LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN069916.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.143	413	430	457	rVB	568624	1289818	1.51%	0.253%
2	5.082	1127	1153	1159	rBV3	336493	978784	1.15%	0.192%
3	5.618	1320	1353	1387	rBV2	731601	2532234	2.97%	0.497%
4	6.122	1514	1541	1569	rBV2	344432	1047622	1.23%	0.205%
5	6.468	1644	1670	1698	rVB2	735064	2216208	2.60%	0.435%
6	6.611	1699	1723	1742	rBV2	364148	1126026	1.32%	0.221%
7	6.903	1810	1832	1864	rBV3	378647	1130731	1.33%	0.222%
8	7.150	1900	1924	1944	rBV	3193115	9325138	10.94%	1.829%
9	7.844	2170	2183	2203	rVB2	566787	1380634	1.62%	0.271%
10	8.021	2227	2249	2259	rBV	958365	2397815	2.81%	0.470%
11	8.088	2260	2274	2293	rVV4	3112657	8284309	9.72%	1.625%
12	8.174	2296	2306	2331	rVB3	646911	1720622	2.02%	0.337%
13	8.298	2334	2352	2366	rBV2	502824	1160287	1.36%	0.228%
14	8.458	2387	2412	2437	rBV	10015754	24858052	29.16%	4.875%
15	8.585	2440	2459	2472	rBV6	1114011	3507756	4.11%	0.688%
16	8.708	2495	2505	2526	rVB2	484324	1152431	1.35%	0.226%
17	8.804	2527	2541	2579	rVB6	270349	930781	1.09%	0.183%
18	8.968	2580	2602	2629	rBV2	3847391	9417033	11.05%	1.847%
19	9.244	2697	2705	2727	rVB	519054	1060492	1.24%	0.208%
20	9.459	2750	2785	2802	rBV3	1811596	5514119	6.47%	1.081%
21	9.641	2841	2853	2868	rVB	460698	897399	1.05%	0.176%
22	9.883	2934	2943	2961	rVB	529893	1030668	1.21%	0.202%
23	9.971	2961	2976	2985	rBV	1475557	2853016	3.35%	0.560%
24	10.017	2987	2993	3010	rVB3	974109	1792924	2.10%	0.352%
25	10.322	3092	3107	3120	rBV	1070677	2026307	2.38%	0.397%
26	10.440	3135	3151	3167	rBV	4651459	8825866	10.35%	1.731%
27	10.859	3293	3307	3328	rVB5	563421	1317104	1.54%	0.258%
28	11.744	3620	3637	3653	rBV	4929275	8972523	10.52%	1.760%
29	11.843	3664	3674	3697	rVB2	726102	1410824	1.65%	0.277%
30	11.948	3698	3713	3726	rBV	681267	1238890	1.45%	0.243%
31	12.578	3933	3948	3969	rVB	7501483	12377471	14.52%	2.427%
32	12.731	3989	4005	4030	rBV	4147956	7323909	8.59%	1.436%
33	12.919	4059	4075	4098	rBV	19630178	32836420	38.51%	6.440%
34	13.058	4113	4127	4146	rVB	12869411	20908177	24.52%	4.101%
35	13.219	4172	4187	4205	rBV	1741772	2896577	3.40%	0.568%
36	13.366	4230	4242	4257	rVB	909520	1517812	1.78%	0.298%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-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\82N120221W.M
Title : SW846 8260

37	13.495	4273	4290	4305	rVB3	1177524	2705861	3.17%	0.531%
38	13.672	4342	4356	4382	rBV2	4738154	9240788	10.84%	1.812%
39	13.836	4403	4417	4422	rBV	13094177	19477339	22.84%	3.820%
40	13.876	4423	4432	4467	rVB3	42444984	85259676	100.00%	16.721%
41	14.002	4467	4479	4493	rVB	2610342	4121419	4.83%	0.808%
42	14.131	4515	4527	4544	rBV2	489521	1065160	1.25%	0.209%
43	14.217	4544	4559	4572	rBV2	26759611	43151147	50.61%	8.463%
44	14.278	4572	4582	4589	rVV	2787120	4553402	5.34%	0.893%
45	14.327	4589	4600	4620	rVB2	11481338	19626485	23.02%	3.849%
46	14.539	4661	4679	4688	rBV	12715043	21162382	24.82%	4.150%
47	14.576	4688	4693	4704	rVV	4738583	6935184	8.13%	1.360%
48	14.619	4704	4709	4718	rVB2	774228	1020000	1.20%	0.200%
49	14.807	4767	4779	4791	rBV	9144007	14625185	17.15%	2.868%
50	14.852	4792	4796	4806	rVB	732750	895547	1.05%	0.176%
51	14.930	4806	4825	4839	rBV3	19470501	40276777	47.24%	7.899%
52	15.083	4868	4882	4900	rBV	3193037	5675474	6.66%	1.113%
53	15.193	4901	4923	4933	rBV6	2051980	4656537	5.46%	0.913%
54	15.308	4951	4966	4988	rVB3	1893536	4450154	5.22%	0.873%
55	15.504	5023	5039	5055	rVB	12622746	23708522	27.81%	4.650%
56	15.614	5069	5080	5090	rBV3	455671	890630	1.04%	0.175%
57	15.668	5093	5100	5131	rVB	555528	1091352	1.28%	0.214%
58	15.804	5135	5151	5169	rBV	874234	1683985	1.98%	0.330%
59	15.981	5203	5217	5251	rVB3	575721	1782817	2.09%	0.350%
60	16.617	5437	5454	5484	rVB	1122183	2580532	3.03%	0.506%

