LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070625.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	1098	1148	1183	rBV4	147162	610090	6.87%	0.850%
2	5.559	1308	1331	1360	rVB3	57945	200035	2.25%	0.279%
3	7.354	1978	2000	2032	rBV2	78457	265432	2.99%	0.370%
4	7.812	2150	2171	2196	rBV2	155082	405612	4.57%	0.565%
5	8.019	2225	2248	2256	rBV	661594	1625334	18.30%	2.265%
6	8.075	2260	2269	2288	rVV	1149122	2694902	30.34%	3.756%
7	8.158	2289	2300	2323	rVB3	98669	242745	2.73%	0.338%
8	8.282	2324	2346	2367	rBV2	412789	955686	10.76%	1.332%
9	8.432	2382	2402	2426	rBV2	815824	1872668	21.08%	2.610%
10	8.547	2429	2445	2460	rBV6	52196	136454	1.54%	0.190%
11	8.815	2528	2545	2579	rBV	376366	832568	9.37%	1.160%
12	8.963	2581	2600	2636	rVB	1593197	3342240	37.62%	4.658%
13	9.451	2757	2782	2802	rBV3	256378	598149	6.73%	0.834%
14	10.073	3003	3014	3044	rVB5	54413	135774	1.53%	0.189%
15	10.210	3046	3065	3092	rBV3	49044	125010	1.41%	0.174%
16	10.440	3132	3151	3162	rBV	2682327	5021840	56.53%	6.999%
17	10.505	3162	3175	3204	rVV	4710842	8883653	100.00%	12.381%
18	10.620	3205	3218	3240	rVB2	174866	350006	3.94%	0.488%
19	11.291	3461	3468	3478	rVB	86567	124882	1.41%	0.174%
20	11.344	3479	3488	3501	rVB4	69458	129220	1.45%	0.180%
21	11.452	3517	3528	3537	rBV4	59057	99239	1.12%	0.138%
22	11.524	3539	3555	3580	rVB7	238125	612020	6.89%	0.853%
23	11.626	3581	3593	3606	rBV	223658	364938	4.11%	0.509%
24	11.747	3622	3638	3661	rBV	1956938	3534660	39.79%	4.926%
25	11.846	3662	3675	3693	rBV	306874	603677	6.80%	0.841%
26	11.953	3695	3715	3736	rBV3	2035129	4027359	45.33%	5.613%
27	12.280	3812	3837	3853	rBV2	592036	1594774	17.95%	2.223%
28	12.366	3862	3869	3879	rVB	210089	311229	3.50%	0.434%
29	12.455	3894	3902	3906	rBV5	118582	174335	1.96%	0.243%
30	12.581	3941	3949	3954	rBV4	80710	130787	1.47%	0.182%
31	12.734	3994	4006	4029	rVB2	2097184	4001244	45.04%	5.576%
32	12.916	4061	4074	4085	rVB2	246028	520055	5.85%	0.725%
33	12.983	4086	4099	4107	rBV	989576	1711650	19.27%	2.385%
34	13.047	4114	4123	4139	rVB2	2475114	4430015	49.87%	6.174%
35	13.109	4140	4146	4157	rVB4	244671	368479	4.15%	0.514%
36	13.283	4205	4211	4227	rVB4	351843	594279	6.69%	0.828%

LSC Area Percent Report

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Sample : N1141-06
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

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\82N122721W.M
Title : SW846 8260

37	13.369	4230	4243	4256	rBV	1846696	3061239	34.46%	4.266%
38	13.562	4305	4315	4325	rVB8	501907	848426	9.55%	1.182%
39	13.675	4346	4357	4377	rVB2	2092846	4195379	47.23%	5.847%
40	13.871	4422	4430	4438	rBV3	642712	943851	10.62%	1.315%
41	13.994	4465	4476	4488	rBV3	1763099	2787403	31.38%	3.885%
42	14.131	4522	4527	4532	rBV	184363	212187	2.39%	0.296%
43	14.217	4551	4559	4570	rVB	550905	855126	9.63%	1.192%
44	14.327	4590	4600	4611	rVB2	605373	989741	11.14%	1.379%
45	14.506	4659	4667	4675	rBV4	461131	682160	7.68%	0.951%
46	14.579	4689	4694	4702	rVB	434774	535529	6.03%	0.746%
47	14.622	4704	4710	4718	rVV2	274314	355296	4.00%	0.495%
48	14.667	4719	4727	4740	rVB7	382572	650871	7.33%	0.907%
49	14.812	4772	4781	4788	rBV4	378949	690739	7.78%	0.963%
50	14.927	4809	4824	4837	rBV6	771462	1974132	22.22%	2.751%
51	15.086	4874	4883	4897	rVB	425076	726430	8.18%	1.012%
52	16.620	5445	5455	5487	rVB3	240158	615132	6.92%	0.857%

