LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

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: VN069925.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.242	85	94	102	rBV3	54043	97712	1.13%	0.120%
2	3.140	421	429	451	rVB3	56080	119666	1.38%	0.147%
3	4.259	816	846	879	rBV3	369792	1348299	15.53%	1.658%
4	5.079	1114	1152	1191	rBV2	1557802	5863506	67.54%	7.209%
5	5.382	1238	1265	1292	rVB4	49459	179202	2.06%	0.220%
6	5.618	1329	1353	1379	rVB4	50287	185706	2.14%	0.228%
7	6.892	1805	1828	1843	rBV3	50532	153684	1.77%	0.189%
8	7.045	1863	1885	1912	rVB	709115	2117969	24.39%	2.604%
9	7.324	1972	1989	2030	rVB4	80680	300856	3.47%	0.370%
10	7.783	2140	2160	2168	rBV6	38355	99136	1.14%	0.122%
11	7.844	2170	2183	2210	rVB2	129304	365726	4.21%	0.450%
12	8.021	2219	2249	2261	rBV2	950931	2360726	27.19%	2.902%
13	8.086	2261	2273	2289	rVV	1674346	3799048	43.76%	4.671%
14	8.174	2289	2306	2333	rVB2	2013958	5022142	57.85%	6.174%
15	8.357	2359	2374	2386	rBV4	100308	231334	2.66%	0.284%
16	8.437	2387	2404	2429	rVV	1099693	2593909	29.88%	3.189%
17	8.555	2430	2448	2454	rVV6	143824	346668	3.99%	0.426%
18	8.617	2455	2471	2493	rVV	1802264	4454752	51.31%	5.477%
19	8.705	2494	2504	2525	rVB3	146423	344804	3.97%	0.424%
20	8.968	2581	2602	2627	rBV	2742690	5803849	66.85%	7.135%
21	9.199	2672	2688	2704	rBV2	193950	406758	4.69%	0.500%
22	9.427	2753	2773	2779	rBV3	258846	560507	6.46%	0.689%
23	9.512	2797	2805	2821	rVB5	135333	274659	3.16%	0.338%
24	9.593	2822	2835	2848	rBV2	154943	318743	3.67%	0.392%
25	9.732	2866	2887	2904	rVB5	182930	453773	5.23%	0.558%
26	9.883	2925	2943	2964	rVB	1218065	2530559	29.15%	3.111%
27	10.014	2969	2992	3020	rBV	1910938	4171127	48.04%	5.128%
28	10.119	3021	3031	3045	rVB8	60791	137214	1.58%	0.169%
29	10.199	3047	3061	3076	rBV4	218729	460204	5.30%	0.566%
30	10.368	3112	3124	3135	rVB4	253013	458864	5.29%	0.564%
31	10.440	3135	3151	3182	rBV	4496445	8470986	97.57%	10.414%
32	10.631	3201	3222	3238	rVB	109965	410452	4.73%	0.505%
33	10.722	3243	3256	3267	rVV3	70288	141392	1.63%	0.174%
34	10.781	3267	3278	3291	rVV3	132136	244483	2.82%	0.301%
35	10.859	3292	3307	3328	rVV5	514459	1208209	13.92%	1.485%
36	10.947	3330	3340	3358	rVB5	64246	153690	1.77%	0.189%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

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	11.130	3401	3408	3420	rVB4	110585	178289	2.05%	0.219%
38	11.258	3447	3456	3467	rVB5	84913	138140	1.59%	0.170%
39	11.315	3468	3477	3493	rVB5	49759	95611	1.10%	0.118%
40	11.401	3498	3509	3518	rBV7	57271	107126	1.23%	0.132%
41	11.452	3520	3528	3540	rVB6	82173	137509	1.58%	0.169%
42	11.744	3621	3637	3667	rBV	4660021	8681991	100.00%	10.674%
43	12.449	3892	3900	3919	rVB8	45203	89979	1.04%	0.111%
44	12.731	3988	4005	4027	rBV	3690750	6576077	75.74%	8.085%
45	13.498	4277	4291	4305	rVB4	72633	173707	2.00%	0.214%
46	13.675	4340	4357	4384	rBV	4012331	7058206	81.30%	8.677%
47	13.839	4405	4418	4432	rBV	743425	1210112	13.94%	1.488%
48	14.394	4615	4625	4639	rVB8	44611	95450	1.10%	0.117%
49	14.463	4642	4651	4662	rBV3	73010	118226	1.36%	0.145%
50	14.619	4699	4709	4716	rBV2	61942	93408	1.08%	0.115%
51	14.657	4717	4723	4737	rVB4	57050	88907	1.02%	0.109%
52	14.823	4770	4785	4797	rBV4	97925	182924	2.11%	0.225%
53	15.507	5032	5040	5054	rVB	69649	123822	1.43%	0.152%