Sum of corrected areas: 509893134

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
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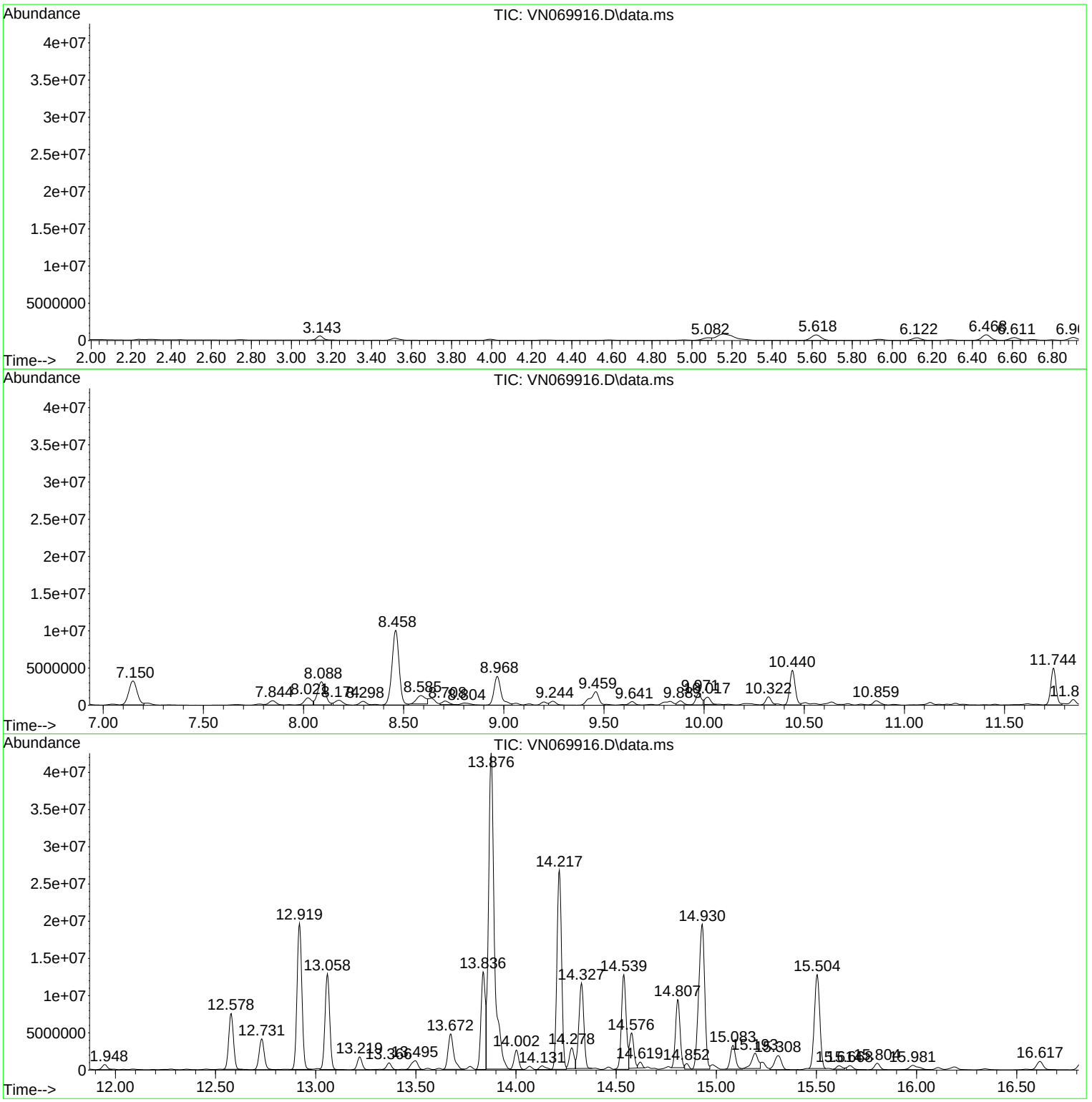
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

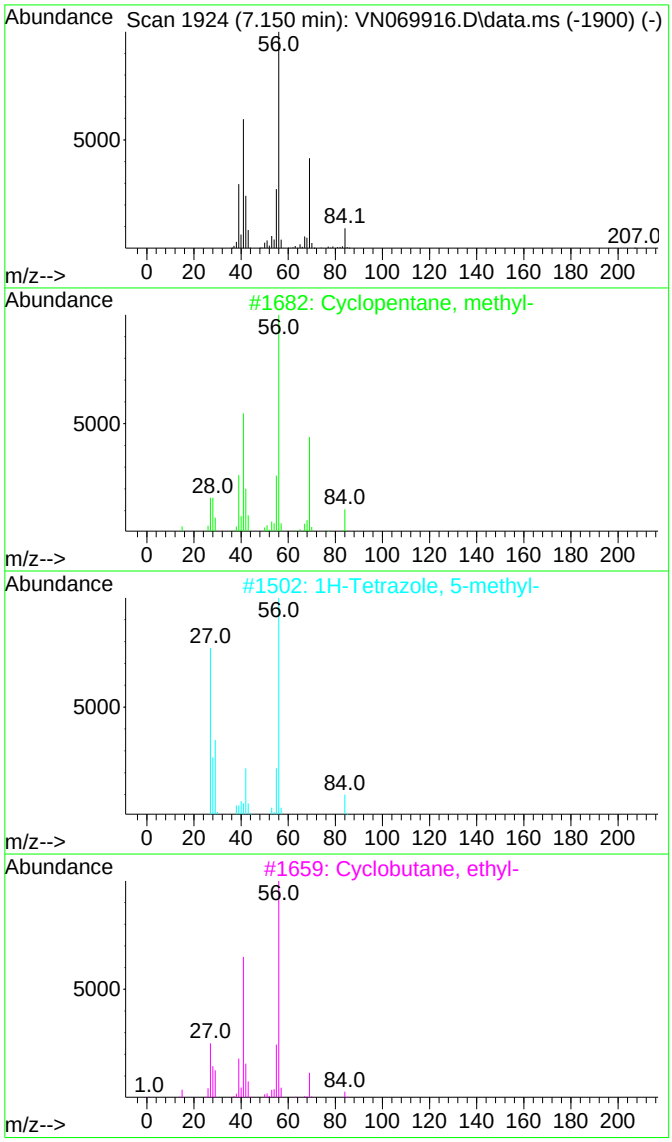
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

