343916	9883587	8.02%	1.665%
44	14.579	4687	4694	4703	rVB	5015478	7155509	5.81%	1.206%
45	14.812	4771	4781	4790	rBV4	1080859	1931577	1.57%	0.325%
46	14.914	4806	4819	4837	rBV2	11034583	21682579	17.60%	3.653%
47	15.083	4871	4882	4896	rVB	1875298	3055361	2.48%	0.515%
48	15.306	4955	4965	4981	rVB3	1087138	2557252	2.08%	0.431%
49	15.504	5025	5039	5056	rVB	8565385	16258176	13.19%	2.739%

Sum of corrected areas: 593544134

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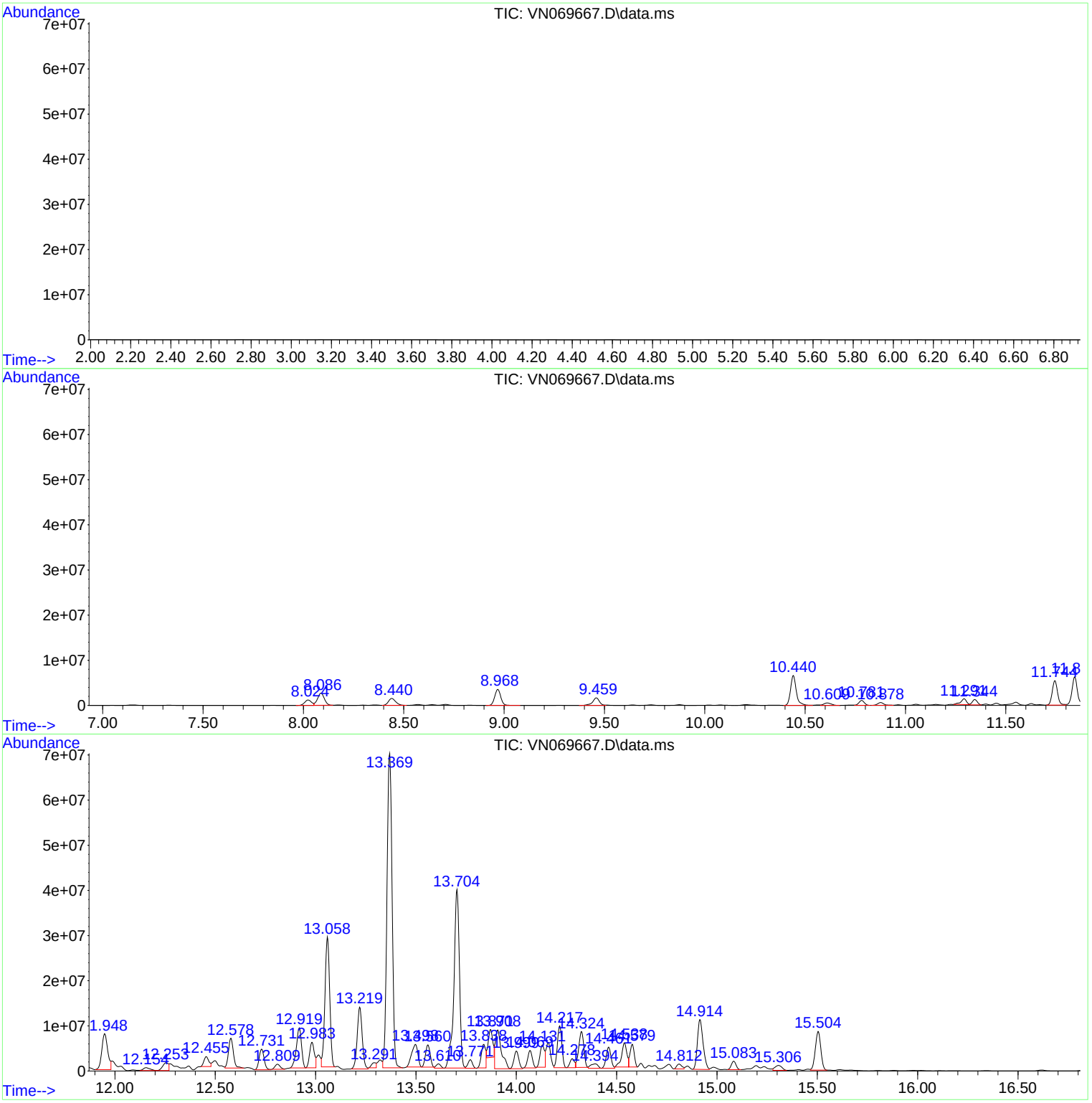
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