Sum of corrected areas: 81339798

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Data File : VN069925.D
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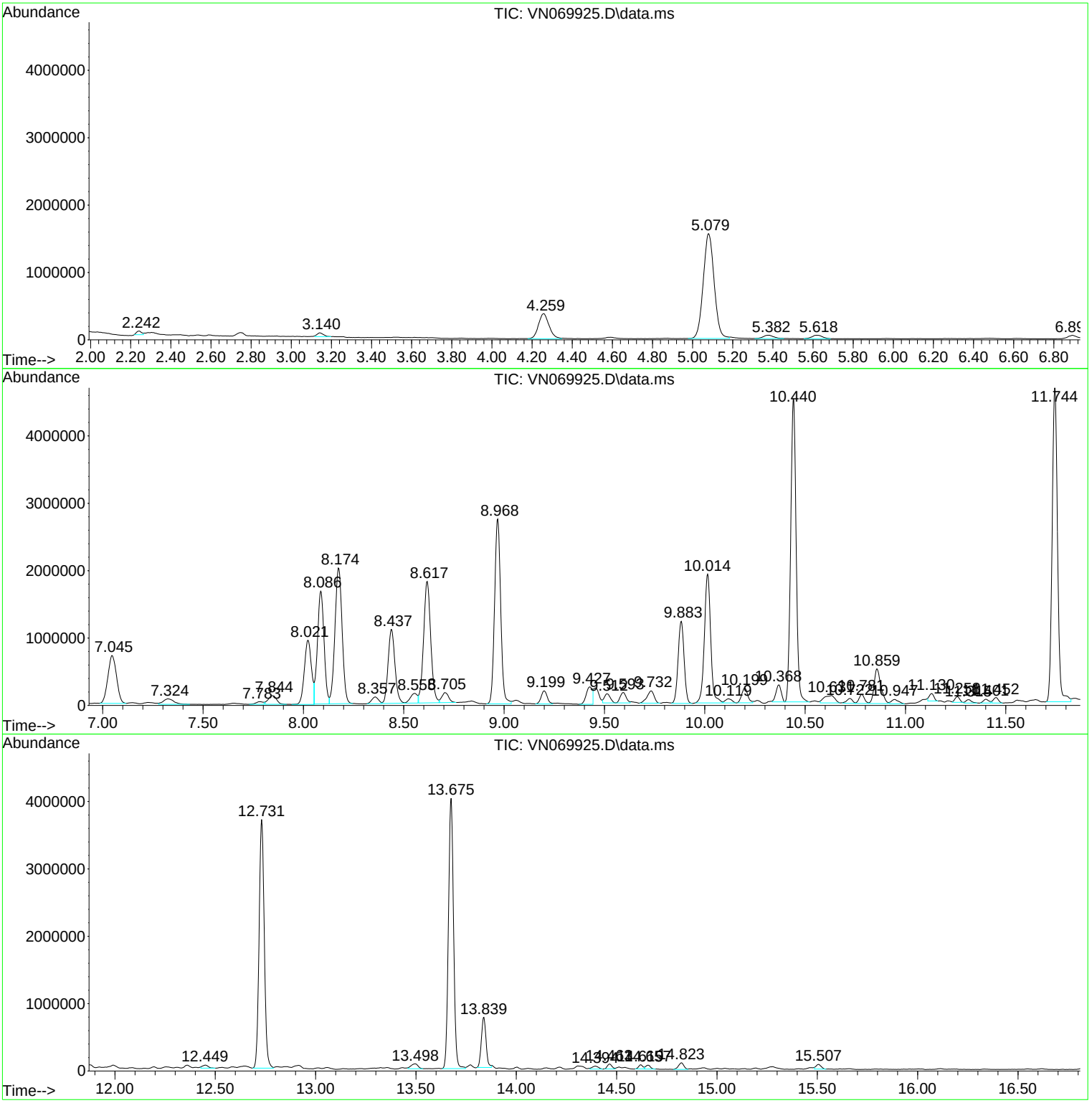
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