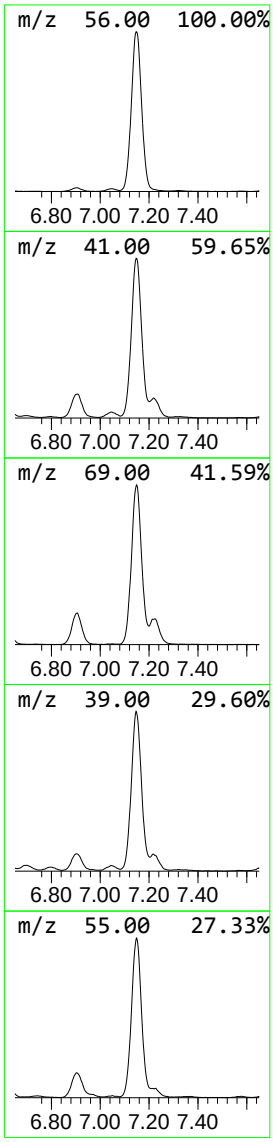
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.150	56.28 ug/l	9325140	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclobutane	56	C4H8	000287-23-0	53
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

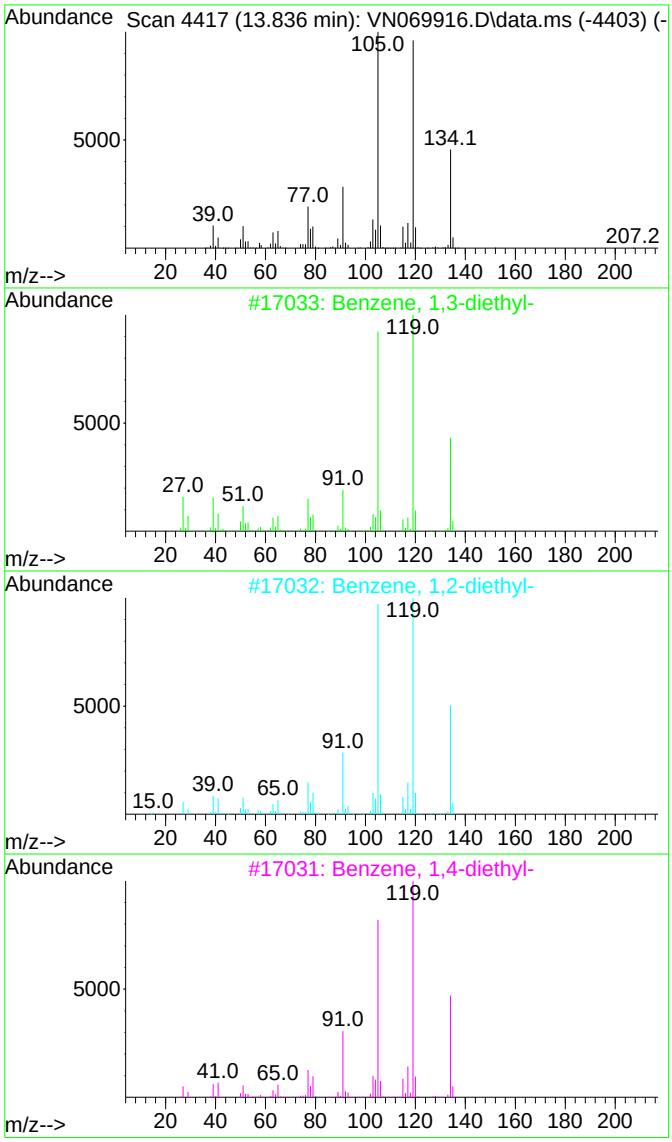
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

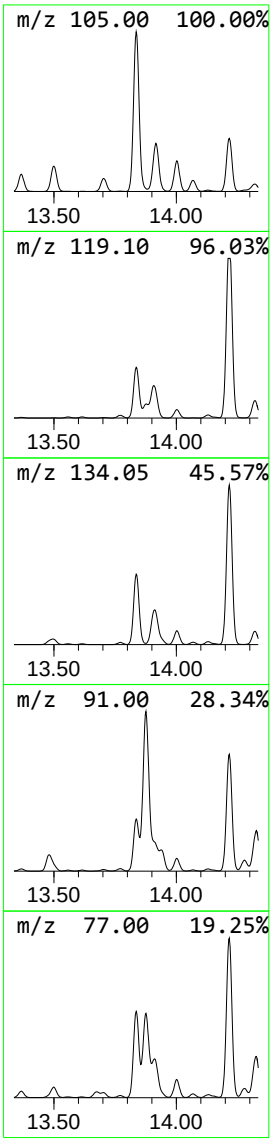
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,3-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.836	105.39 ug/l	19477300	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	94
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