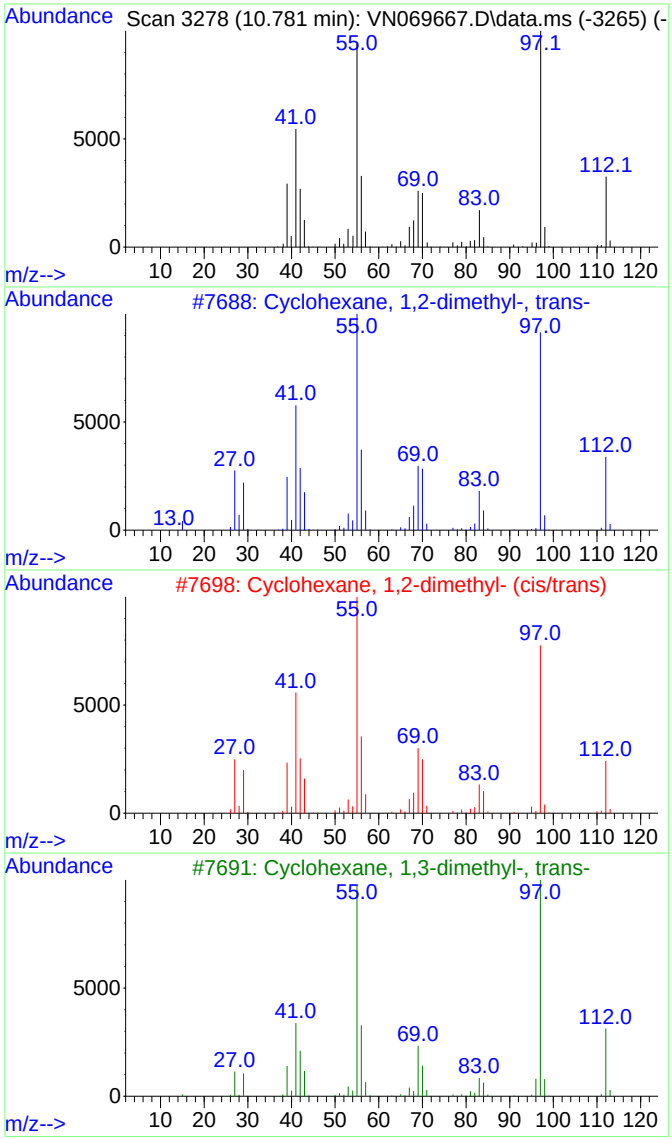
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

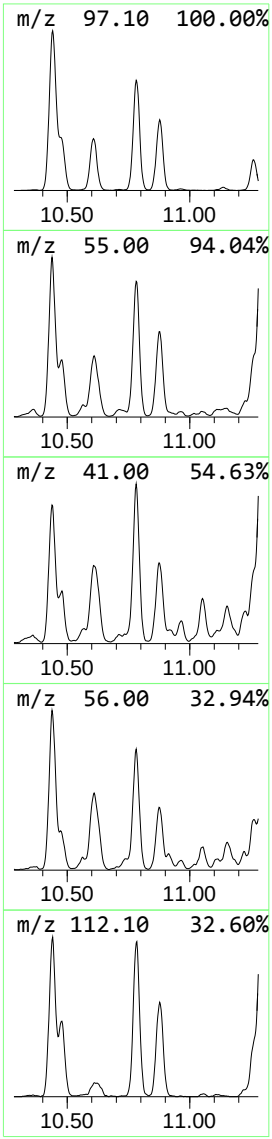
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	10.13 ug/l	2025430	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	94
2	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	91
3	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	87
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	80
5	1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

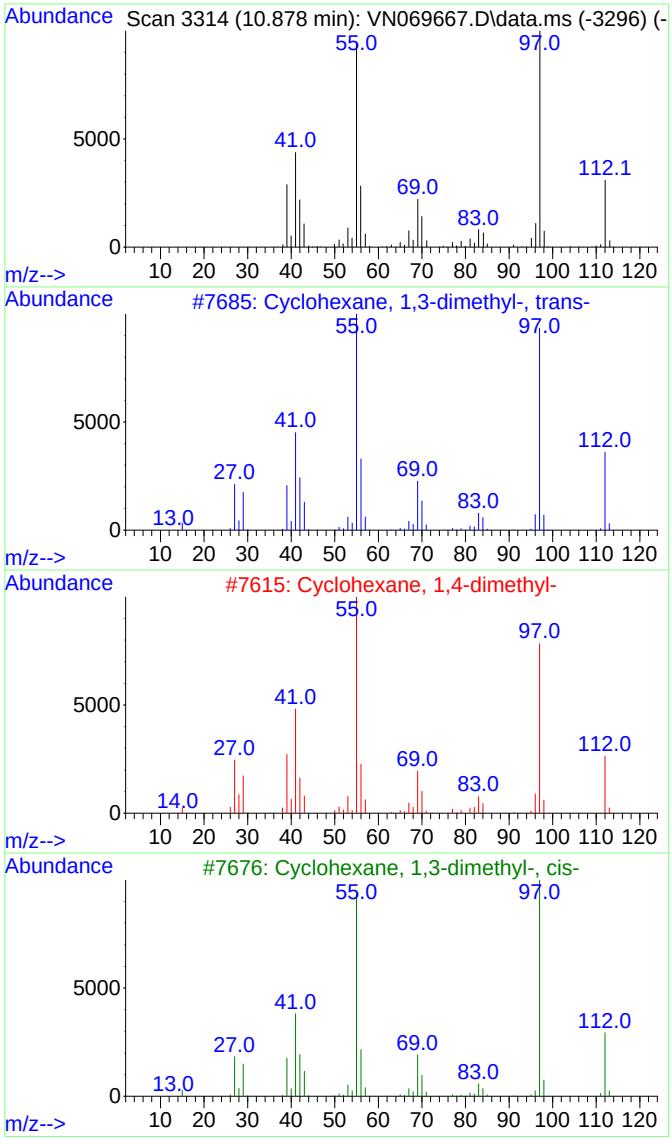
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