Sum of corrected areas: 71754681

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
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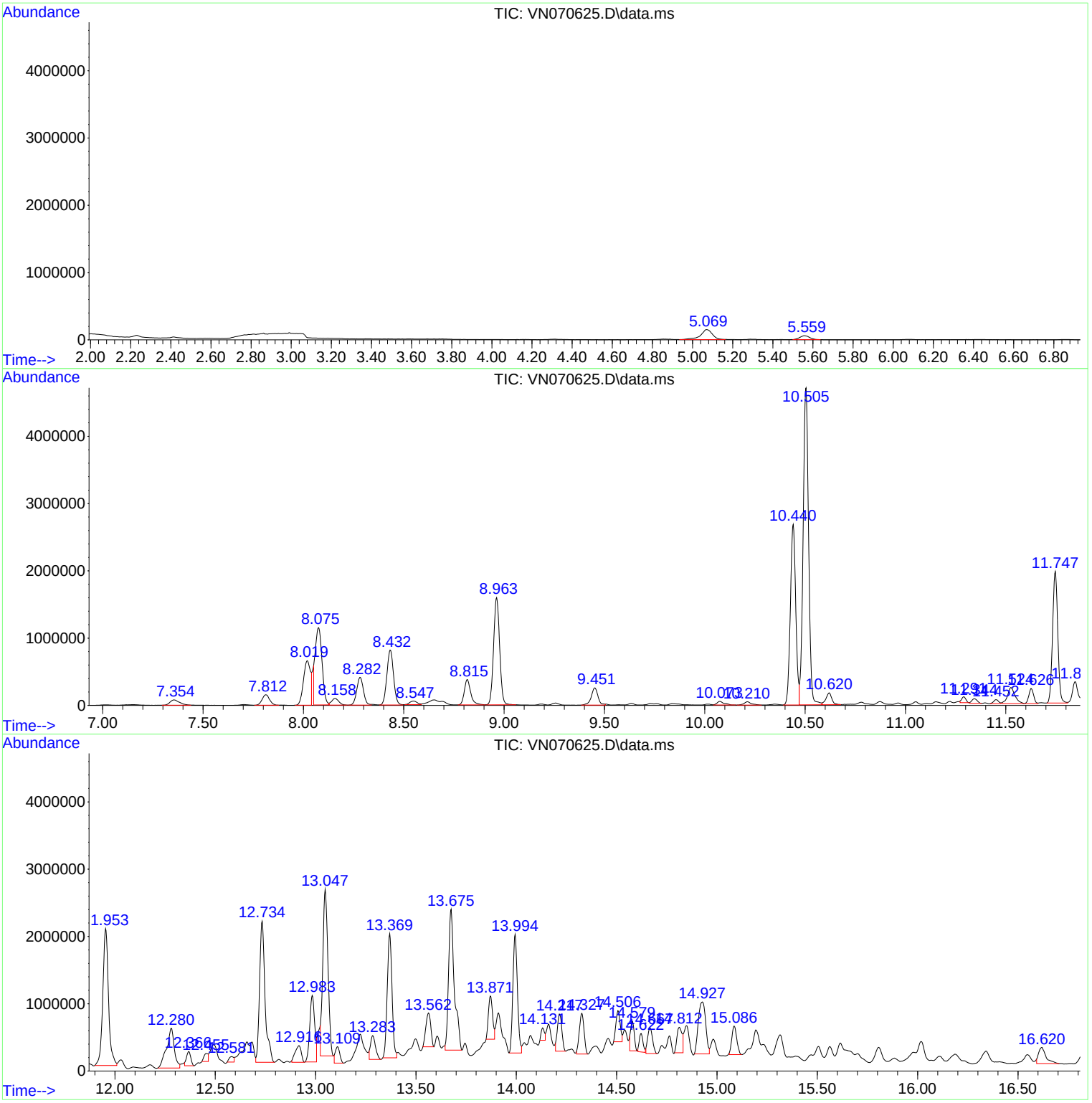
Instrument :
MSVOA_N
ClientSampleId :
101224

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

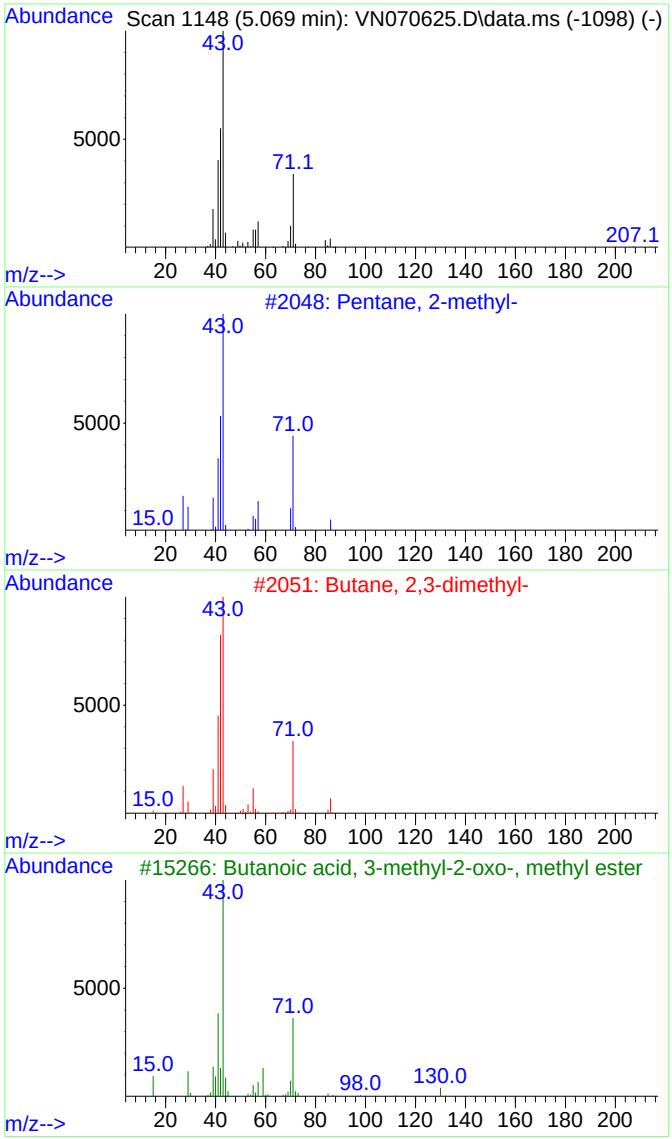
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

