LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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: VN070012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.137	409	428	456	rBV	2450010	5593361	4.04%	0.628%
2	3.510	546	567	597	rBV3	1819838	4680910	3.38%	0.525%
3	3.988	724	745	776	rVB2	760204	2069145	1.49%	0.232%
4	5.085	1126	1154	1156	rBV2	965423	2555059	1.85%	0.287%
5	5.618	1320	1353	1395	rBV2	2635847	9142076	6.60%	1.026%
6	5.932	1443	1470	1506	rBV3	441011	1418145	1.02%	0.159%
7	6.120	1509	1540	1576	rBV2	2327017	7118765	5.14%	0.799%
8	6.468	1654	1670	1698	rVB3	1027087	3138997	2.27%	0.352%
9	6.608	1699	1722	1740	rBV3	600957	1850142	1.34%	0.208%
10	6.900	1810	1831	1860	rVB5	1210176	3583674	2.59%	0.402%
11	7.045	1862	1885	1903	rBV	1109810	3308200	2.39%	0.371%
12	7.147	1903	1923	1943	rBV	3392431	9595784	6.93%	1.077%
13	7.847	2168	2184	2203	rVB2	1857338	4456189	3.22%	0.500%
14	8.029	2230	2252	2253	rBV2	955962	1740682	1.26%	0.195%
15	8.080	2256	2271	2291	rVV7	4340257	14158404	10.23%	1.589%
16	8.177	2292	2307	2331	rVB2	3276092	8551849	6.18%	0.960%
17	8.298	2332	2352	2369	rBV	3278411	7553302	5.46%	0.848%
18	8.461	2389	2413	2435	rBV	9676205	23935365	17.29%	2.686%
19	8.619	2437	2472	2495	rBV2	4891532	17791940	12.85%	1.996%
20	8.708	2496	2505	2527	rVB3	993978	2562851	1.85%	0.288%
21	8.829	2528	2550	2580	rVB3	2595019	6628487	4.79%	0.744%
22	8.968	2581	2602	2616	rBV4	5302444	12507583	9.03%	1.404%
23	9.244	2697	2705	2739	rVB2	978316	2199613	1.59%	0.247%
24	9.459	2750	2785	2798	rBV2	4808986	12988787	9.38%	1.458%
25	9.513	2800	2805	2822	rVV2	1088800	1882968	1.36%	0.211%
26	9.641	2843	2853	2867	rVV	960677	1844814	1.33%	0.207%
27	9.883	2930	2943	2963	rVB	3378212	6933062	5.01%	0.778%
28	9.974	2964	2977	2983	rBV	2172920	3858348	2.79%	0.433%
29	10.017	2984	2993	3007	rVB2	4714539	9214519	6.66%	1.034%
30	10.081	3008	3017	3025	rBV	928421	1426217	1.03%	0.160%
31	10.218	3049	3068	3093	rBV3	1526458	3835426	2.77%	0.430%
32	10.322	3093	3107	3115	rBV2	1076283	2045137	1.48%	0.229%
33	10.371	3116	3125	3137	rVB3	1387112	2467309	1.78%	0.277%
34	10.443	3137	3152	3163	rBV	5293083	10291712	7.43%	1.155%
35	10.508	3164	3176	3191	rVB	5713873	10630967	7.68%	1.193%
36	10.626	3205	3220	3234	rVB5	1814327	4057390	2.93%	0.455%

LSC Area Percent Report

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Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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	10.864	3296	3309	3332	rVB6	1473714	4055888	2.93%	0.455%
38	11.529	3547	3557	3583	rVB8	574928	1678648	1.21%	0.188%
39	11.747	3623	3638	3653	rBV	5124344	9158808	6.62%	1.028%
40	11.846	3660	3675	3696	rVV2	29282515	50889470	36.76%	5.710%
41	11.950	3697	3714	3754	rVB3	66859338	138447708	100.00%	15.536%
42	12.280	3815	3837	3857	rBV	8650997	15475397	11.18%	1.737%
43	12.581	3936	3949	3963	rBV	3168532	5274585	3.81%	0.592%
44	12.731	3992	4005	4027	rVB	4252086	7759409	5.60%	0.871%
45	12.921	4061	4076	4087	rBV	10942415	17925618	12.95%	2.012%
46	12.983	4087	4099	4108	rBV2	36211734	64586538	46.65%	7.247%
47	13.061	4120	4128	4159	rVB	18698028	30408099	21.96%	3.412%
48	13.222	4172	4188	4206	rBV	14812933	24891491	17.98%	2.793%
49	13.369	4227	4243	4273	rVB2	57279139	98088427	70.85%	11.007%
50	13.495	4274	4290	4303	rBV3	1089503	2698332	1.95%	0.303%
51	13.560	4304	4314	4325	rVB	1707099	2645715	1.91%	0.297%
52	13.707	4345	4369	4403	rVB2	15989356	35906614	25.94%	4.029%
53	13.841	4405	4419	4421	rBV	3714189	4867138	3.52%	0.546%
54	13.873	4422	4431	4439	rBV3	11920763	18541255	13.39%	2.081%
55	14.002	4468	4479	4490	rVB4	1009612	1640220	1.18%	0.184%
56	14.069	4490	4504	4515	rBV2	2988630	5163272	3.73%	0.579%
57	14.134	4515	4528	4533	rBV	5535601	9056271	6.54%	1.016%
58	14.217	4548	4559	4572	rVB	8617101	13362434	9.65%	1.499%
59	14.281	4573	4583	4590	rBV	1255000	1966296	1.42%	0.221%
60	14.329	4590	4601	4614	rVB3	5078775	8540178	6.17%	0.958%
61	14.461	4639	4650	4662	rBV	2157179	3358184	2.43%	0.377%
62	14.541	4662	4680	4687	rBV	4490004	7738136	5.59%	0.868%
63	14.579	4687	4694	4704	rVV	6240460	9775674	7.06%	1.097%
64	14.622	4704	4710	4718	rVV2	1515752	2232347	1.61%	0.250%
65	14.809	4770	4780	4791	rBV	4583666	7518783	5.43%	0.844%
66	14.930	4807	4825	4838	rBV3	7337819	16547474	11.95%	1.857%
67	14.986	4840	4846	4870	rVB3	1026735	2144464	1.55%	0.241%
68	15.086	4871	4883	4899	rBV2	1667457	2928741	2.12%	0.329%
69	15.196	4902	4924	4935	rBV5	2166063	5611790	4.05%	0.630%
70	15.314	4954	4968	4988	rVB3	1913175	4508170	3.26%	0.506%
71	15.507	5015	5040	5054	rBV	7587706	14735139	10.64%	1.653%
72	15.614	5070	5080	5091	rBV5	778869	1410297	1.02%	0.158%
73	15.807	5137	5152	5170	rBV	1073740	2284288	1.65%	0.256%
74	16.620	5439	5455	5491	rVB	4110937	9718227	7.02%	1.091%