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 : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

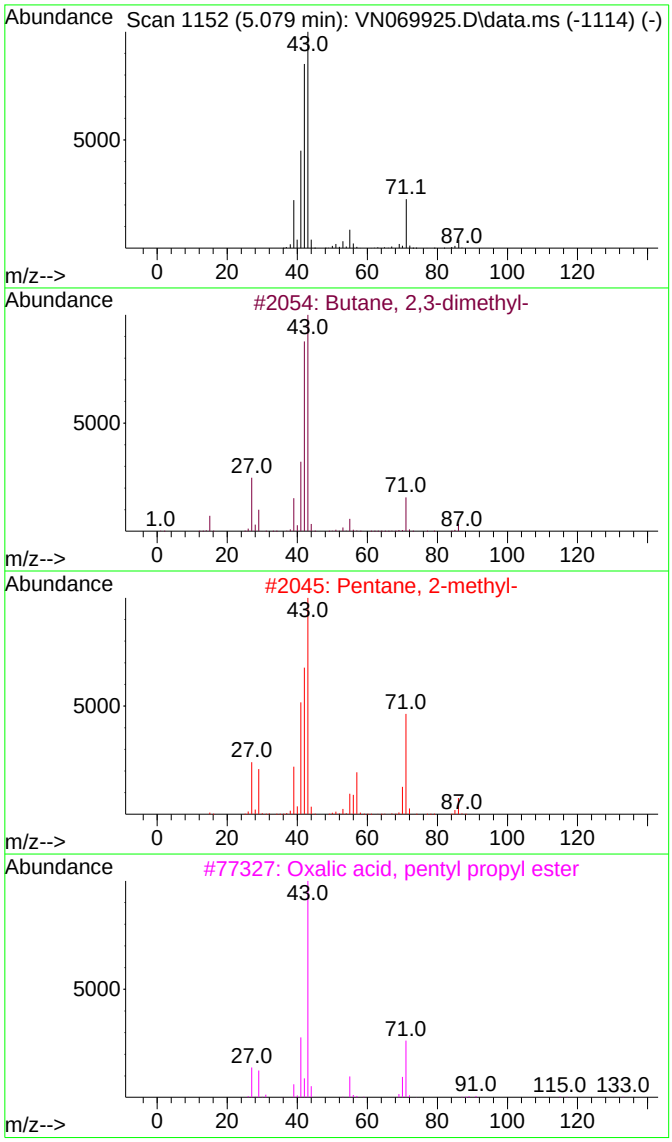
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

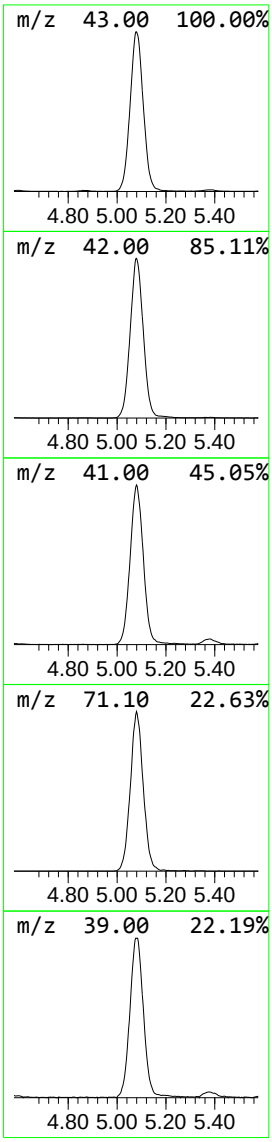
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.079	77.17 ug/l	5863510	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	12
4	Pyrrolidine	71	C4H9N	000123-75-1	9
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