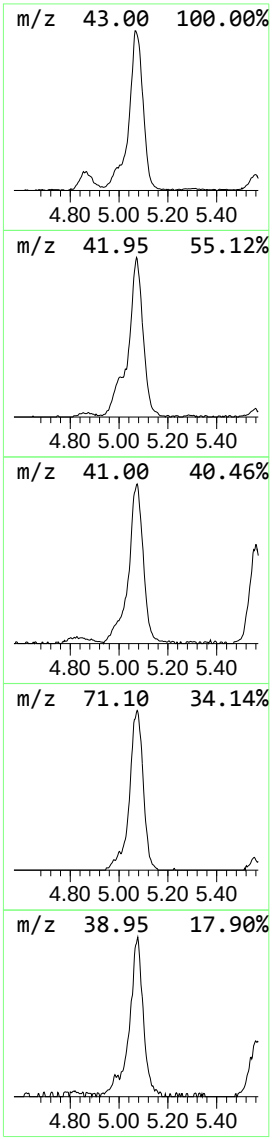
****

Peak Number 1 Pentane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	11.32 ug/l	610090	Pentafluorobenzene	8.078

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	87
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3	Butanoic acid, 3-methyl-2-oxo-, ...	130	C6H10O3	003952-67-8	43
4	trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	40
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

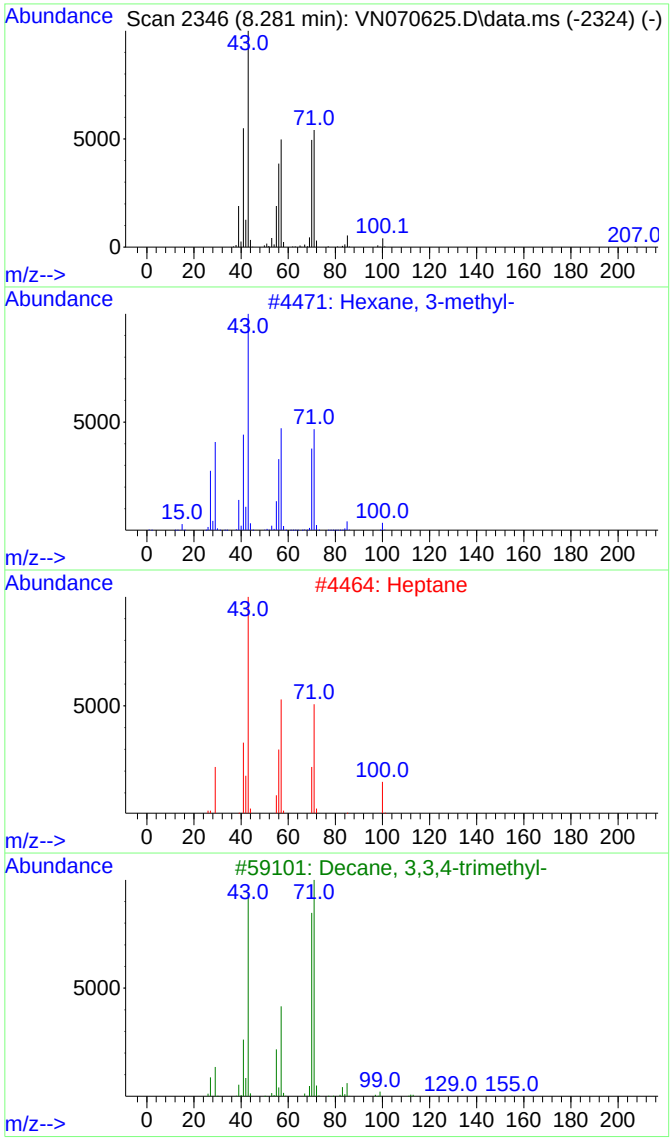
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

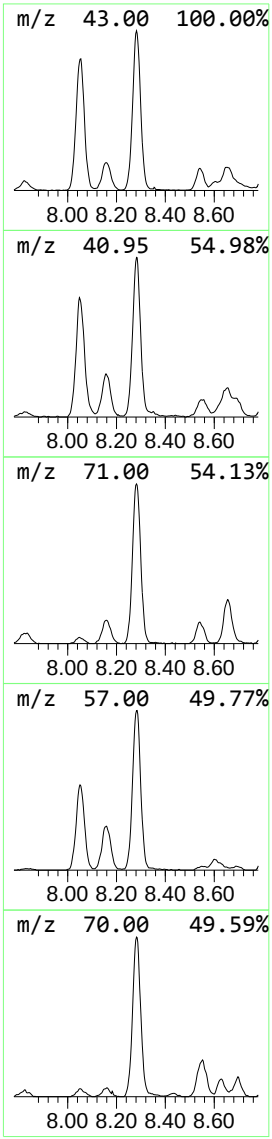
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.281	17.73 ug/l	955686	Pentafluorobenzene	8.078

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	59
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Diisoamyl ether	158	C10H22O	000544-01-4	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