Sum of corrected areas: 891156704

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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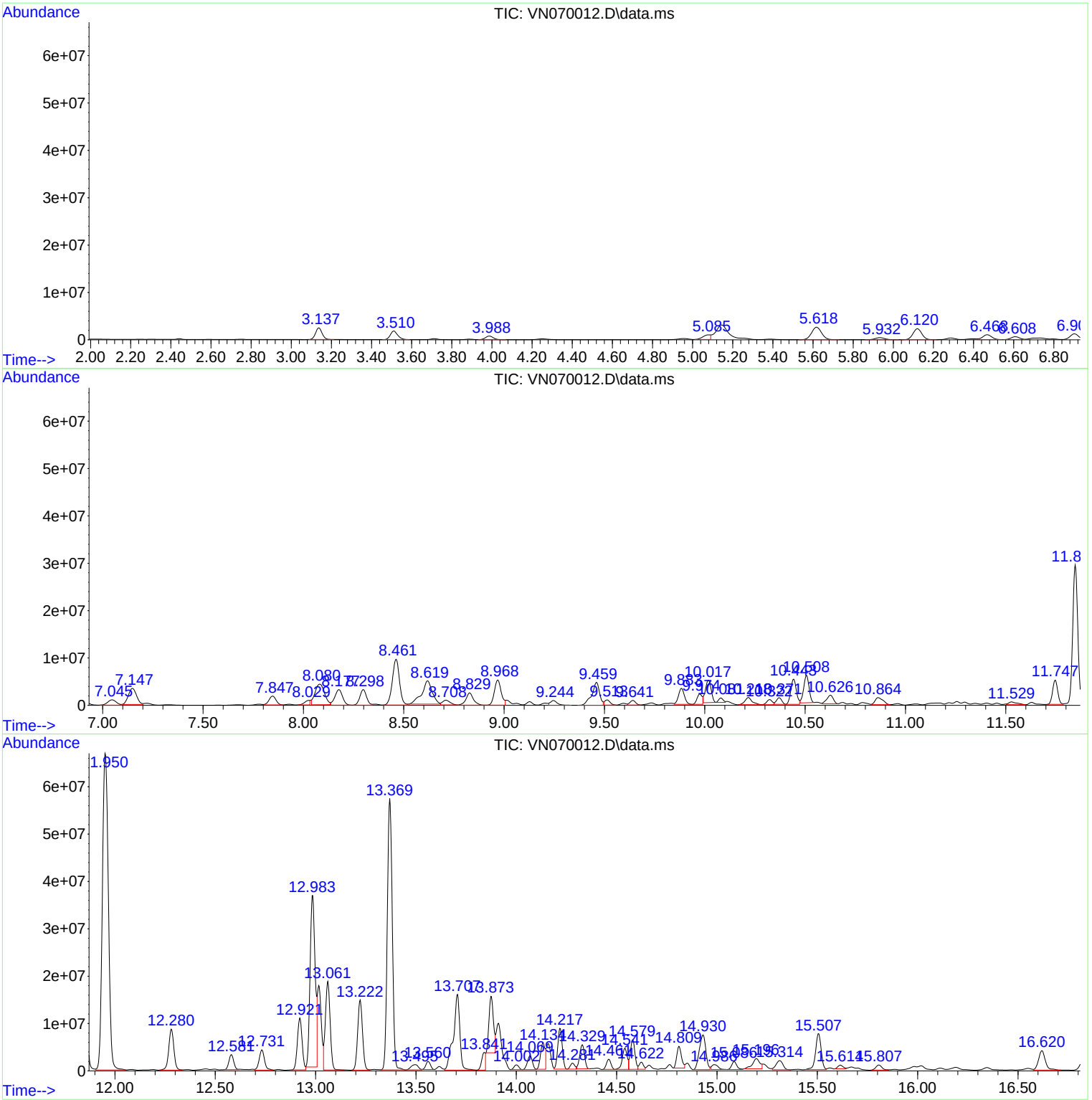
Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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



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Data File : VN070012.D
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ClientSampleId :
A2-8-6.5

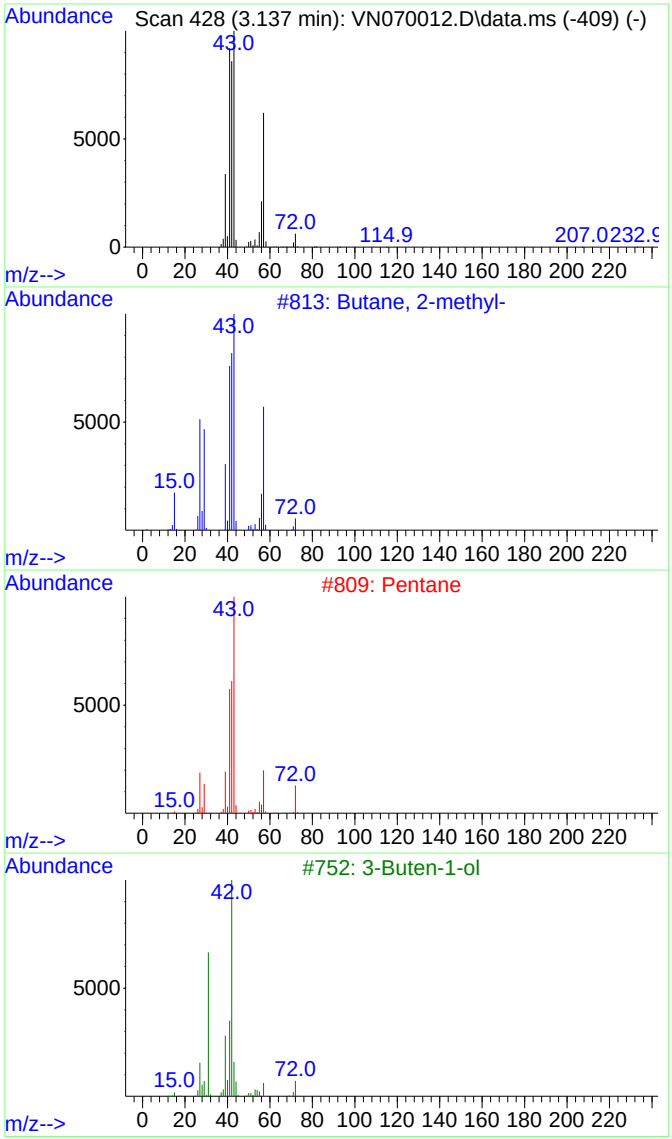
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

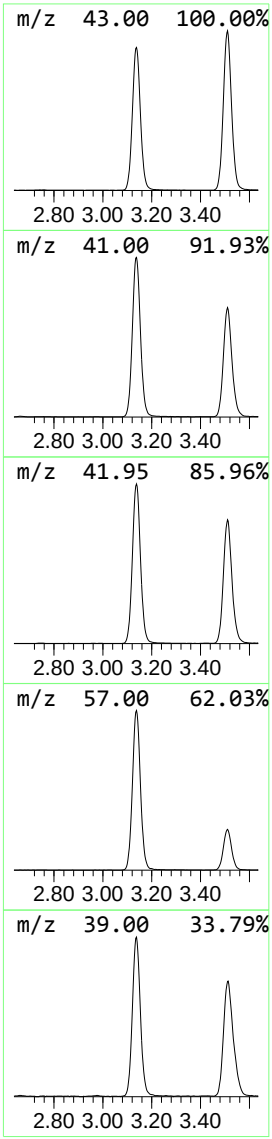
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.137	19.75 ug/l	5593360	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5	Azetidine	57	C3H7N	000503-29-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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

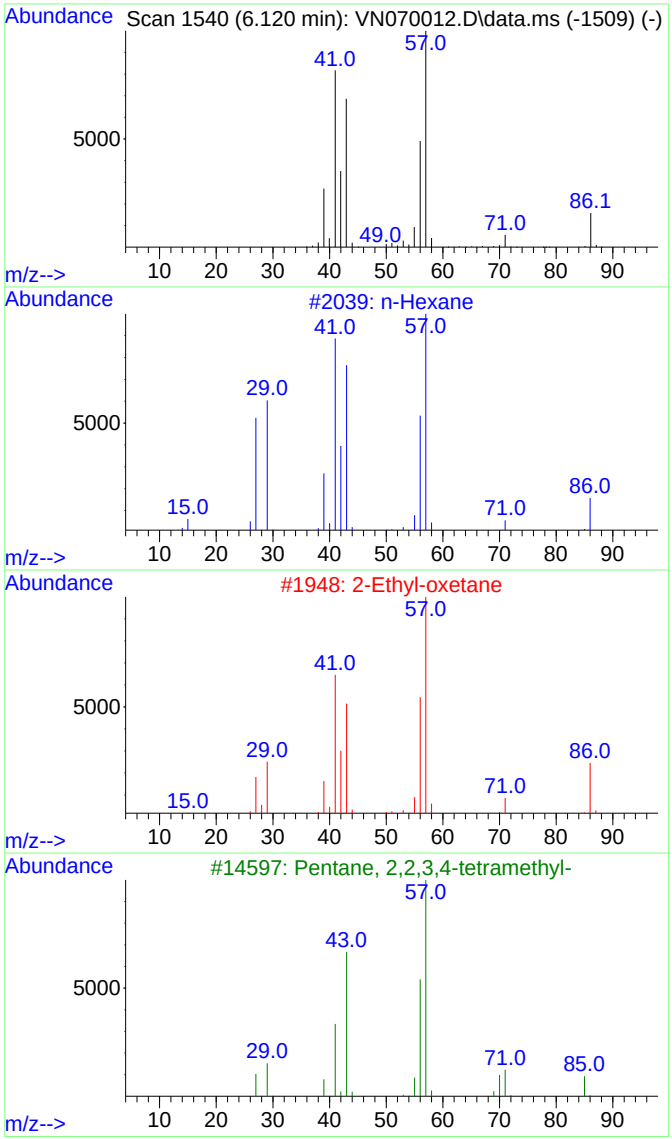
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