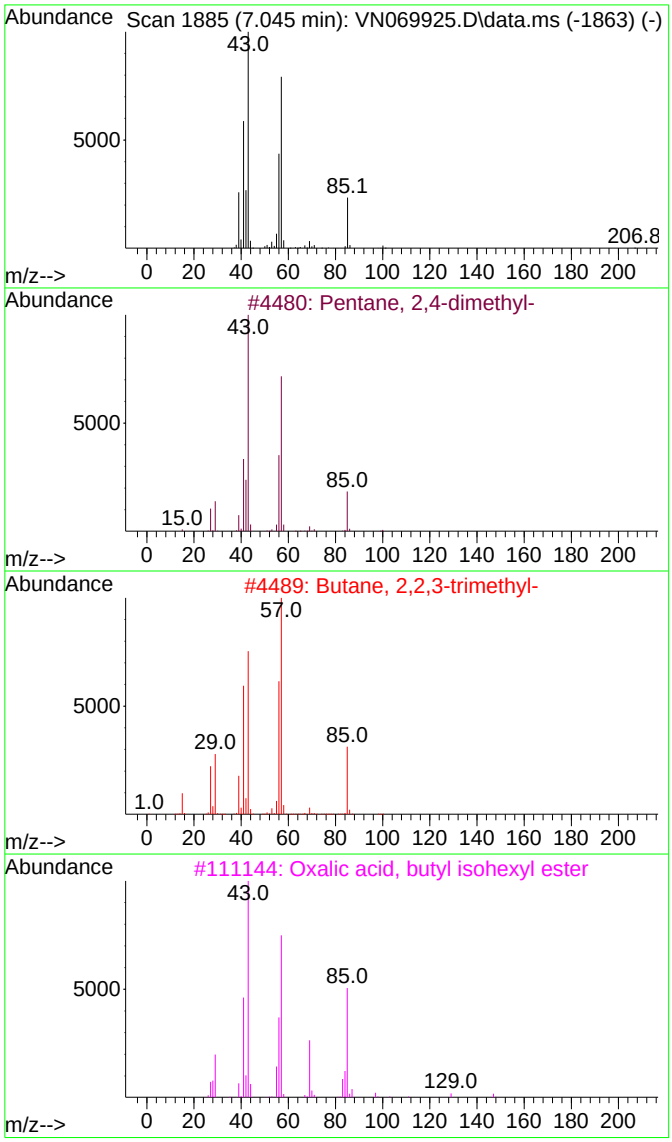
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

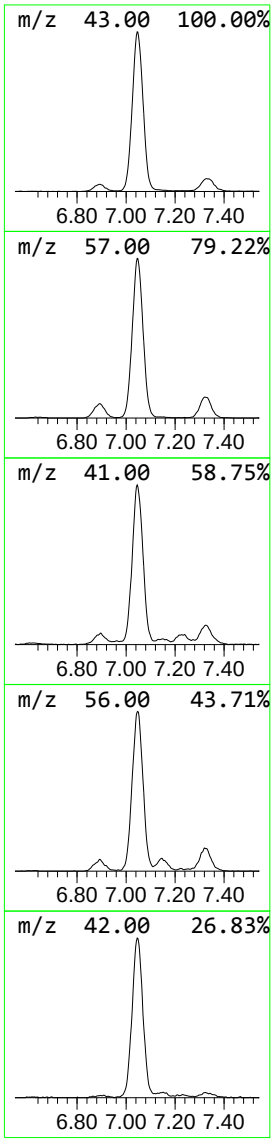
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	27.88 ug/l	2117970	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	56
5	n-Hexane	86	C6H14	000110-54-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