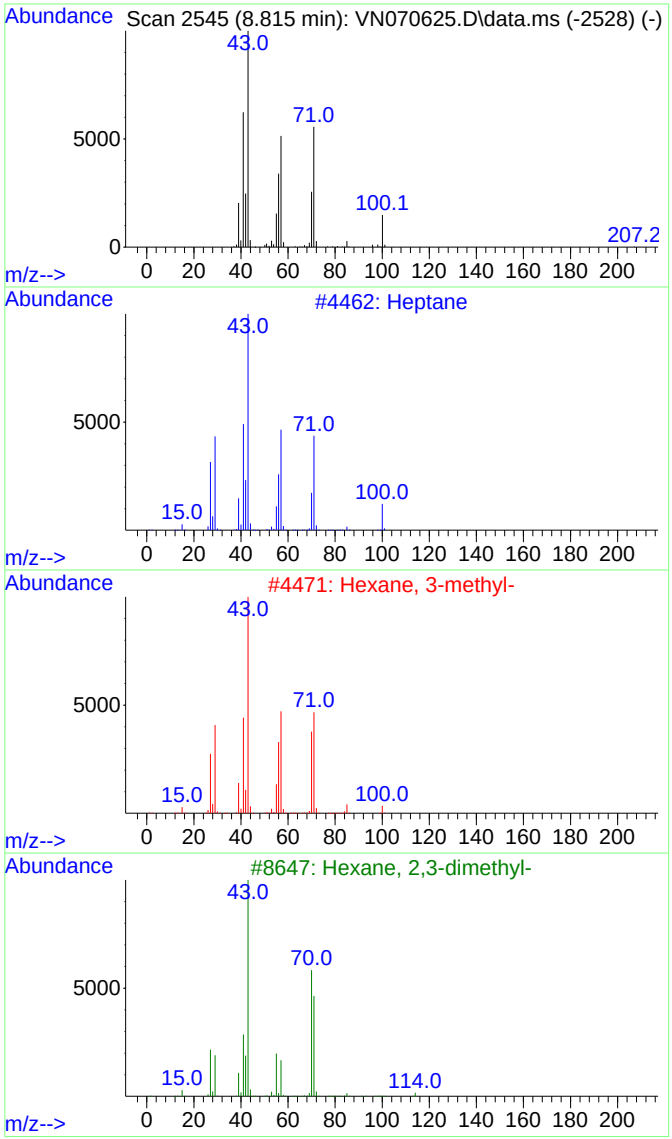
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

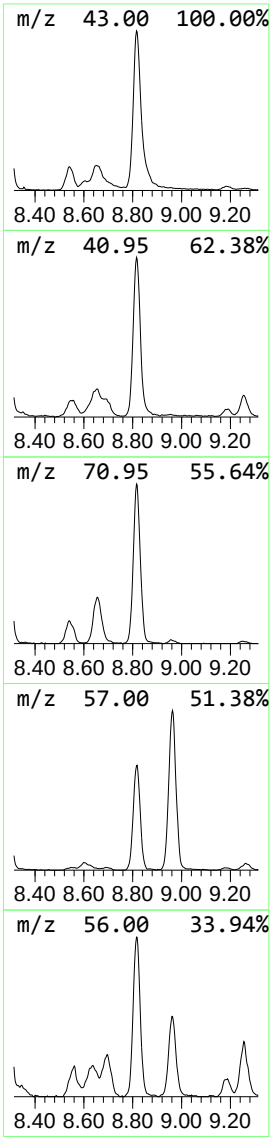
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.815	12.46 ug/l	832568	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	94
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	40
3	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

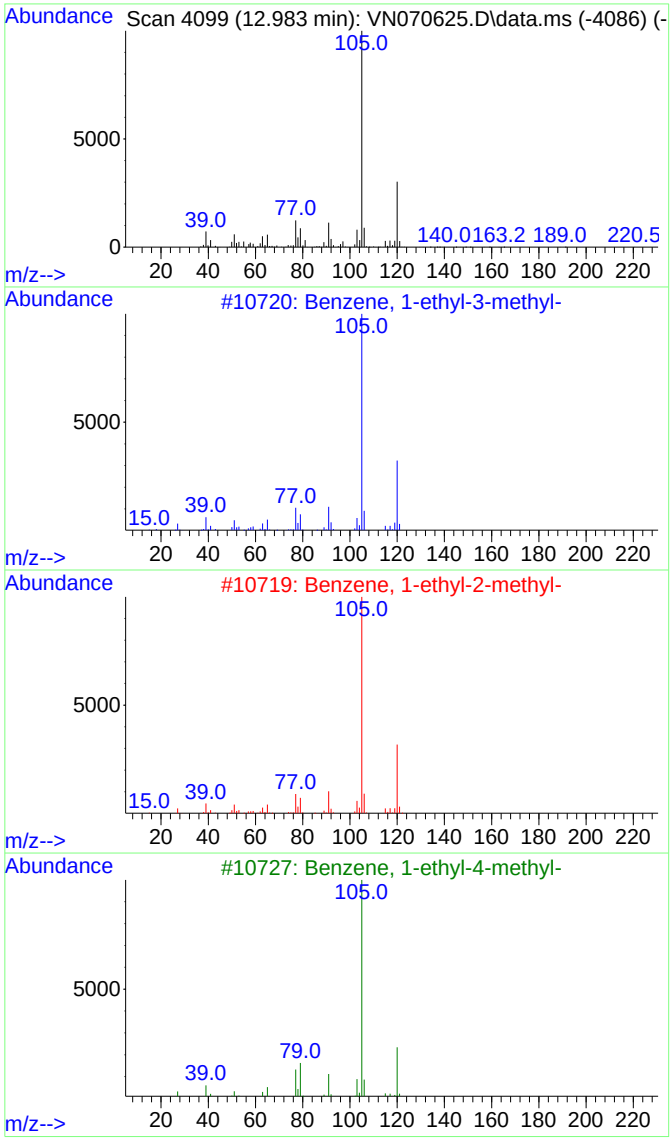
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

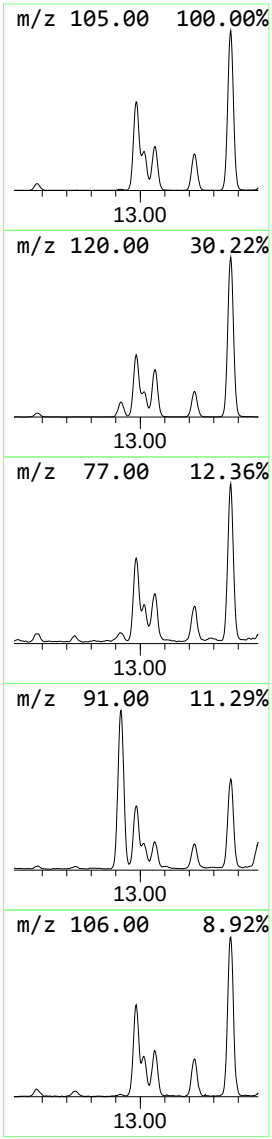
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	20.40 ug/l	1711650	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