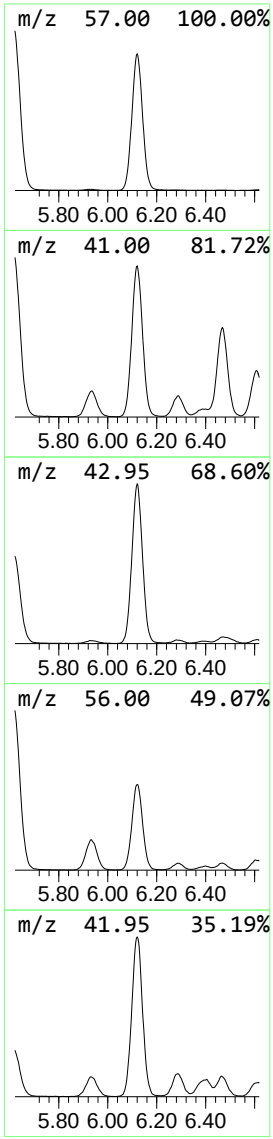
****

Peak Number 2 n-Hexane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.120	25.14 ug/l	7118770	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	83
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

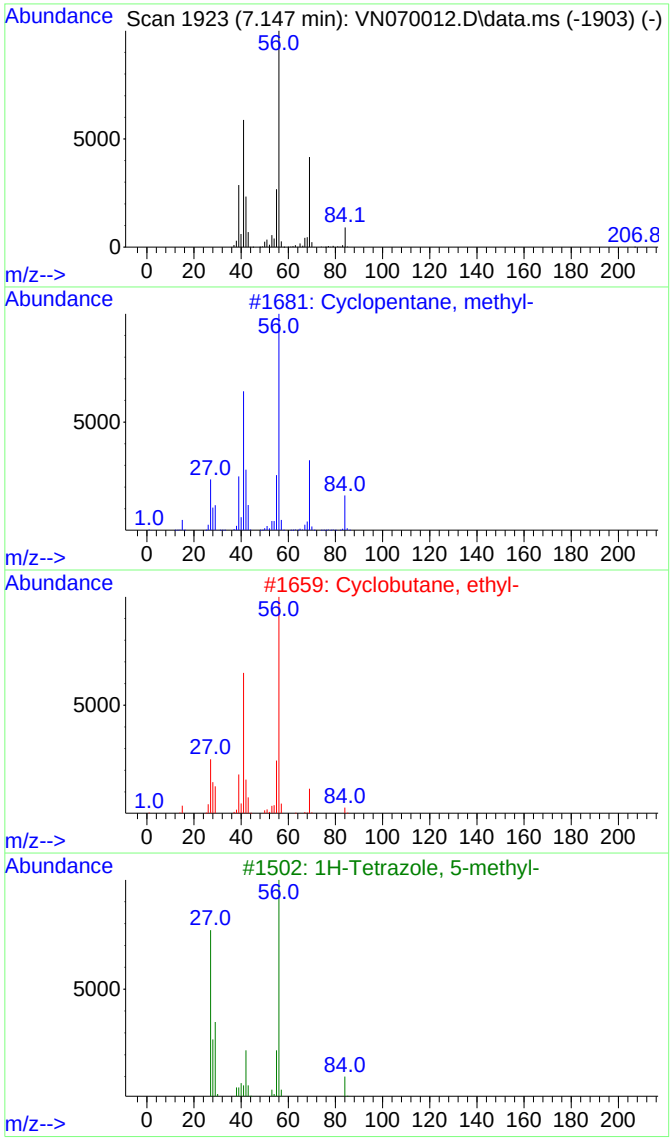
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

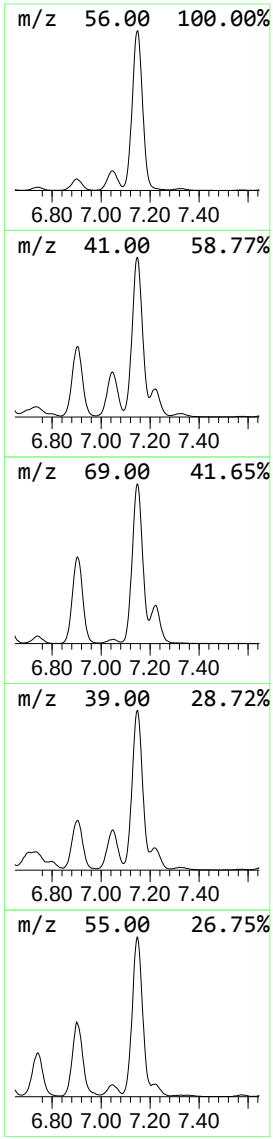
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	33.89 ug/l	9595780	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	39





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

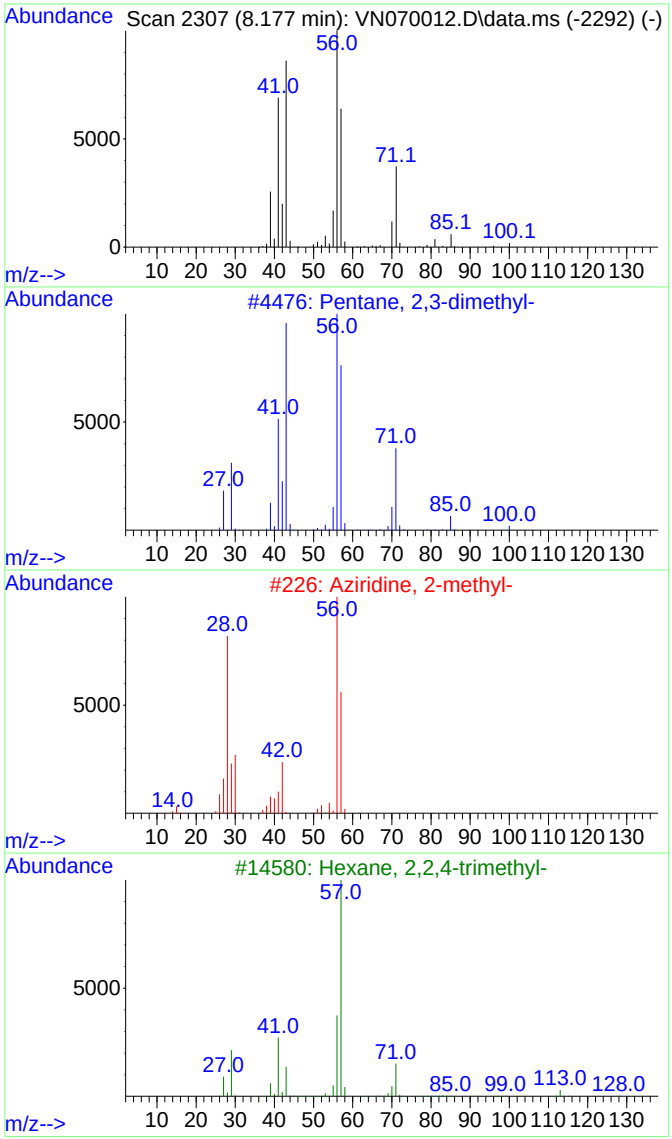
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

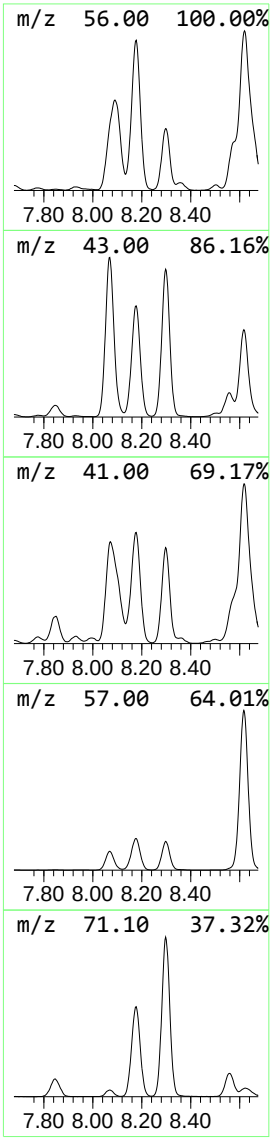
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.177	30.20 ug/l	8551850	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
4	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	37