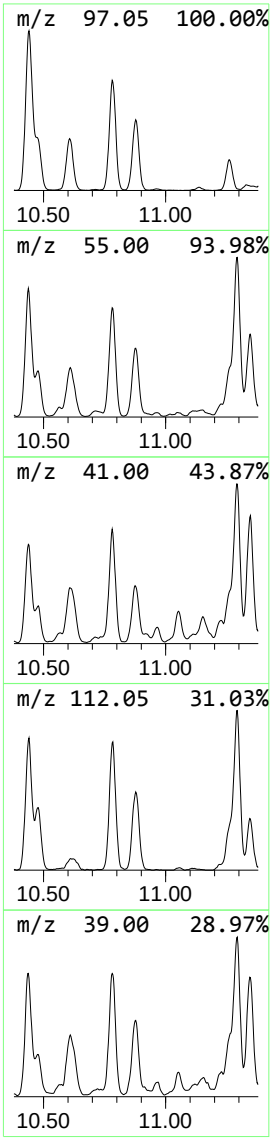
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.878	6.84 ug/l	1366950	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	97
2	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	95
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	93
4	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	93
5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

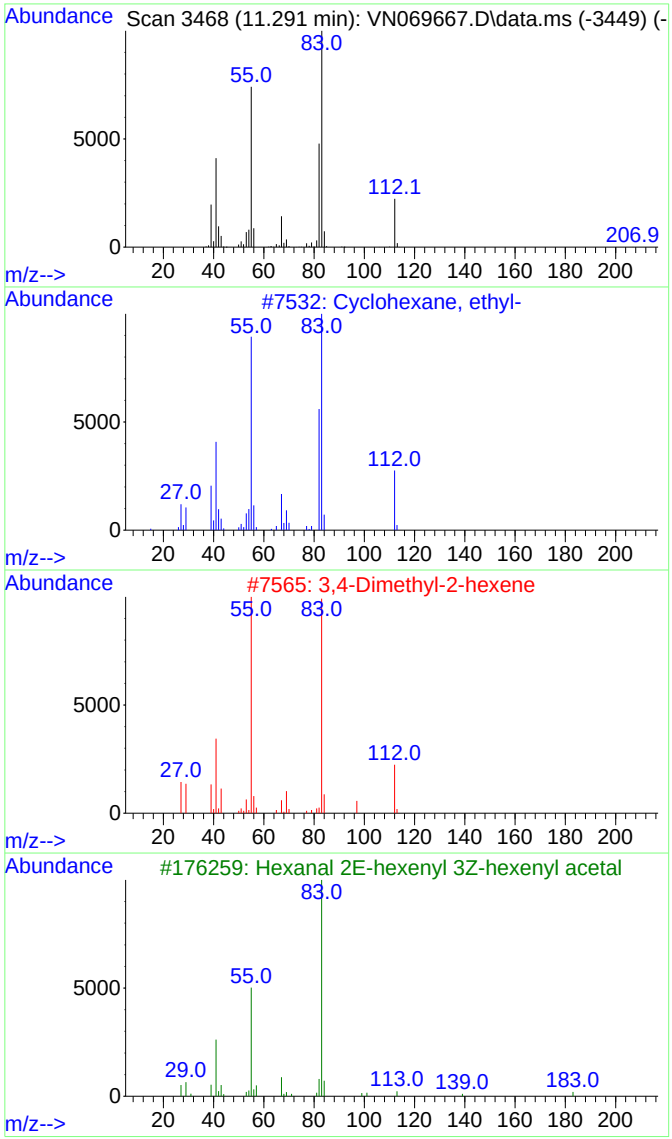
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

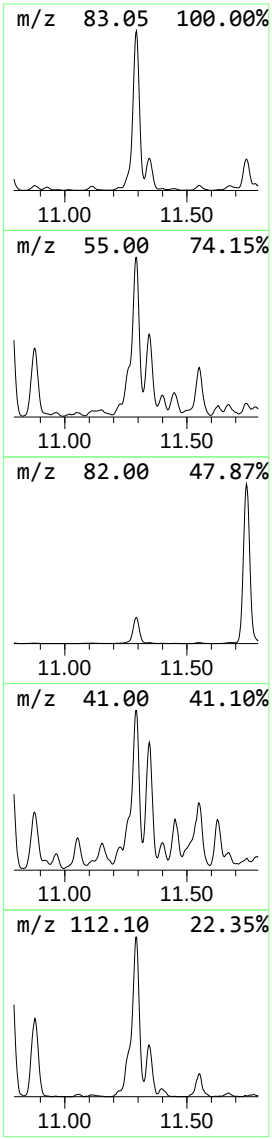
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	12.87 ug/l	2573170	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	94
2	3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	58
3	Hexanal 2E-hexenyl 3Z-hexenyl ac...	282	C18H34O2	1000431-43-4	53
4	4-Hexen-3-one, 5-methyl-	112	C7H12O	013905-10-7	52
5	4-Oxohex-2-enal	112	C6H8O2	020697-55-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