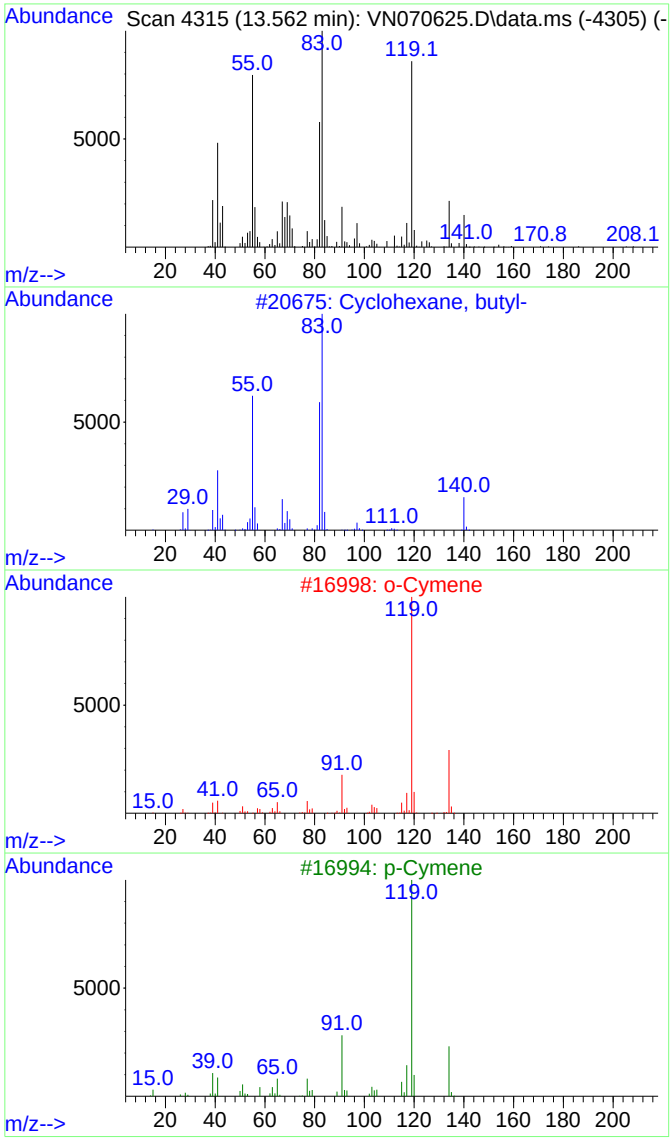
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

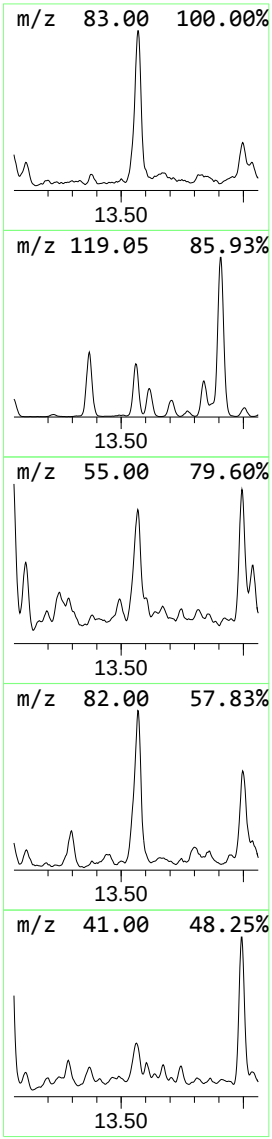
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, butyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.562	10.11 ug/l	848426	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	53
2	o-Cymene	134	C10H14	000527-84-4	47
3	p-Cymene	134	C10H14	000099-87-6	47
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	38
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	38





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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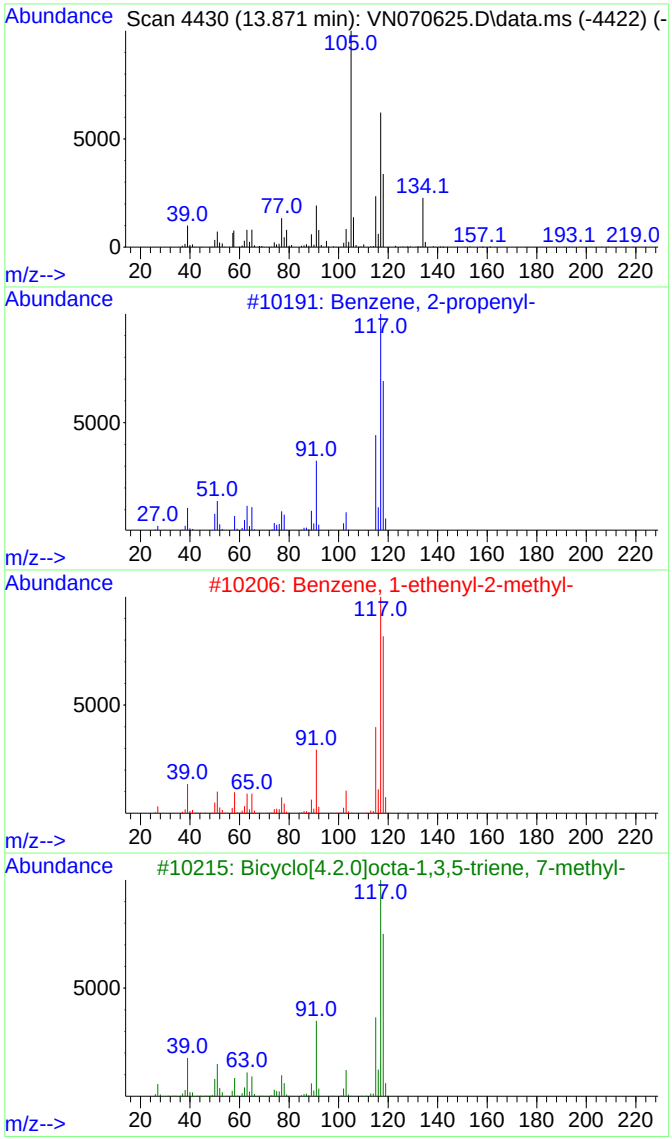
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