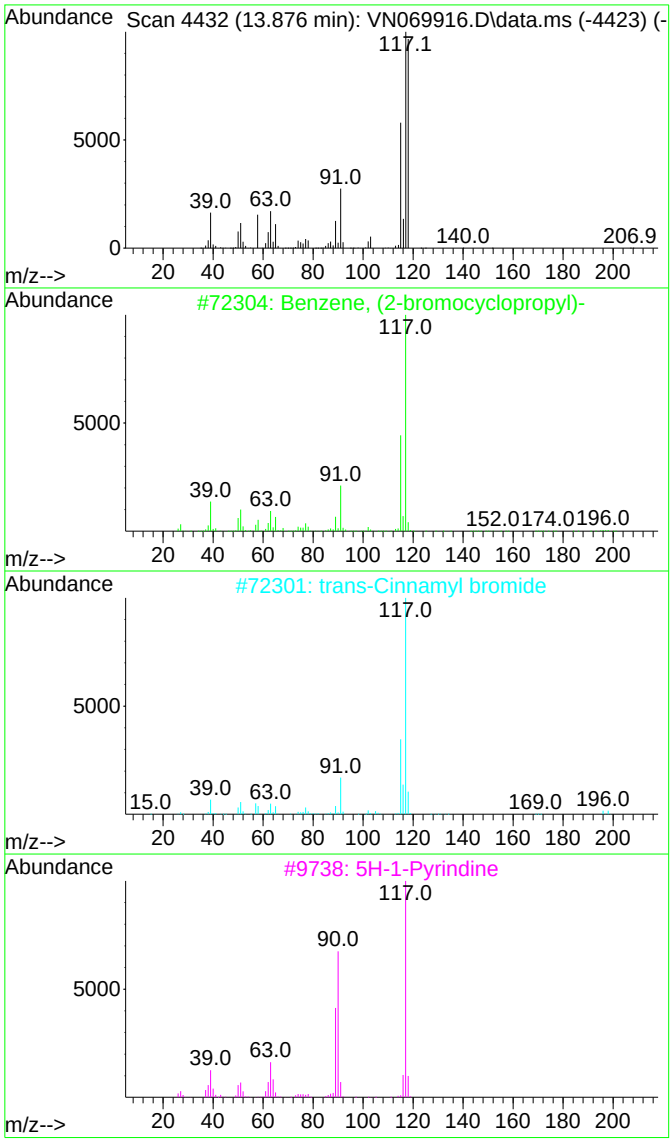
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

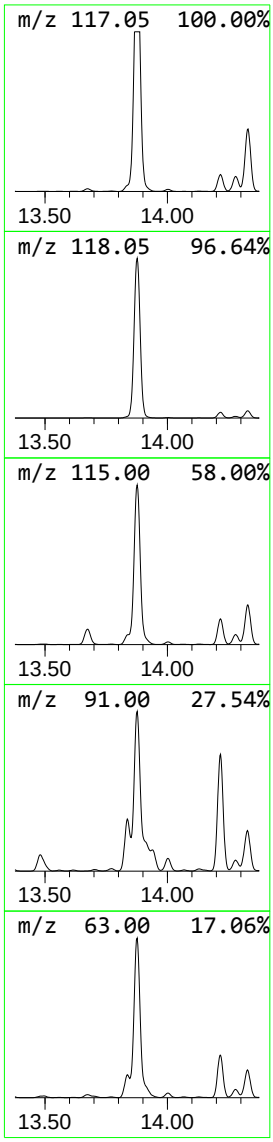
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	461.32 ug/l	85259700	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	52
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	47
3	5H-1-Pyridine	117	C8H7N	000270-91-7	38
4	Indole	117	C8H7N	000120-72-9	35
5	Indolizine	117	C8H7N	000274-40-8	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

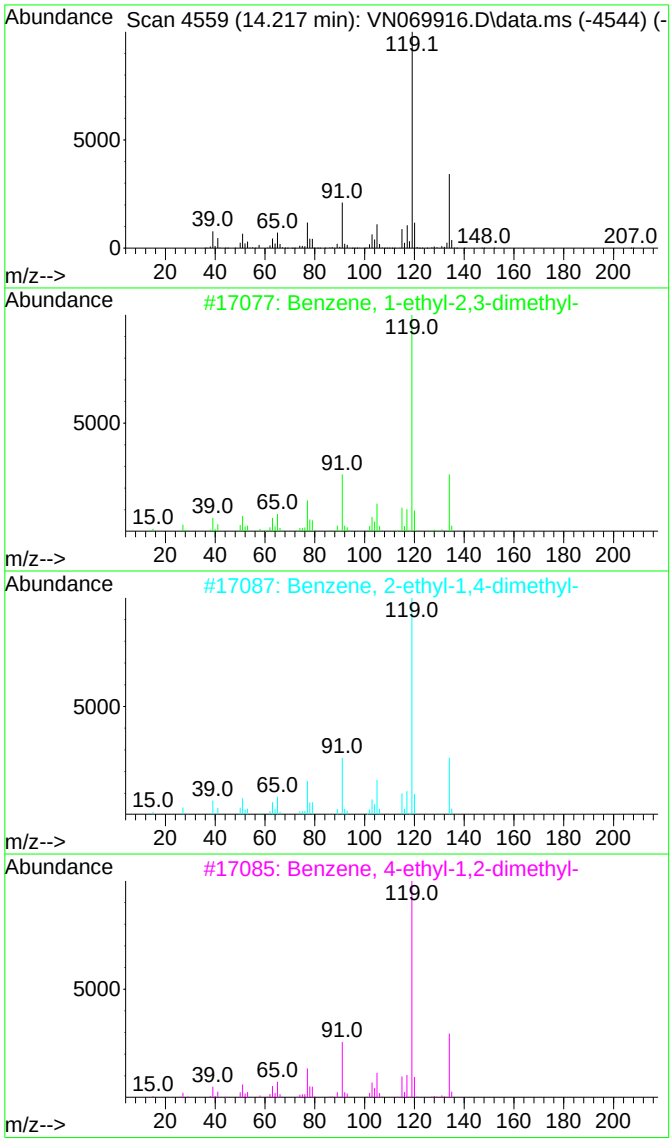
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