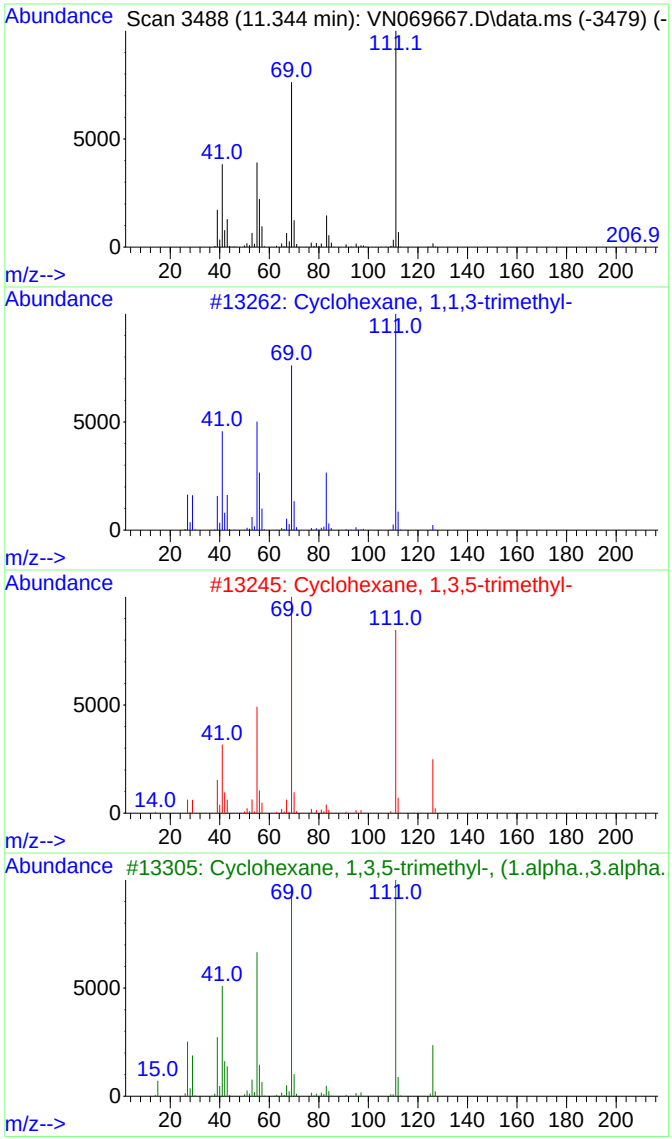
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

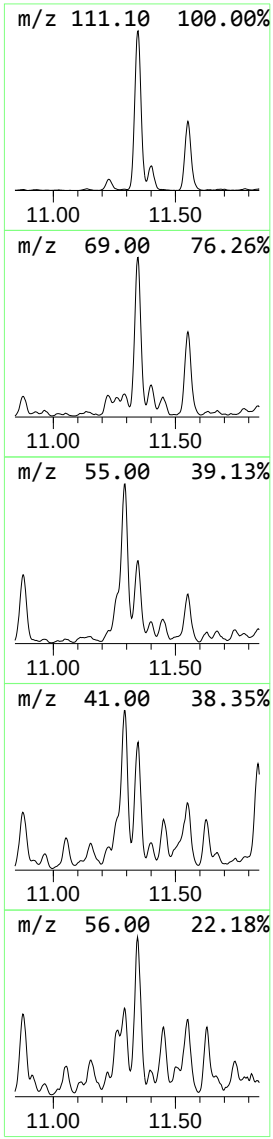
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.344	9.94 ug/l	1988000	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
2	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	72
4	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	60
5	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	50





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Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

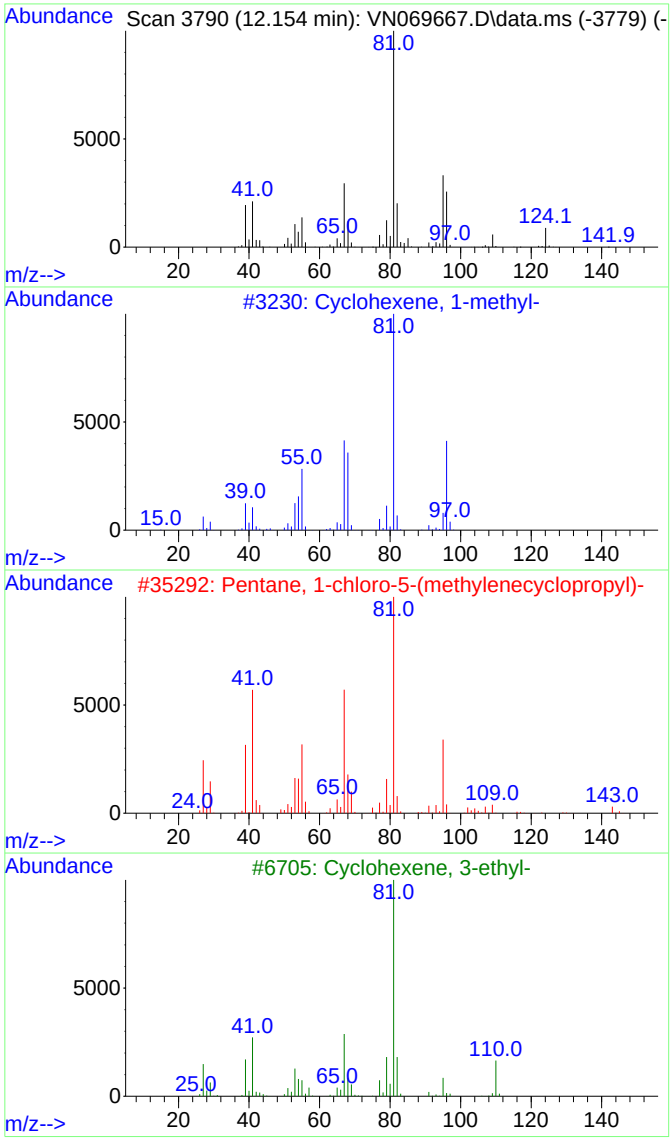
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