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Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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

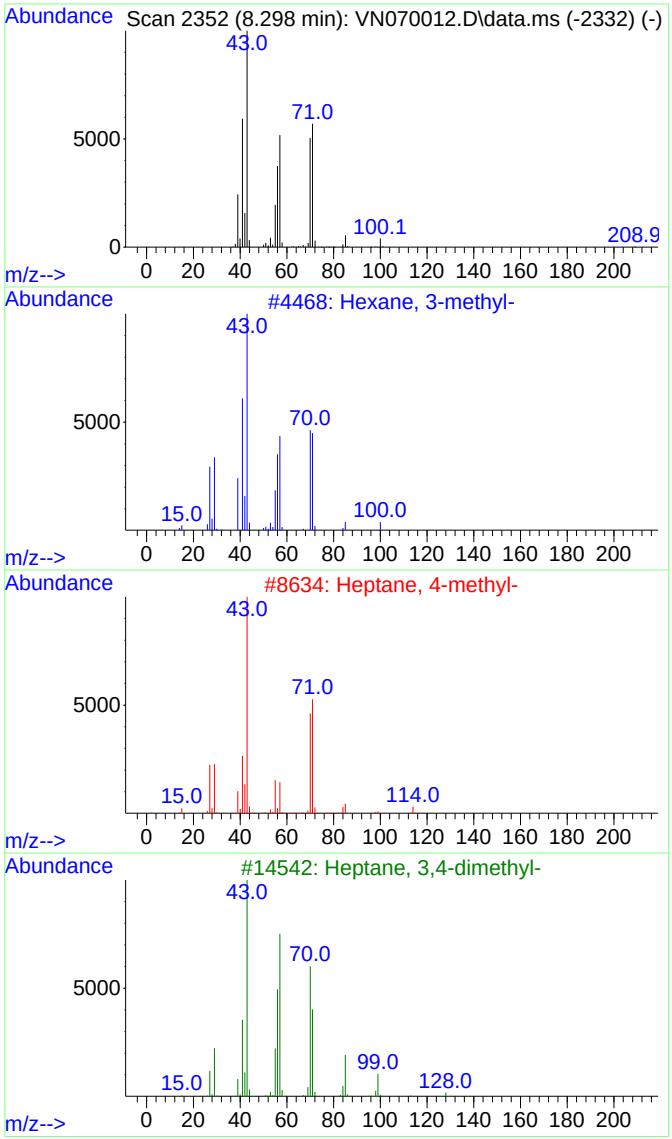
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

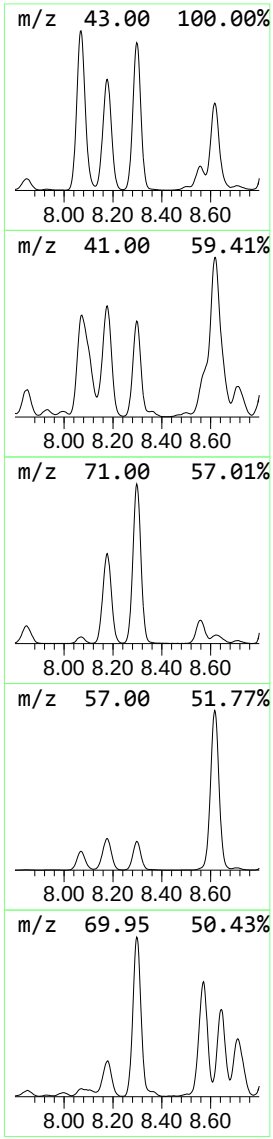
****

Peak Number 5 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	26.67 ug/l	7553300	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	64
4	Heptane	100	C7H16	000142-82-5	64
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	59





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

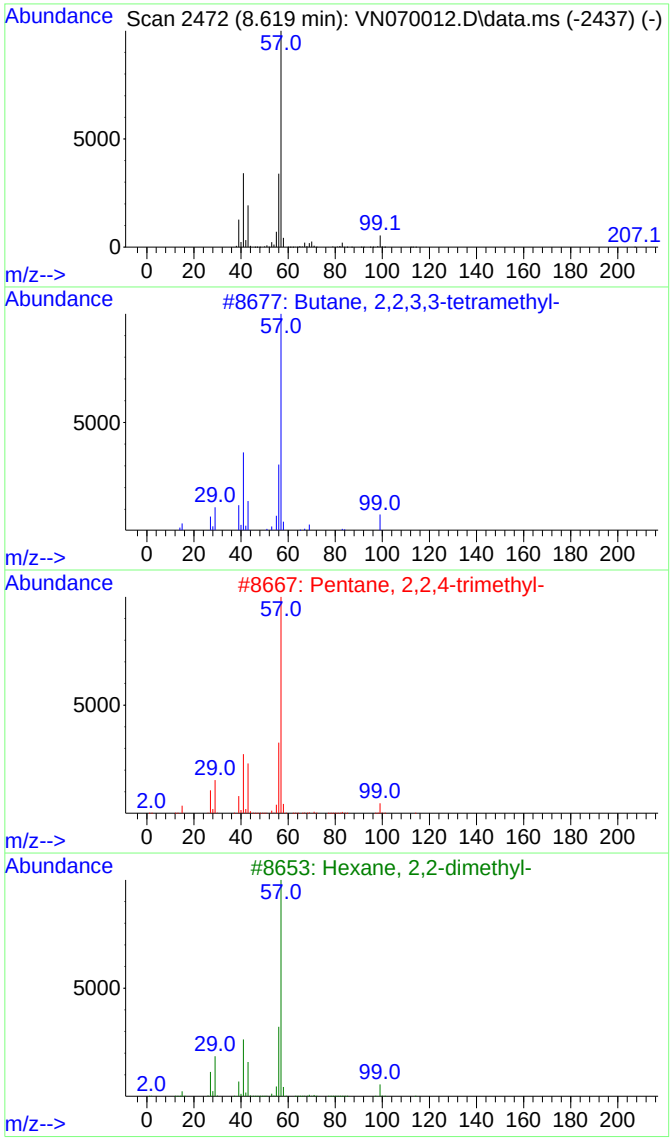
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

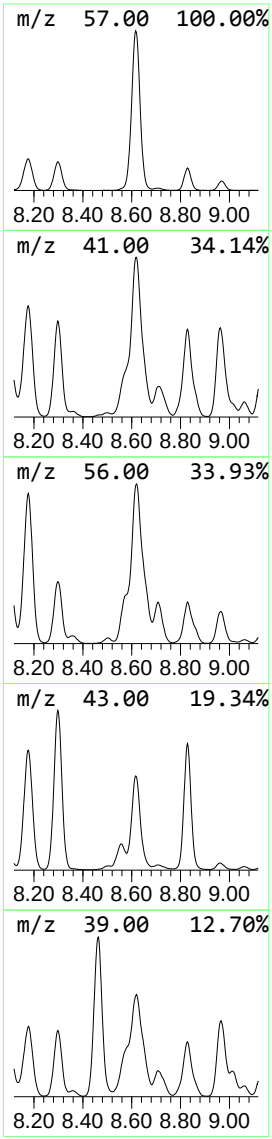
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	71.12 ug/l	17791900	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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

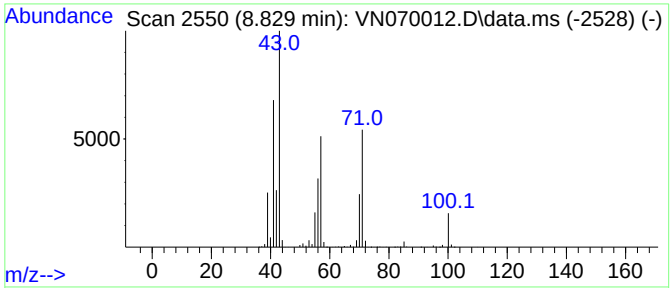
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