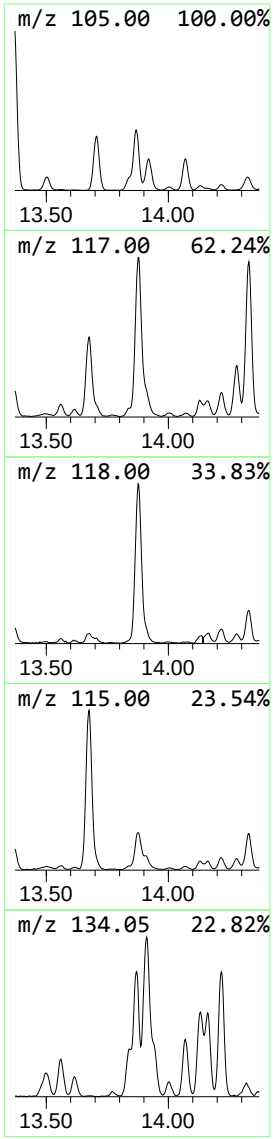
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-propenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	11.25 ug/l	943851	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	50
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	45
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	45
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	43
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	43





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Data File : VN070625.D
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Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

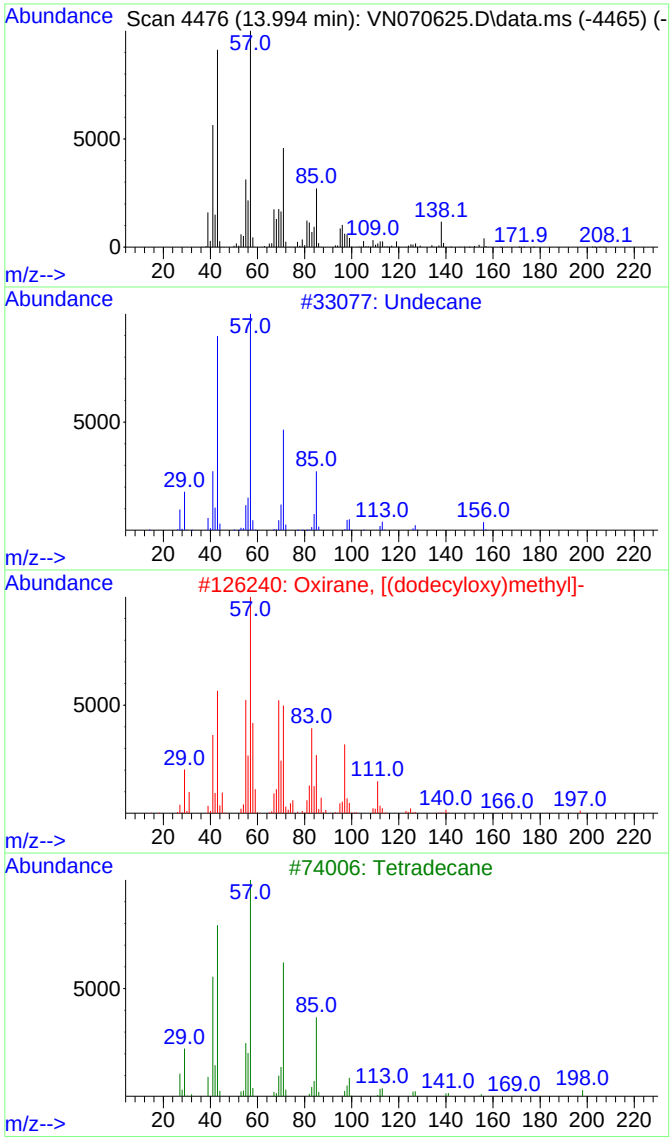
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