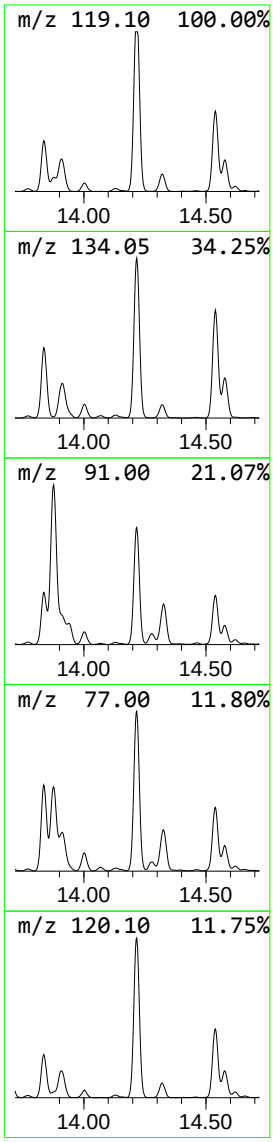
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	233.48 ug/l	43151100	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

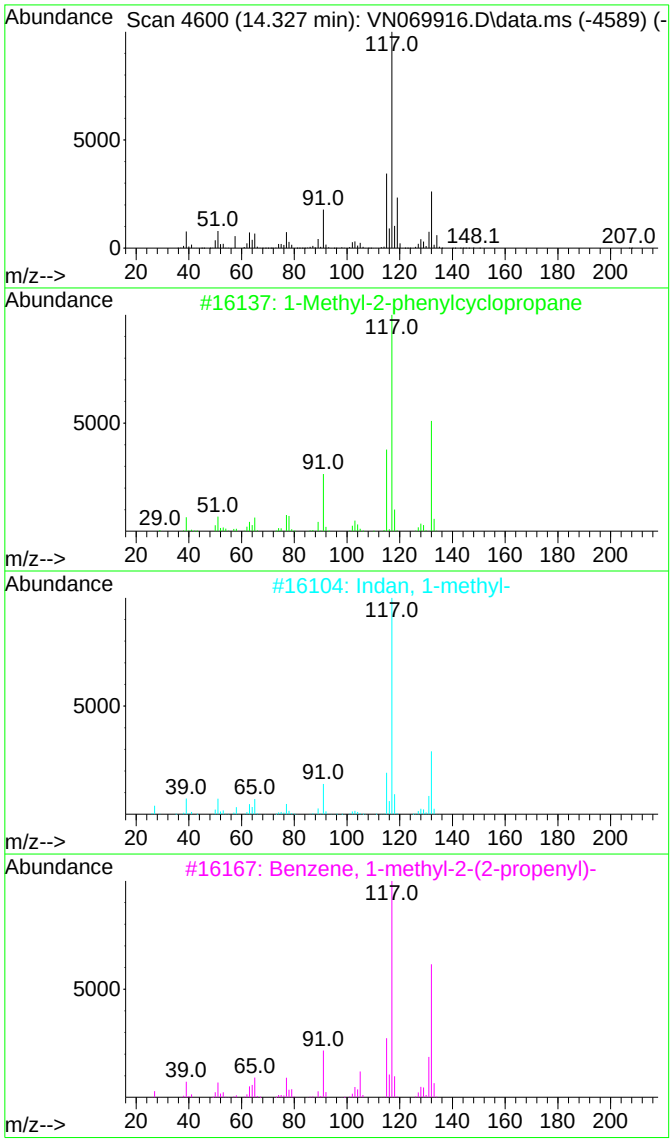
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

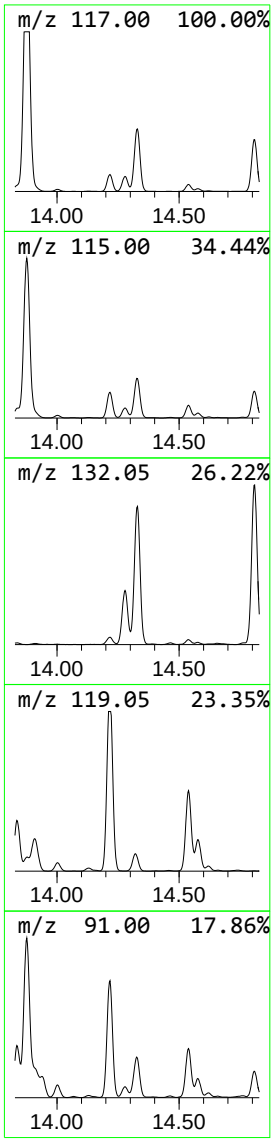
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Methyl-2-phenylcyclopropane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	106.19 ug/l	19626500	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76
2	Indan, 1-methyl-	132	C10H12	000767-58-8	76
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	76
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
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Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

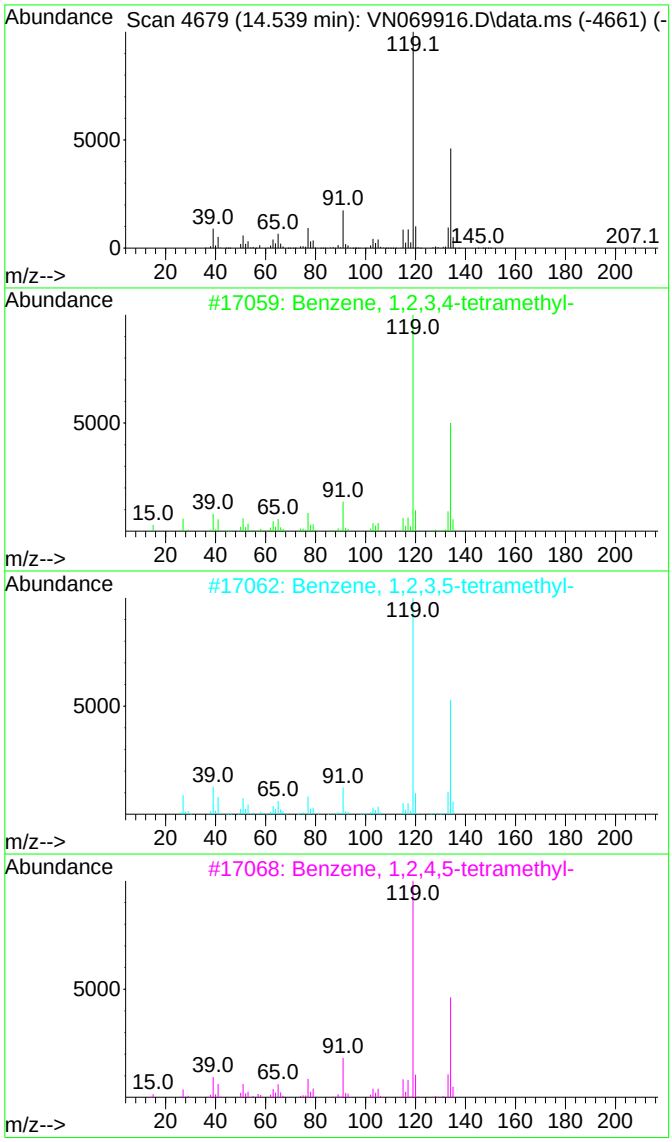
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