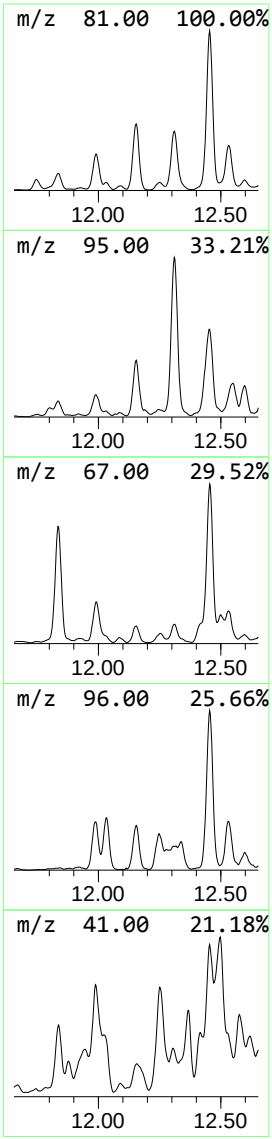
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.154	7.37 ug/l	1474820	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	64
2	Pentane, 1-chloro-5-(methylenecy...	158	C9H15Cl	1000158-49-0	59
3	Cyclohexene, 3-ethyl-	110	C8H14	002808-71-1	53
4	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	53
5	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	53





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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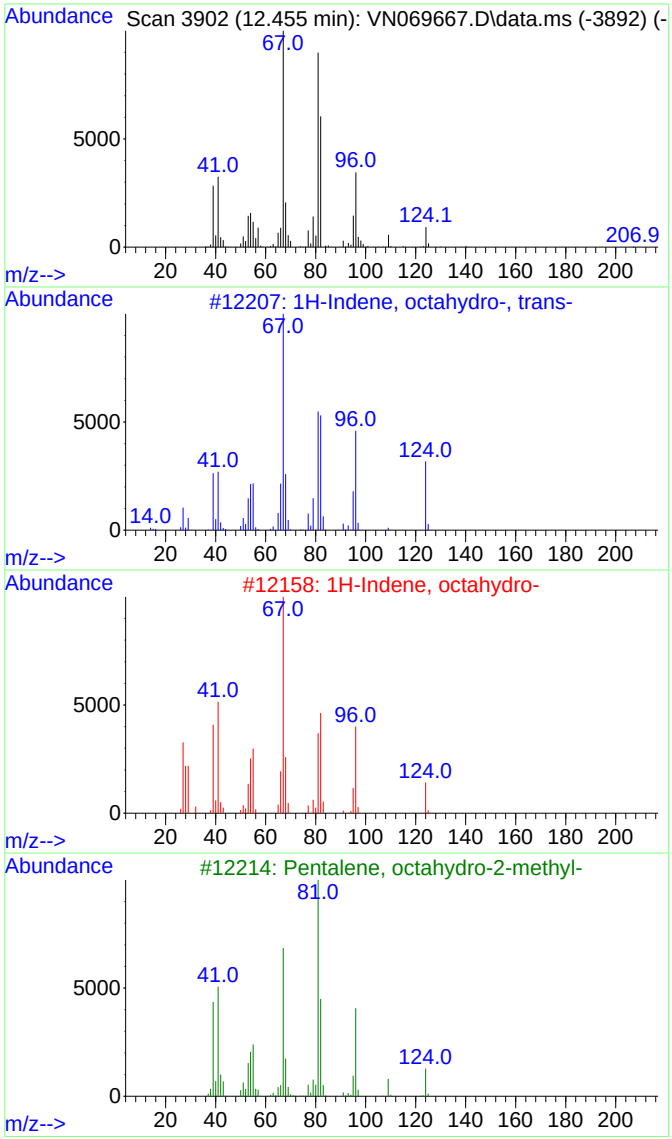
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

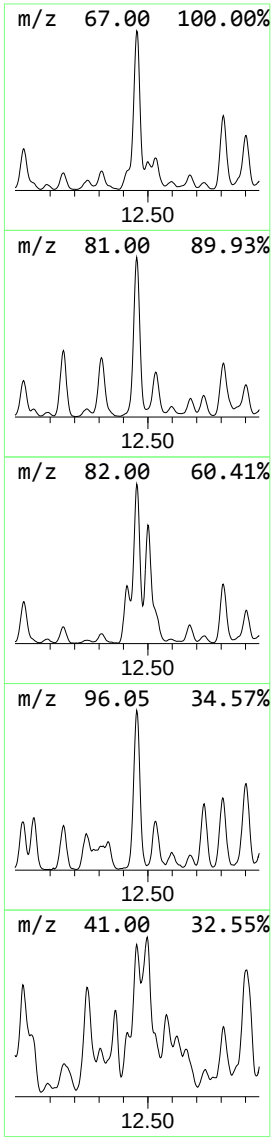
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, octahydro-, trans- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	18.82 ug/l	3763270	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	70
2	1H-Indene, octahydro-	124	C9H16	000496-10-6	62
3	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	58
4	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	50
5	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	49