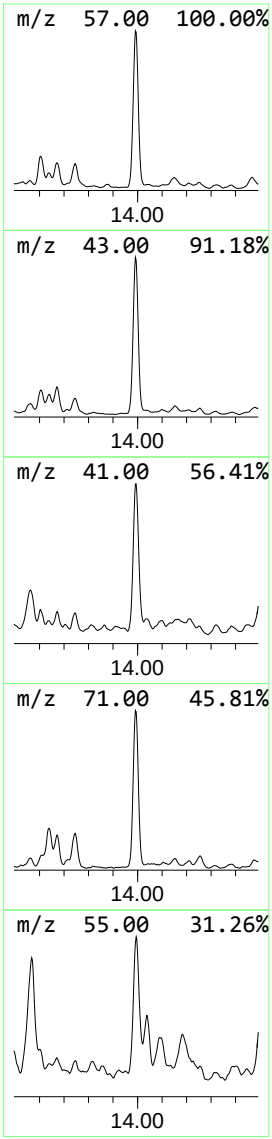
****

Peak Number 7 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	33.22 ug/l	2787400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	81
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	72
3	Tetradecane	198	C14H30	000629-59-4	64
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	64
5	Decane	142	C10H22	000124-18-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
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Acq On : 14 Jan 2022 16:04
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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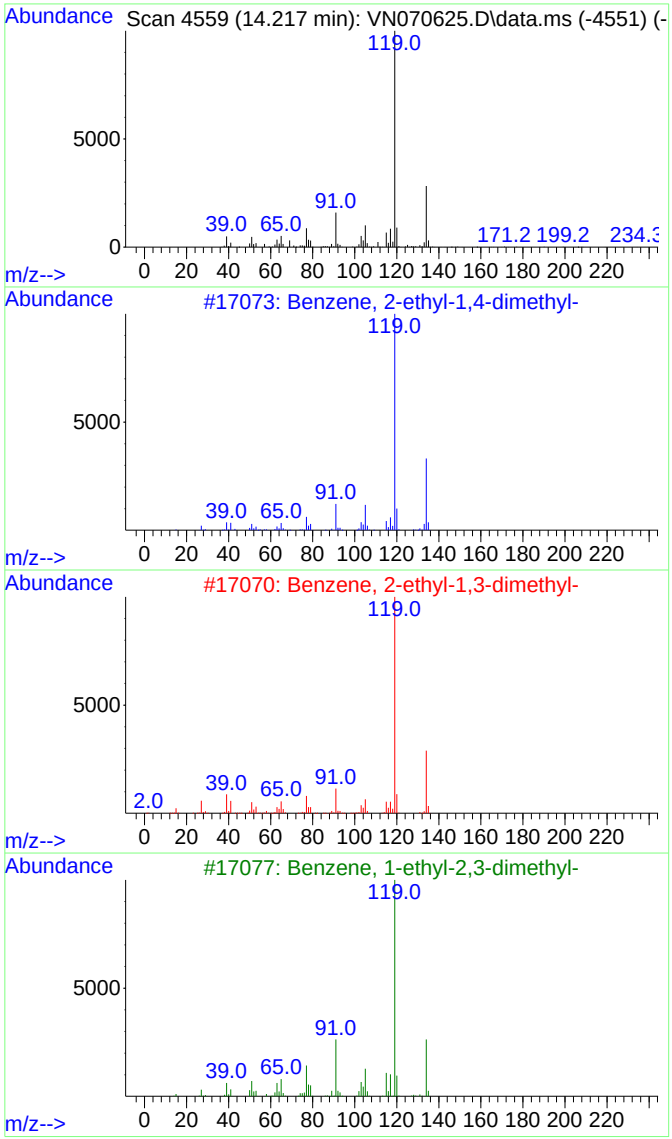
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

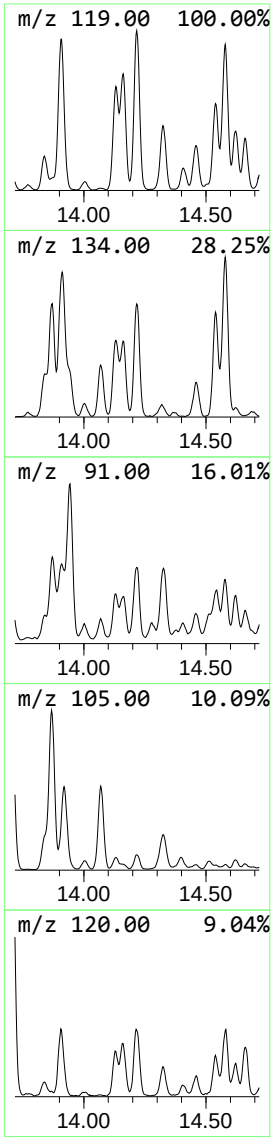
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	10.19 ug/l	855126	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95