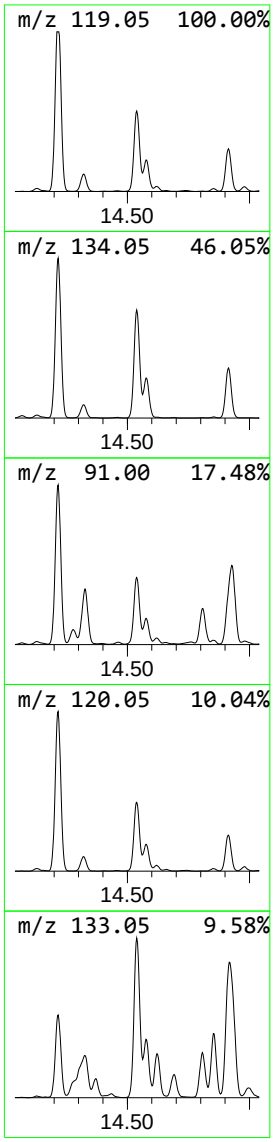
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	114.51 ug/l	21162400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

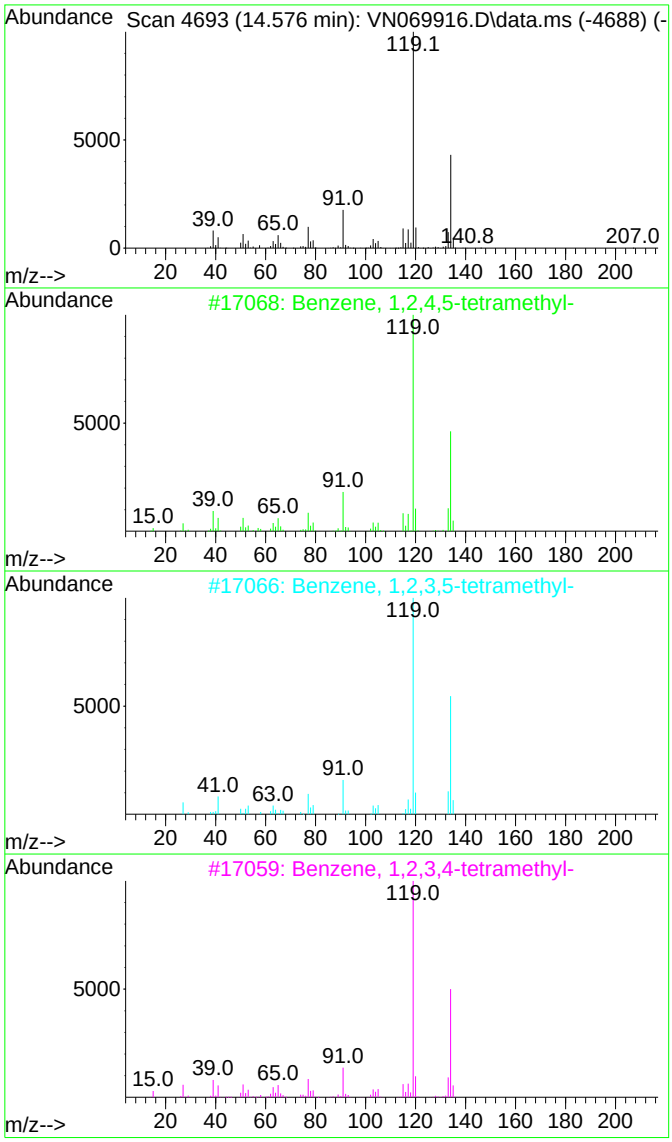
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

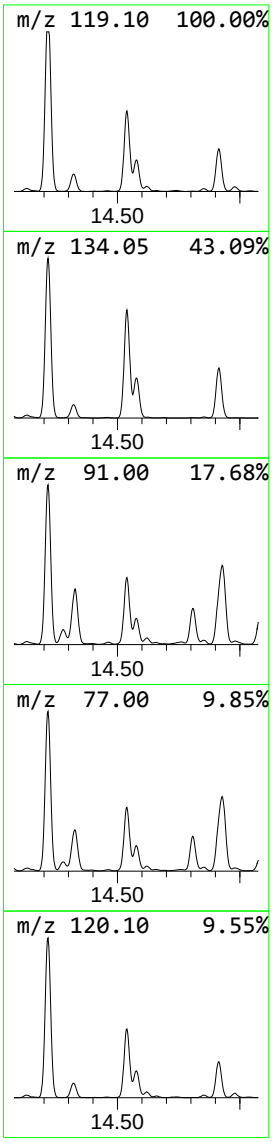
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.576	37.52 ug/l	6935180	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