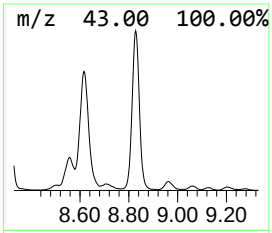
****

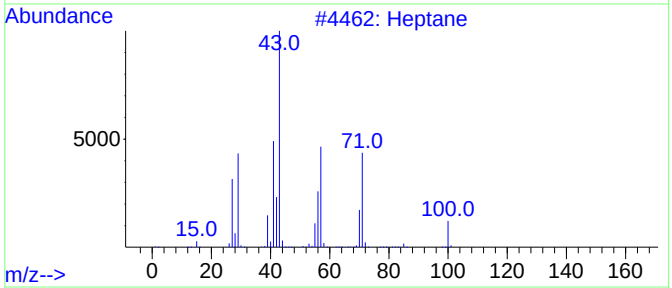
Peak Number 7 Heptane Concentration Rank 9

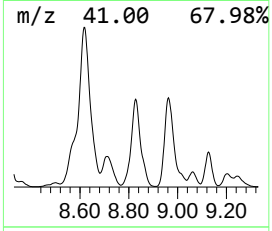
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.829	26.50 ug/l	6628490	1,4-Difluorobenzene	8.971

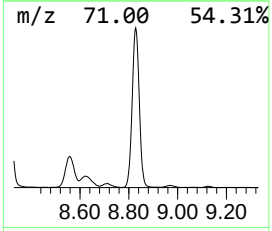
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	94
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	50
3	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	38
5	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38

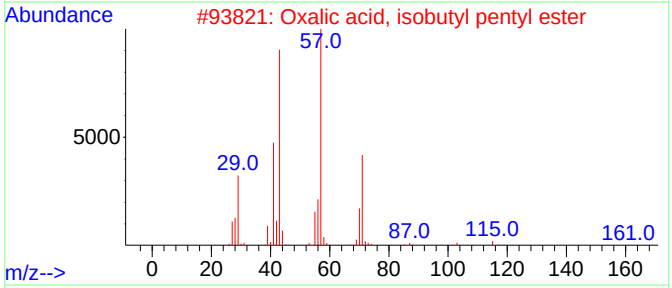


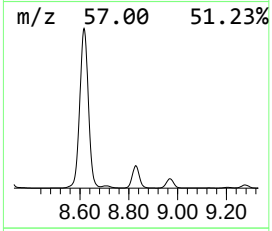


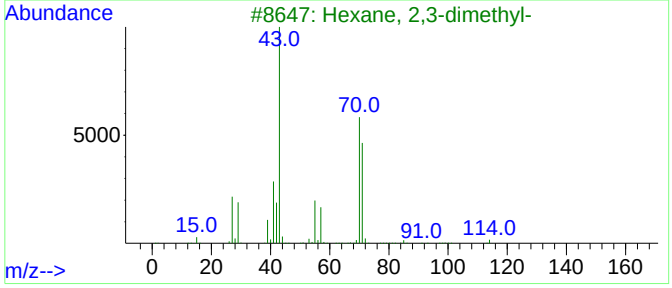


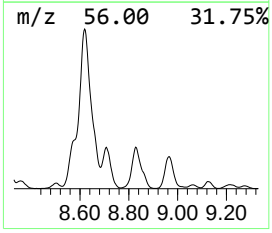












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Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

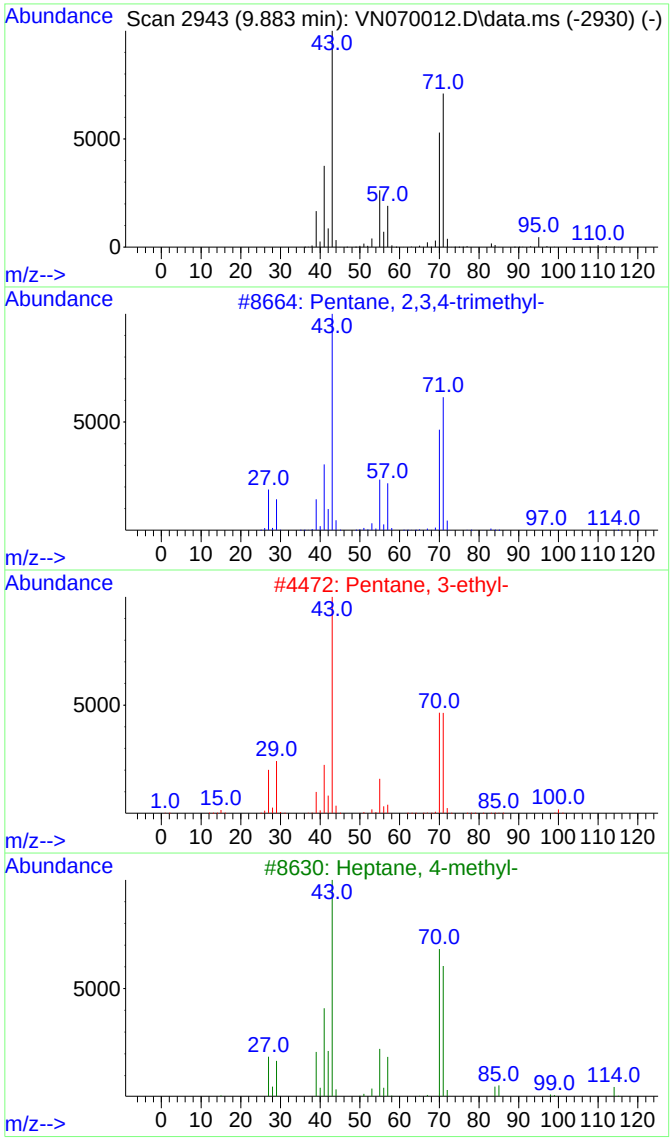
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

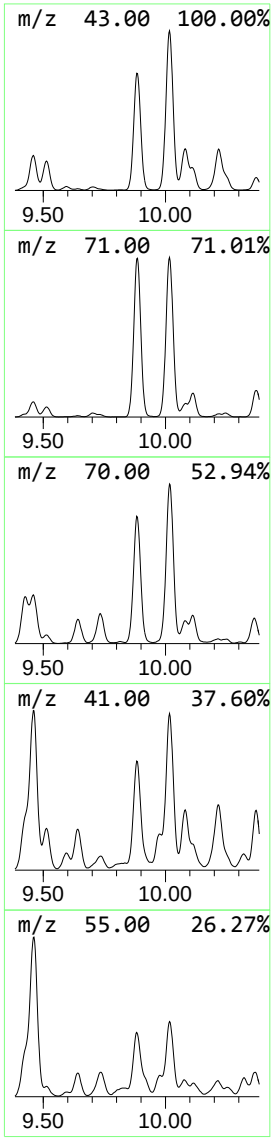
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	27.72 ug/l	6933060	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	87
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64





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Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

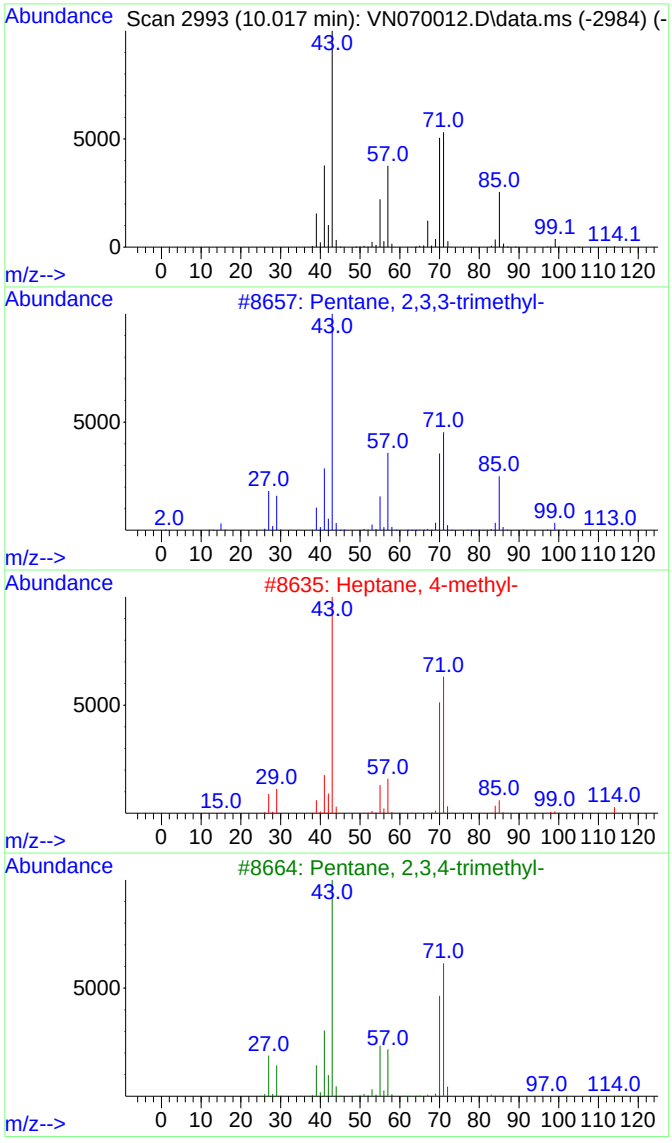
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