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Instrument :
MSVOA_N
ClientSampleId :
MW-2D

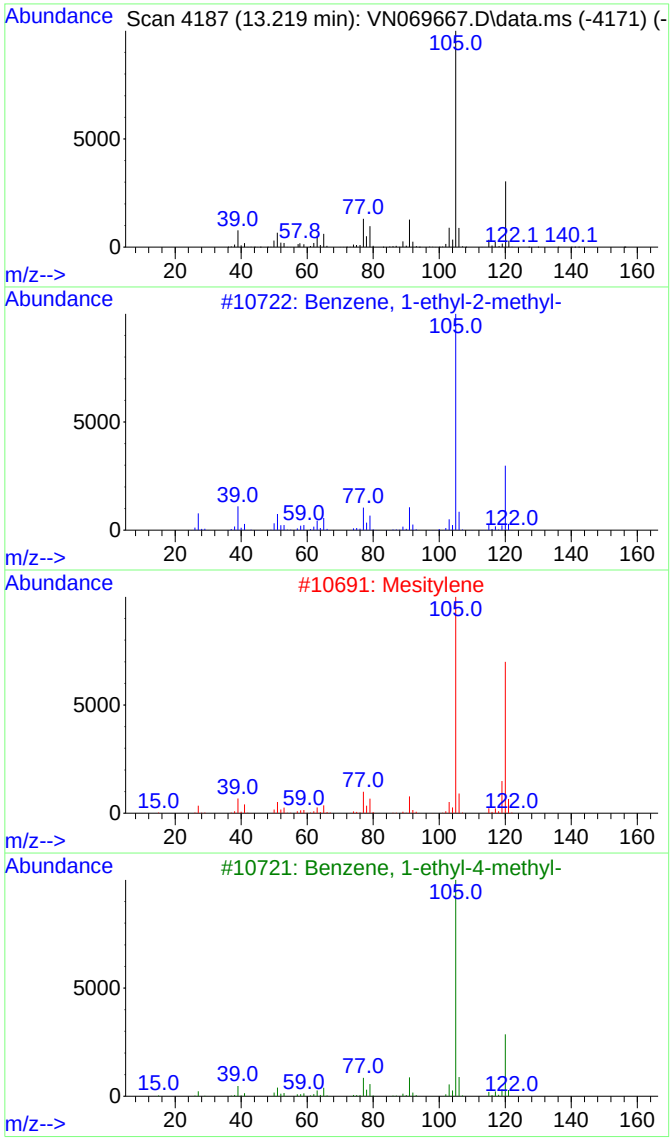
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

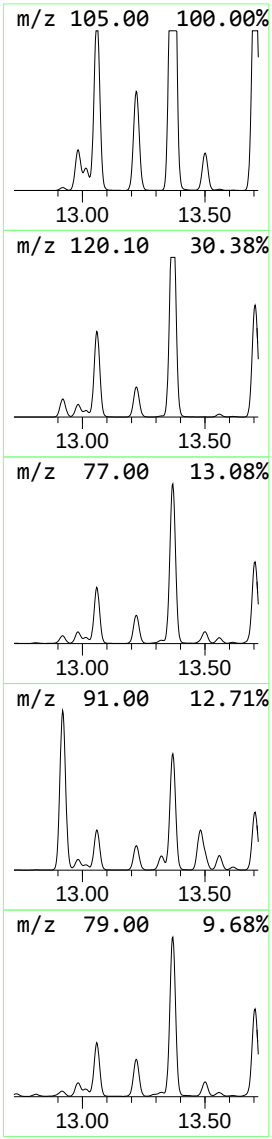
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	15.66 ug/l	23747100	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	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\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

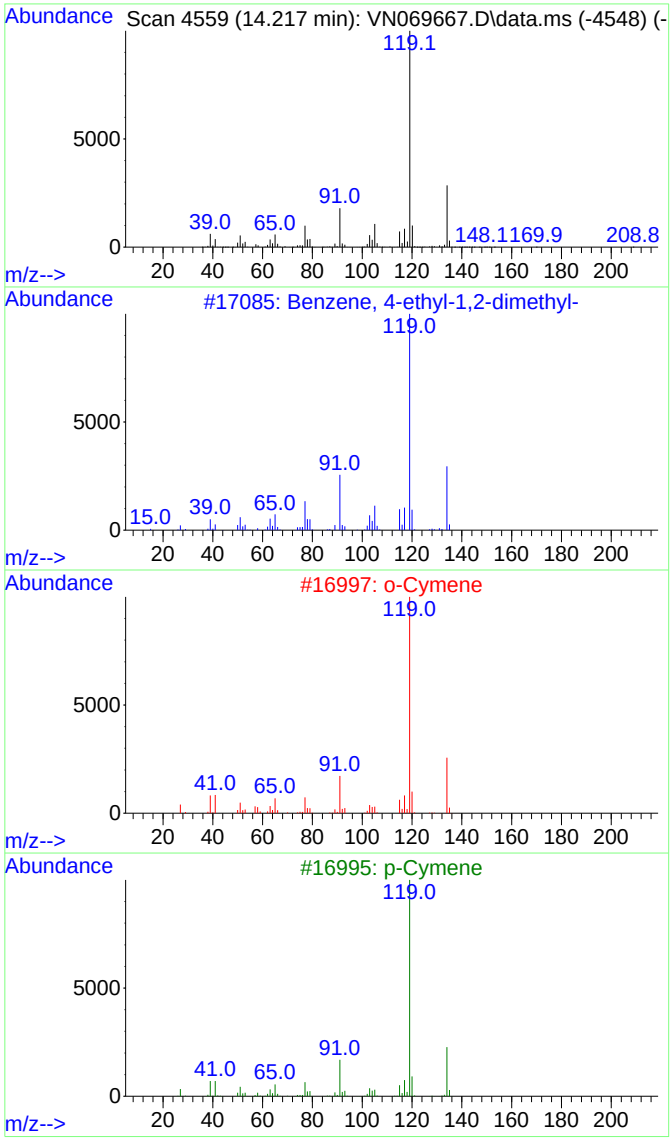
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