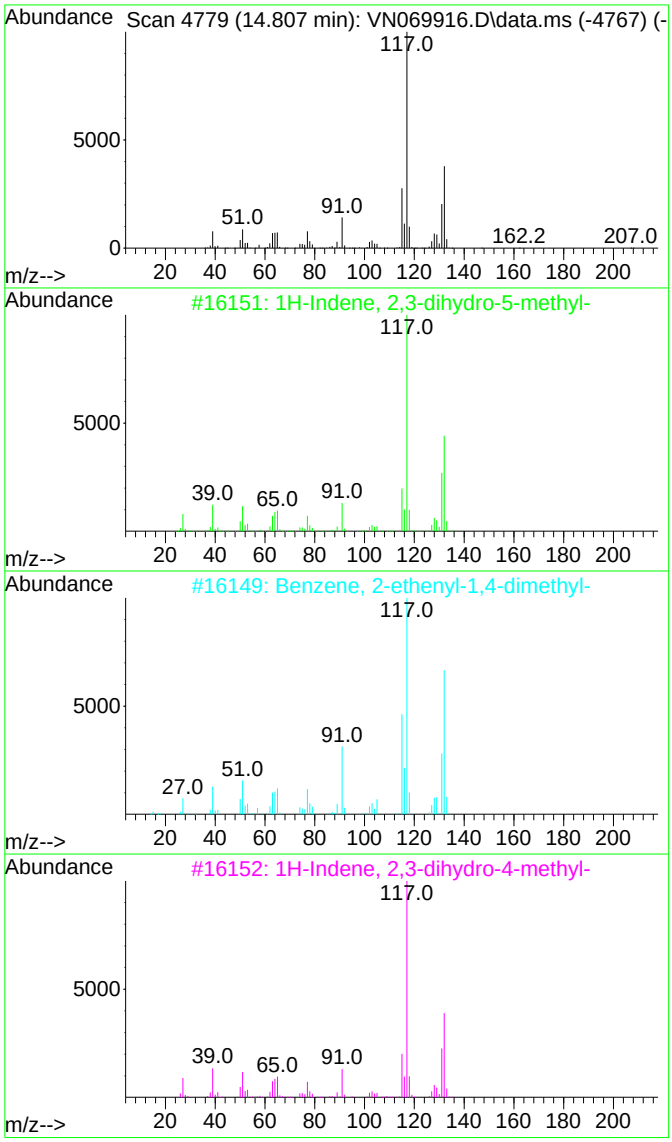
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

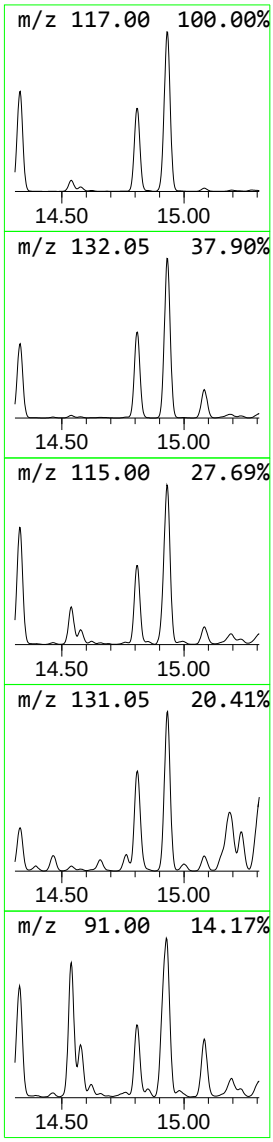
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.807	79.13 ug/l	14625200	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	96
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

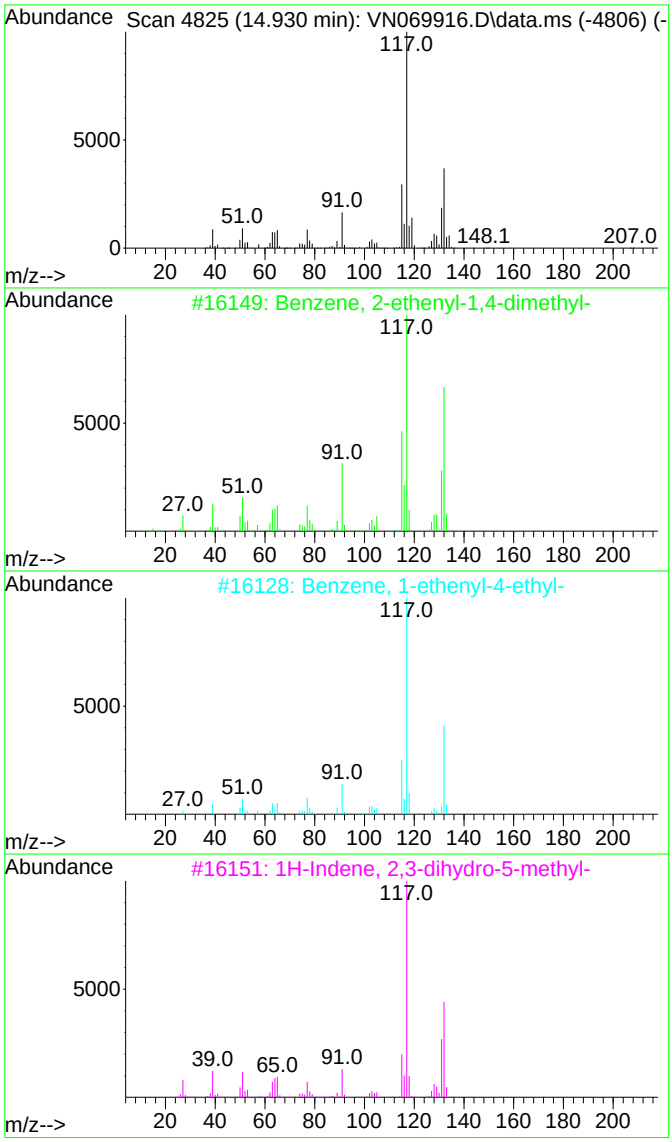
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