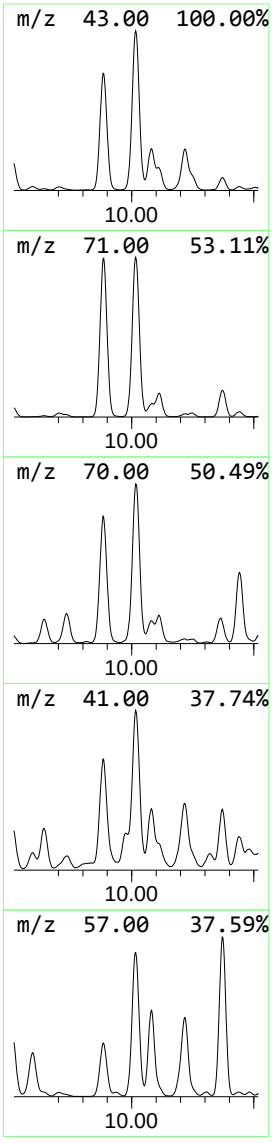
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.017	36.84 ug/l	9214520	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	86
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	58
4	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	53





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Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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

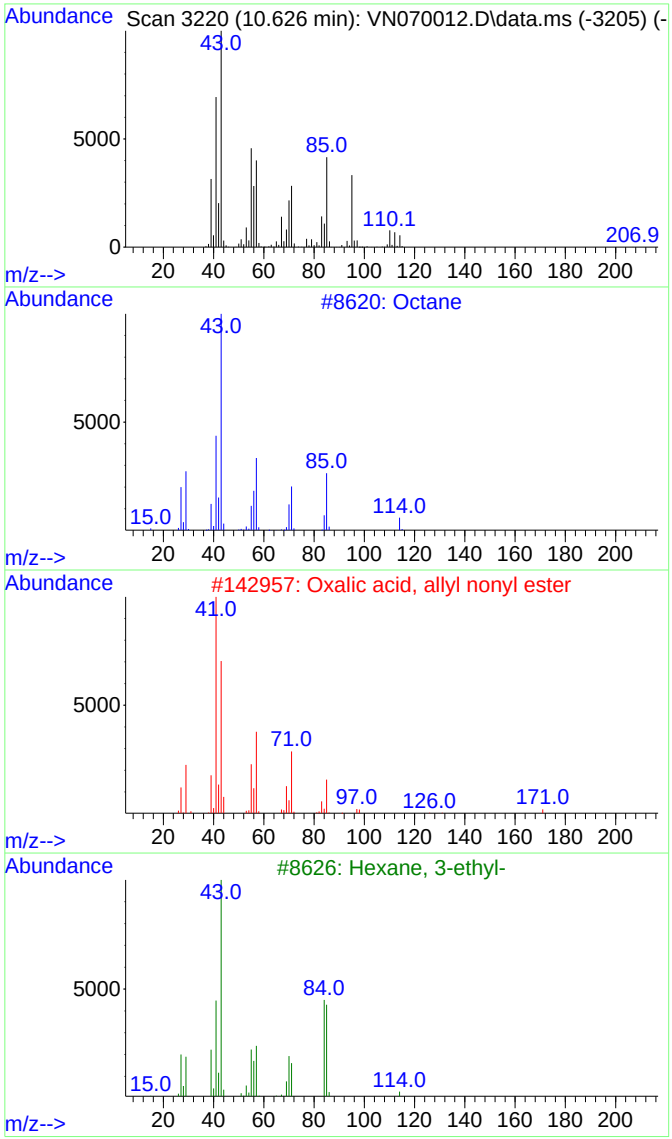
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

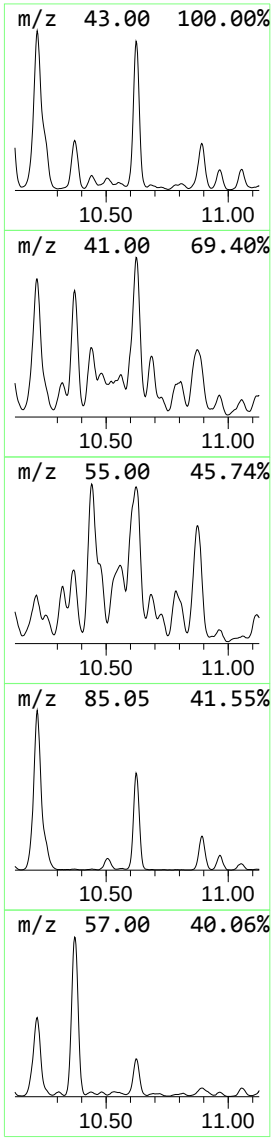
****

Peak Number 10 Octane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.626	22.15 ug/l	4057390	Chlorobenzene-d5	11.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	81
2	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	50
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	46
4	2-Heptenal, (Z)-	112	C7H12O	057266-86-1	42
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38





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Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

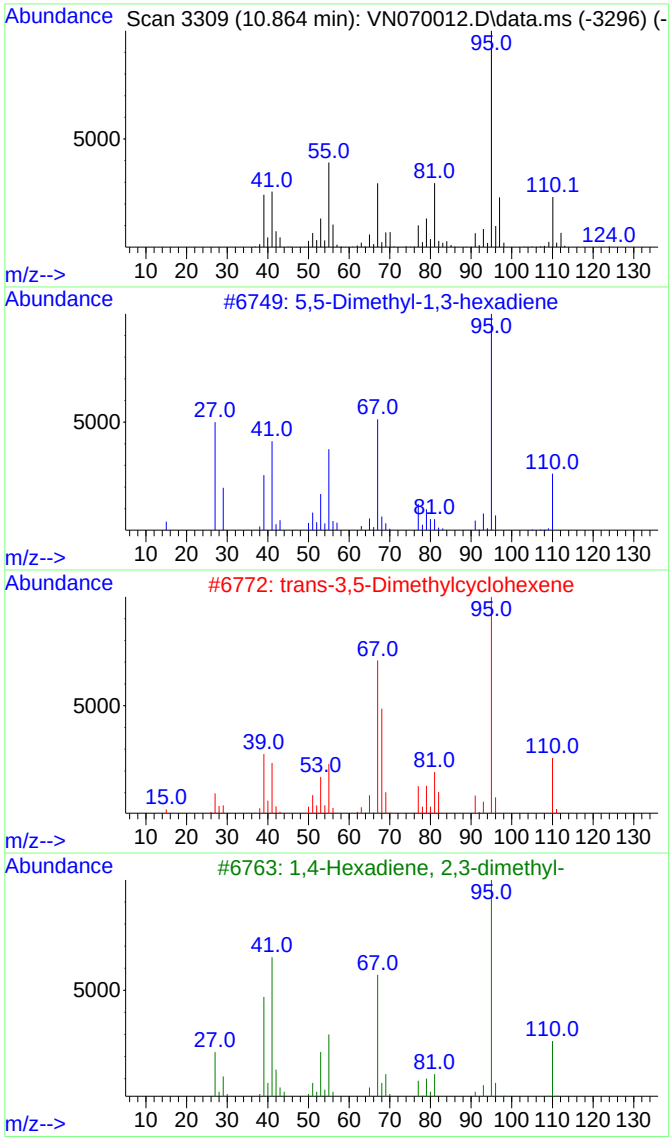
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