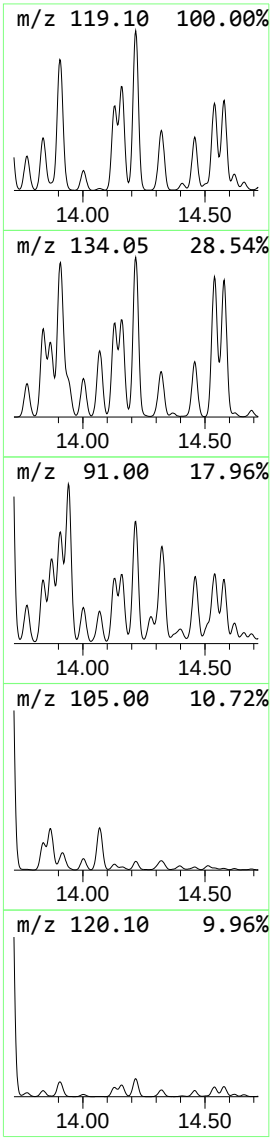
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	9.42 ug/l	14285400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	o-Cymene	134	C10H14	000527-84-4	95
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

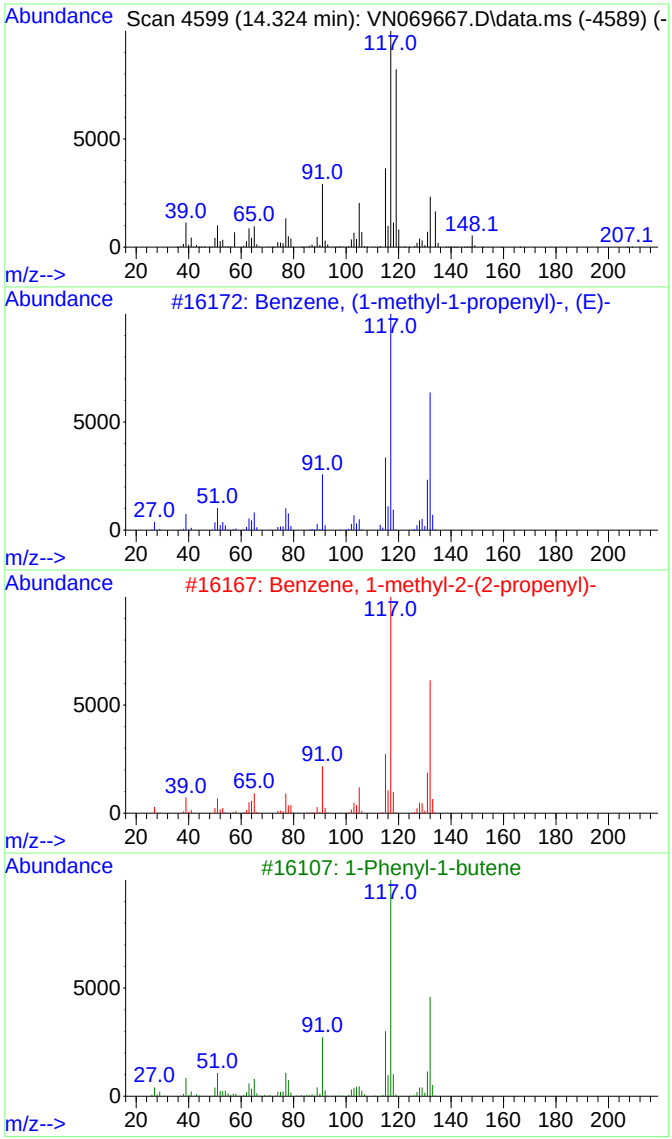
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

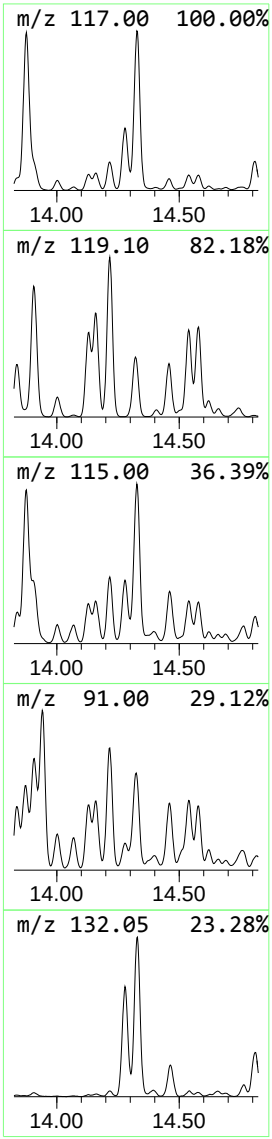
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-methyl-1-propen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.324	9.07 ug/l	13748600	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	60
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	55
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	55
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