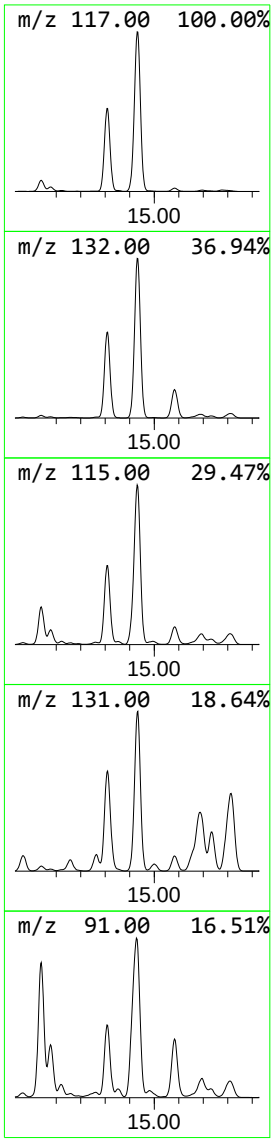
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	217.93 ug/l	40276800	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

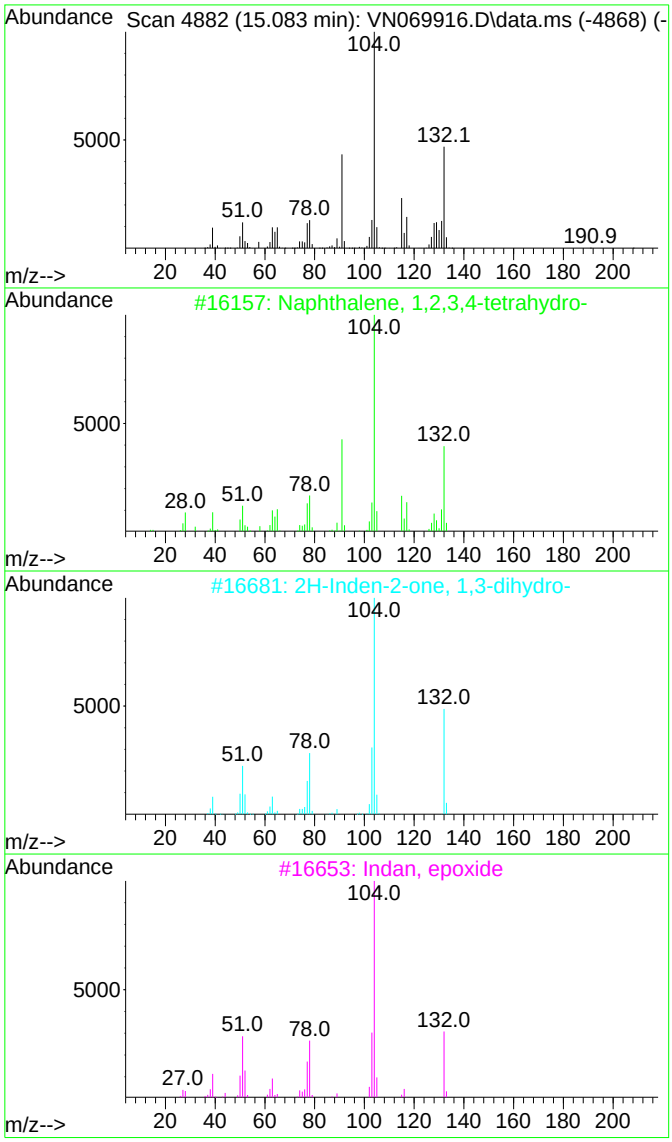
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

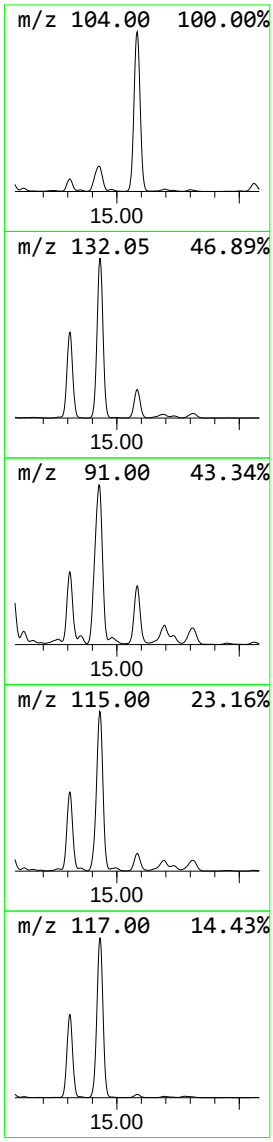
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.083	30.71 ug/l	5675470	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
3	Indan, epoxide	132	C9H8O	000768-22-9	53
4	Benzene, cyclobutyl-	132	C10H12	004392-30-7	40
5	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069916.D
Acq On : 9 Dec 2021 17:12
Operator : JC/MD
Sample : M4969-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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...	7.150	56.3	ug/l	9325140	1	8.086	8284310	50.0
Benzene, 1,3-di...	13.836	105.4	ug/l	19477300	4	13.675	9240790	50.0
Benzene, (2-bro...	13.876	461.3	ug/l	85259700	4	13.675	9240790	50.0
Benzene, 1-ethy...	14.217	233.5	ug/l	43151100	4	13.675	9240790	50.0
1-Methyl-2-phen...	14.327	106.2	ug/l	19626500	4	13.675	9240790	50.0
Benzene, 1,2,3,...	14.539	114.5	ug/l	21162400	4	13.675	9240790	50.0
Benzene, 1,2,4,...	14.576	37.5	ug/l	6935180	4	13.675	9240790	50.0
1H-Indene, 2,3-...	14.807	79.1	ug/l	14625200	4	13.675	9240790	50.0
Benzene, 2-ethe...	14.930	217.9	ug/l	40276800	4	13.675	9240790	50.0
Naphthalene, 1,...	15.083	30.7	ug/l	5675470	4	13.675	9240790	50.0