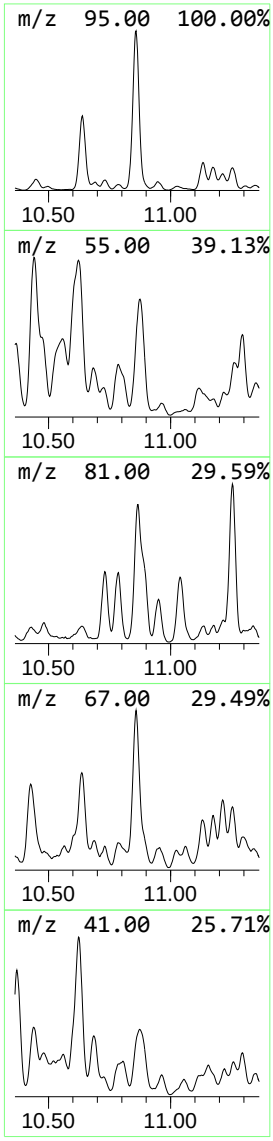
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 5,5-Dimethyl-1,3-hexadiene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.864	22.14 ug/l	4055890	Chlorobenzene-d5	11.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	81
2	trans-3,5-Dimethylcyclohexene	110	C8H14	056021-63-7	70
3	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	70
4	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	70
5	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	70





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Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

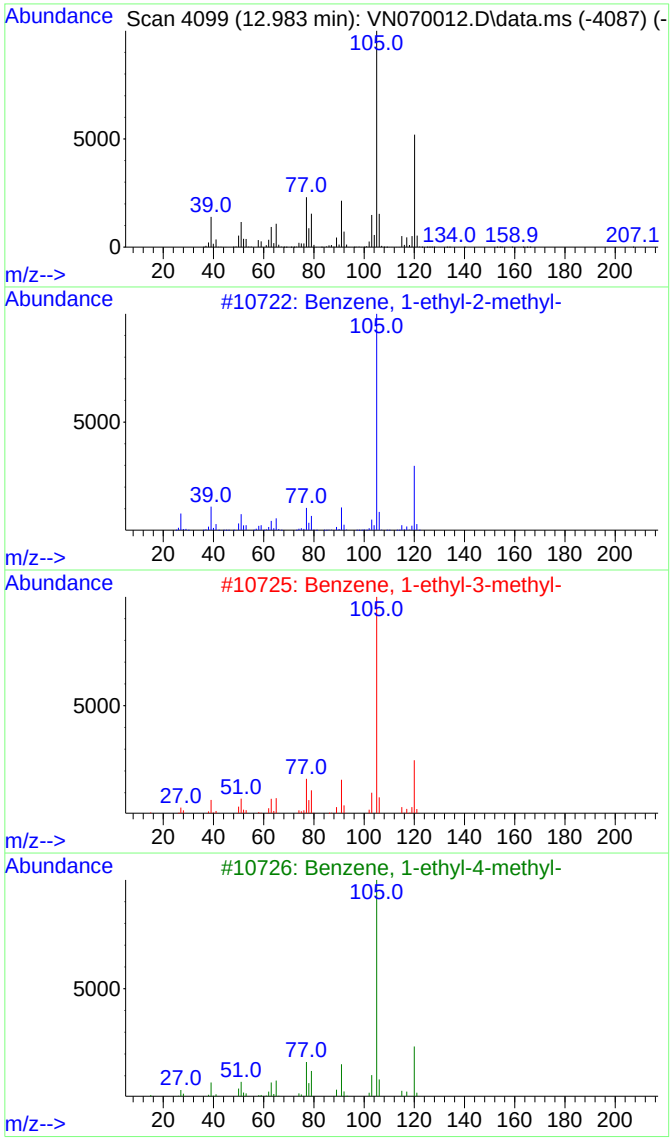
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

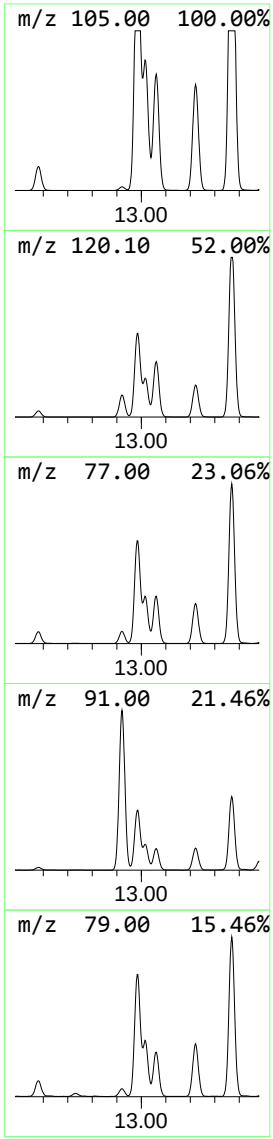
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	89.94 ug/l	64586500	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	90
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	86





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Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

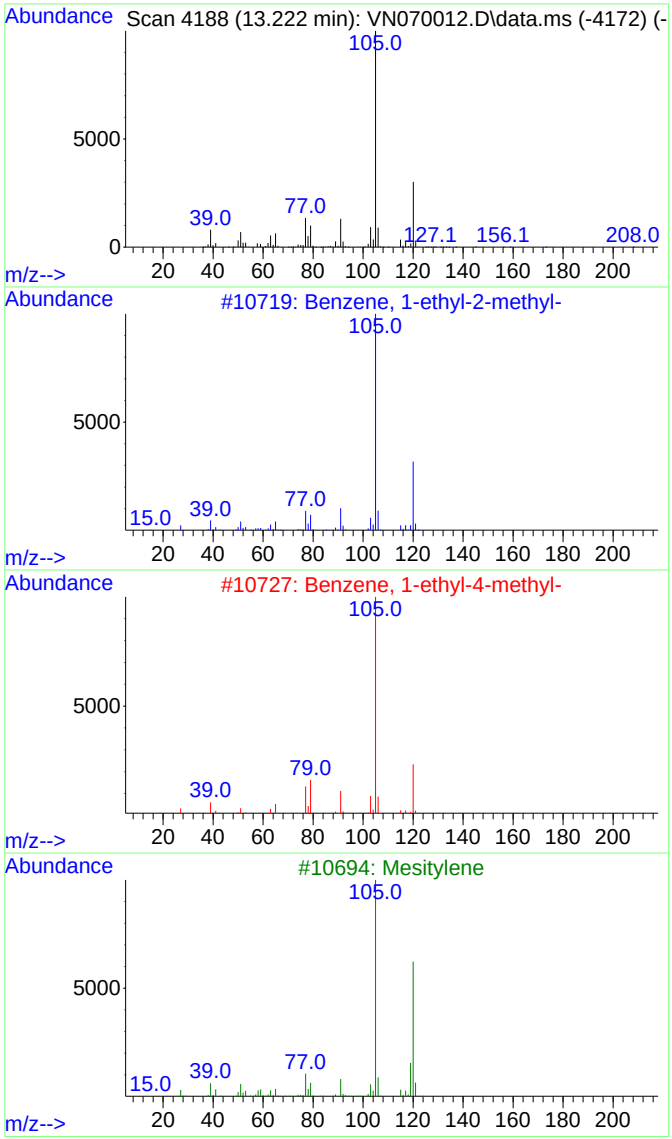
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

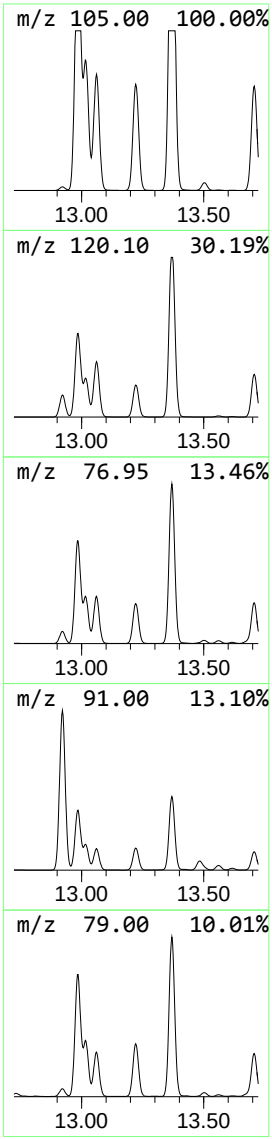
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	34.66 ug/l	24891500	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	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