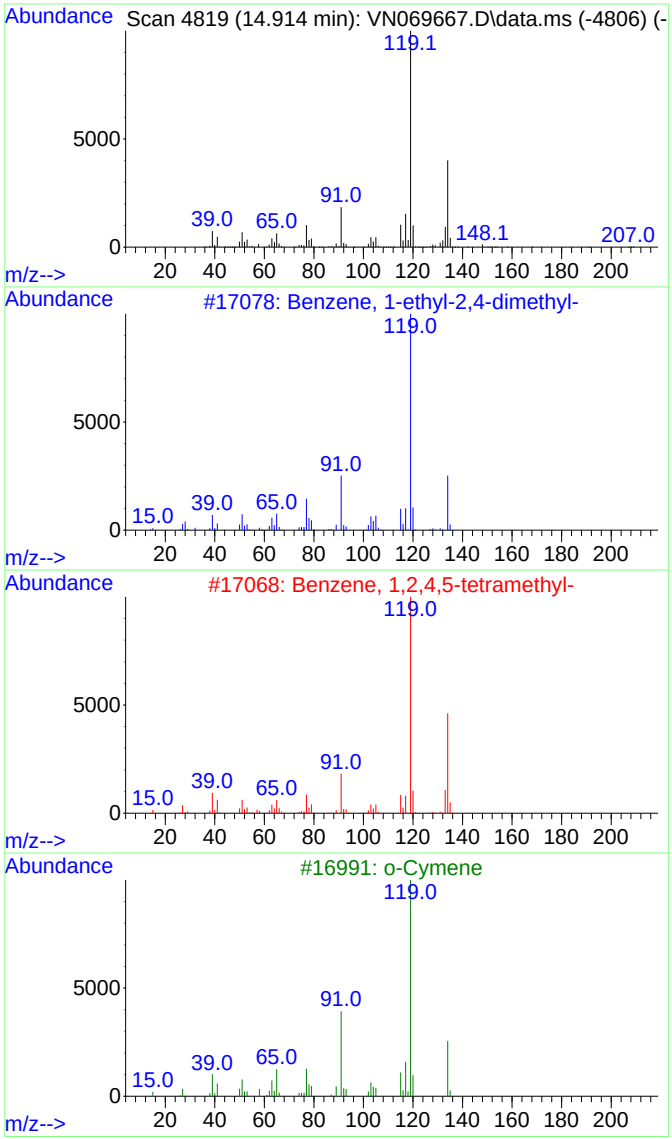
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

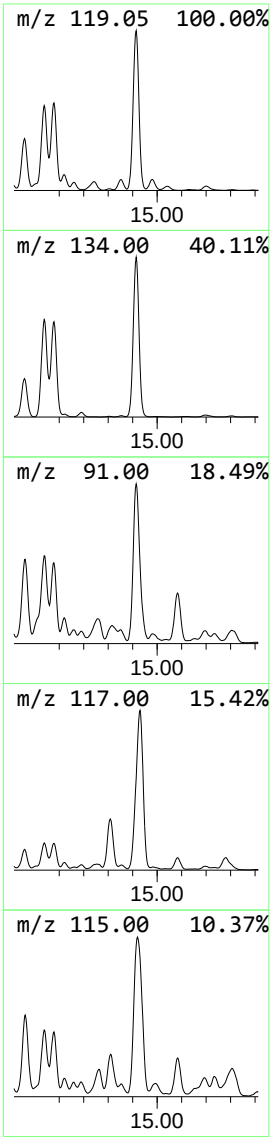
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.914	14.30 ug/l	21682600	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3	o-Cymene	134	C10H14	000527-84-4	94
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
5	p-Cymene	134	C10H14	000099-87-6	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069667.D
Acq On : 29 Nov 2021 16:36
Operator : JC/MD
Sample : M4852-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.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
Cyclohexane, 1,...	10.781	10.1	ug/l	2025430	3	11.744	9999630	50.0
Cyclohexane, 1,...	10.878	6.8	ug/l	1366950	3	11.744	9999630	50.0
Cyclohexane, et...	11.291	12.9	ug/l	2573170	3	11.744	9999630	50.0
Cyclohexane, 1,...	11.344	9.9	ug/l	1988000	3	11.744	9999630	50.0
Cyclohexene, 1-...	12.154	7.4	ug/l	1474820	3	11.744	9999630	50.0
1H-Indene, octa...	12.455	18.8	ug/l	3763270	3	11.744	9999630	50.0
Benzene, 1-ethy...	13.219	15.7	ug/l	23747100	4	13.675	75819100	50.0
Benzene, 4-ethy...	14.217	9.4	ug/l	14285400	4	13.675	75819100	50.0
Benzene, (1-met...	14.324	9.1	ug/l	13748600	4	13.675	75819100	50.0
Benzene, 1-ethy...	14.914	14.3	ug/l	21682600	4	13.675	75819100	50.0