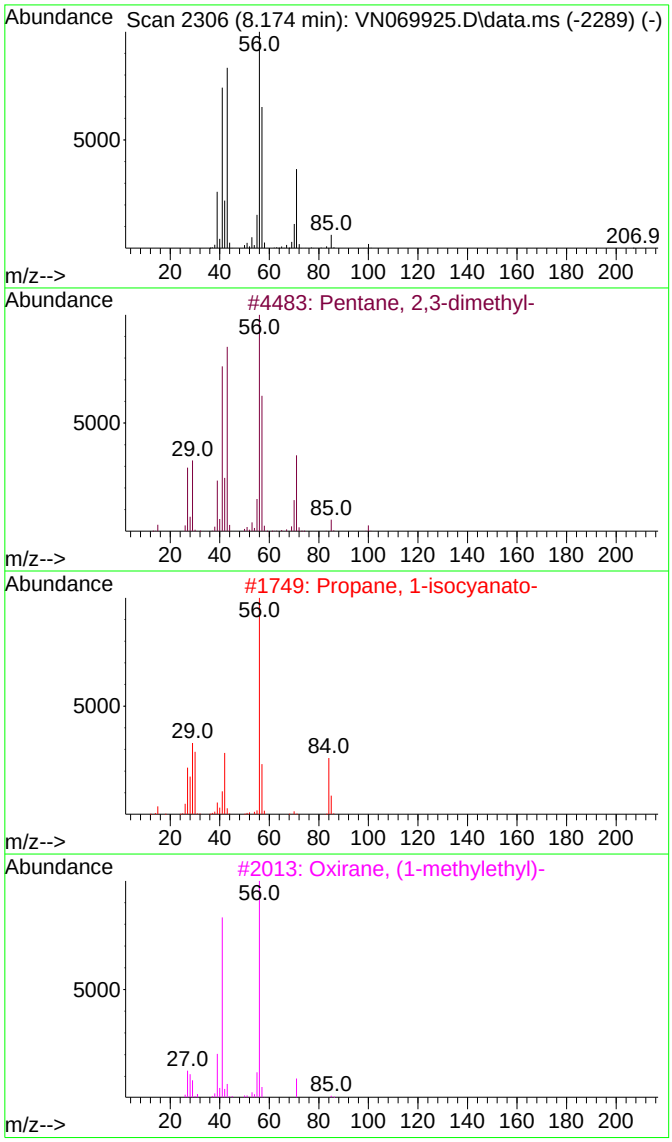
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

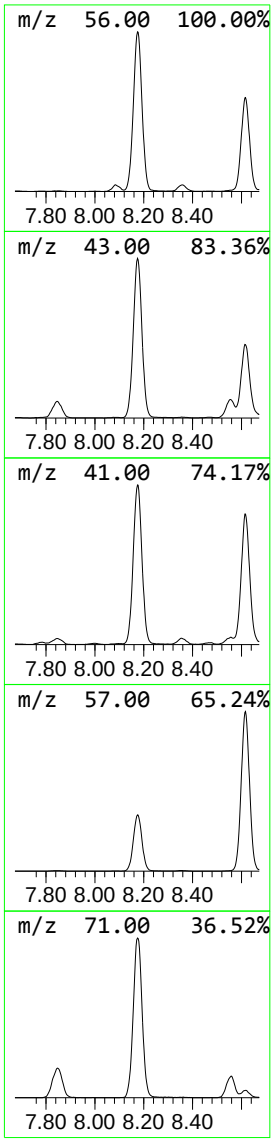
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	66.10 ug/l	5022140	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	47
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
4	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

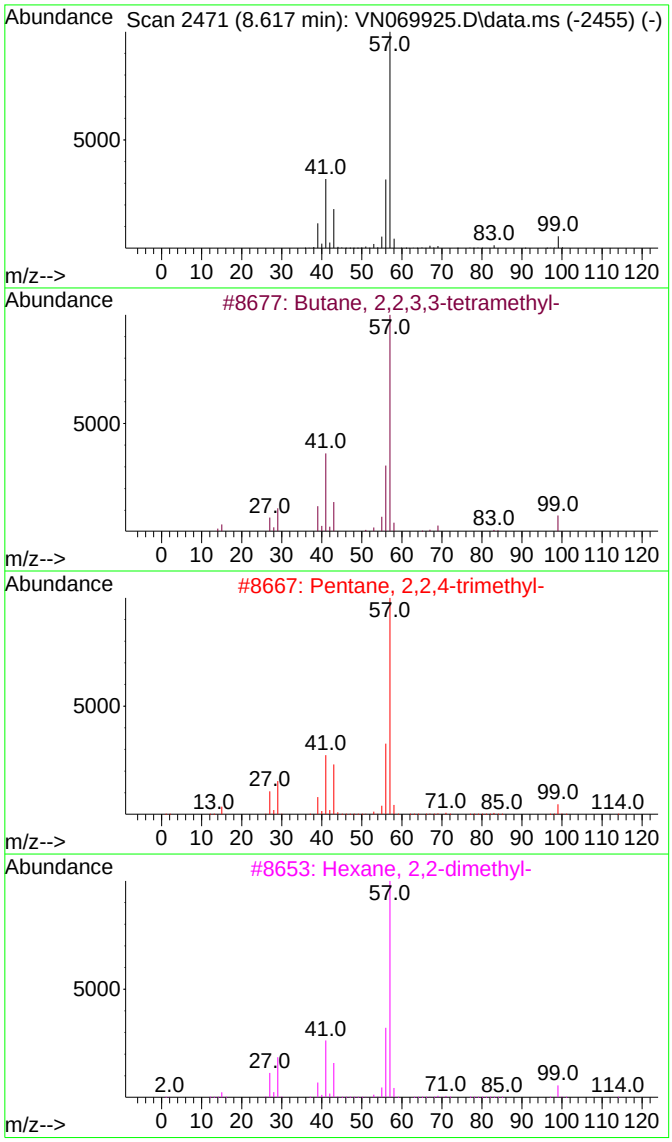
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