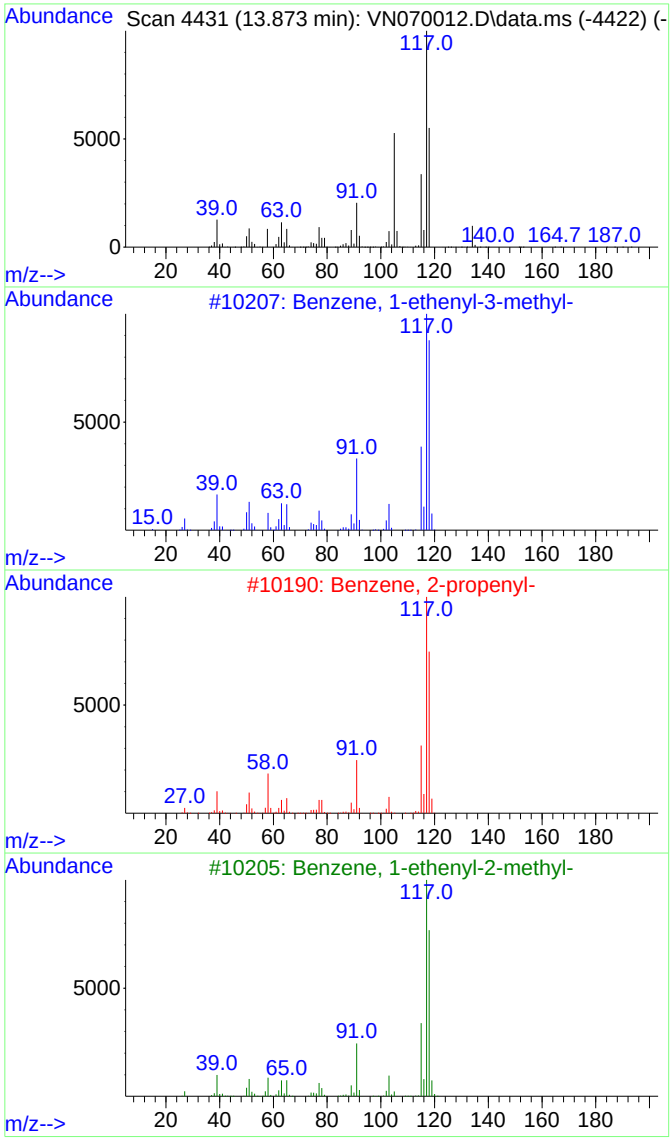
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

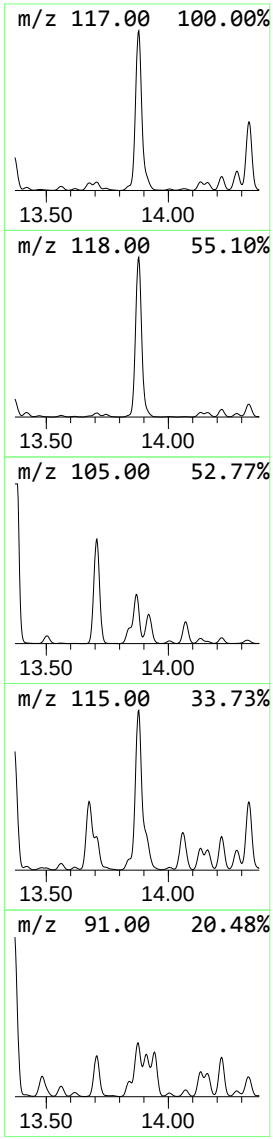
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 1-ethenyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	25.82 ug/l	18541300	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	87
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
4	Indane	118	C9H10	000496-11-7	76
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76





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Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

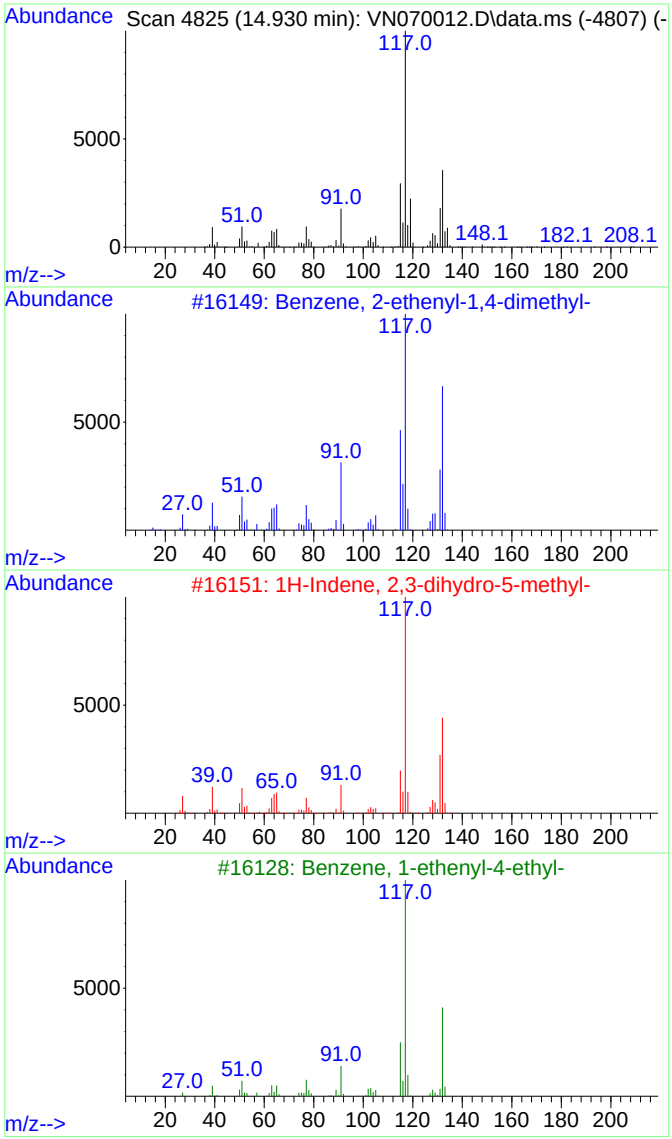
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

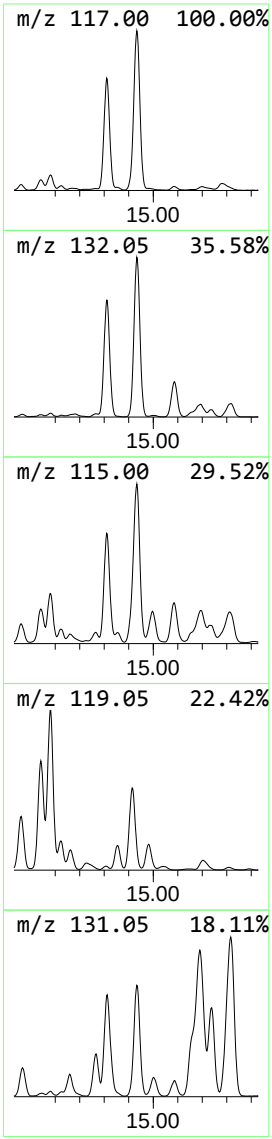
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	23.04 ug/l	16547500	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	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070012.D
Acq On : 11 Dec 2021 16:53
Operator : JC/MD
Sample : M4873-07
Misc : 5.18g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-8-6.5

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
Butane, 2-methyl-	3.137	19.8	ug/l	5593360	1	8.088	14158400	50.0
n-Hexane	6.120	25.1	ug/l	7118770	1	8.088	14158400	50.0
Cyclopentane, m...	7.147	33.9	ug/l	9595780	1	8.088	14158400	50.0
Pentane, 2,3-di...	8.177	30.2	ug/l	8551850	1	8.088	14158400	50.0
Hexane, 3-methyl-	8.298	26.7	ug/l	7553300	1	8.088	14158400	50.0
Butane, 2,2,3,3...	8.619	71.1	ug/l	17791900	2	8.971	12507600	50.0
Heptane	8.829	26.5	ug/l	6628490	2	8.971	12507600	50.0
Pentane, 2,3,4-...	9.883	27.7	ug/l	6933060	2	8.971	12507600	50.0
Pentane, 2,3,3-...	10.017	36.8	ug/l	9214520	2	8.971	12507600	50.0
Octane	10.626	22.1	ug/l	4057390	3	11.747	9158810	50.0
5,5-Dimethyl-1,...	10.864	22.1	ug/l	4055890	3	11.747	9158810	50.0
Benzene, 1-ethy...	12.983	89.9	ug/l	64586500	4	13.675	35906600	50.0
Benzene, 1-ethy...	13.222	34.7	ug/l	24891500	4	13.675	35906600	50.0
Benzene, 1-ethe...	13.873	25.8	ug/l	18541300	4	13.675	35906600	50.0
Benzene, 2-ethe...	14.930	23.0	ug/l	16547500	4	13.675	35906600	50.0