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Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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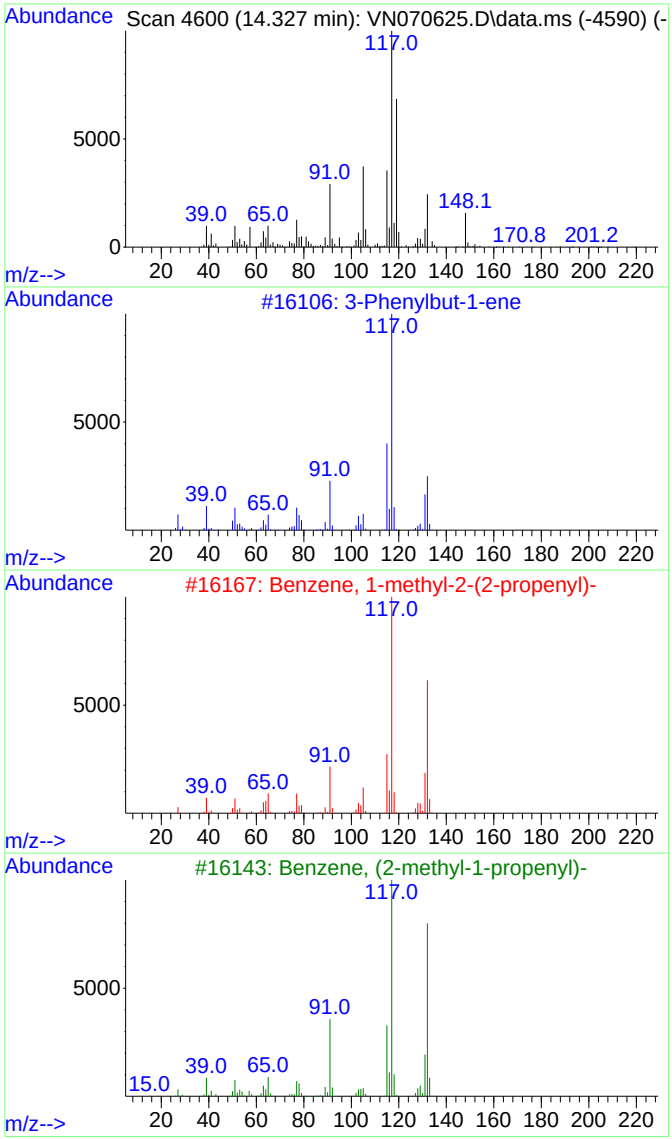
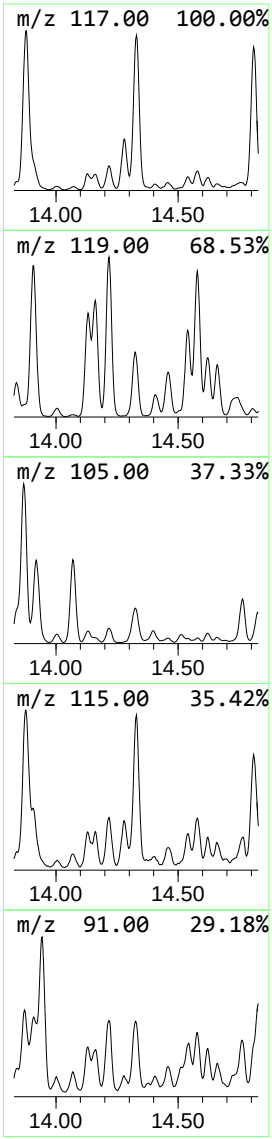
Peak Number 9 3-Phenylbut-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	11.80 ug/l	989741	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	62
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	62
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	62
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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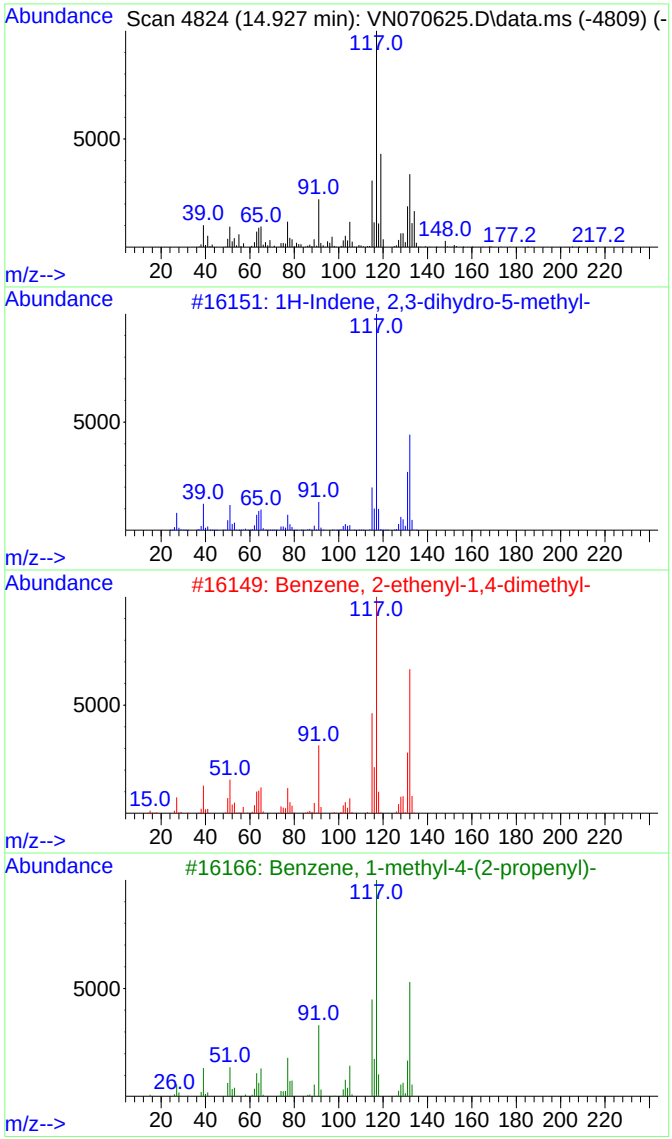
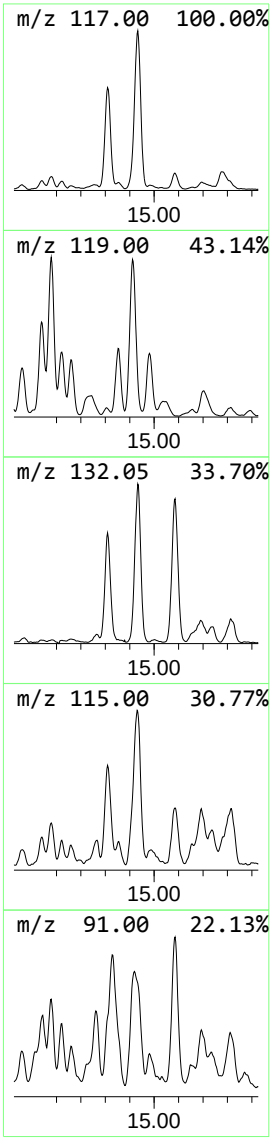
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	23.53 ug/l	1974130	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	91
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070625.D
Acq On : 14 Jan 2022 16:04
Operator : JC/MD
Sample : N1141-06
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101224

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Pentane, 2-methyl-	5.069	11.3	ug/l	610090	1	8.078	2694900	50.0
Hexane, 3-methyl-	8.281	17.7	ug/l	955686	1	8.078	2694900	50.0
Heptane	8.815	12.5	ug/l	832568	2	8.963	3342240	50.0
Benzene, 1-ethy...	12.983	20.4	ug/l	1711650	4	13.675	4195380	50.0
Cyclohexane, bu...	13.562	10.1	ug/l	848426	4	13.675	4195380	50.0
Benzene, 2-prop...	13.871	11.3	ug/l	943851	4	13.675	4195380	50.0
Undecane	13.994	33.2	ug/l	2787400	4	13.675	4195380	50.0
Benzene, 2-ethy...	14.217	10.2	ug/l	855126	4	13.675	4195380	50.0
3-Phenylbut-1-ene	14.327	11.8	ug/l	989741	4	13.675	4195380	50.0
1H-Indene, 2,3-...	14.927	23.5	ug/l	1974130	4	13.675	4195380	50.0