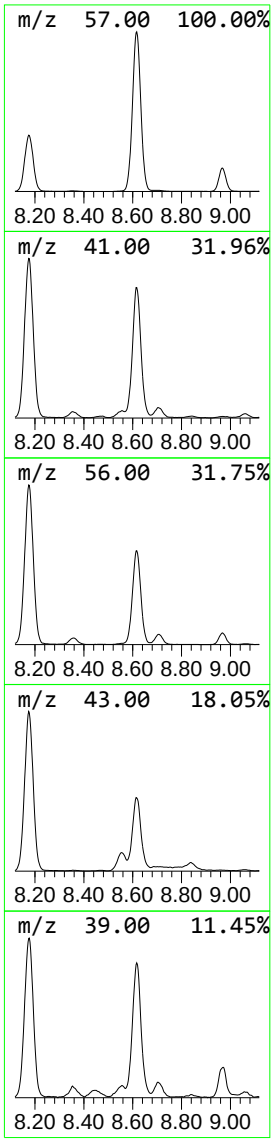
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	38.38 ug/l	4454750	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

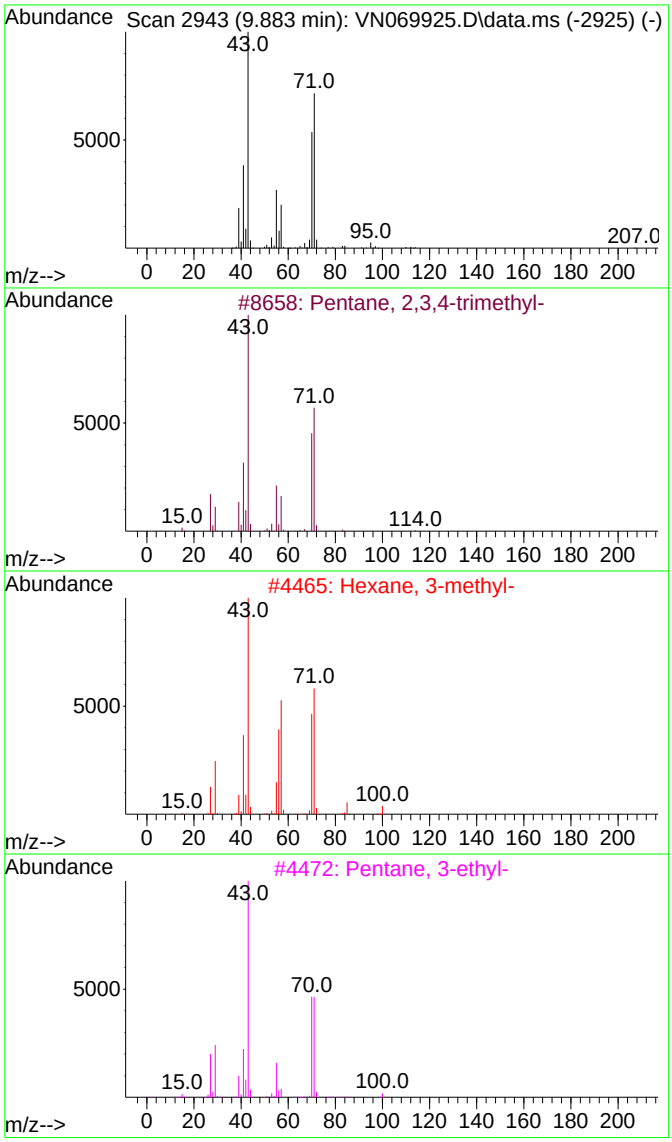
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

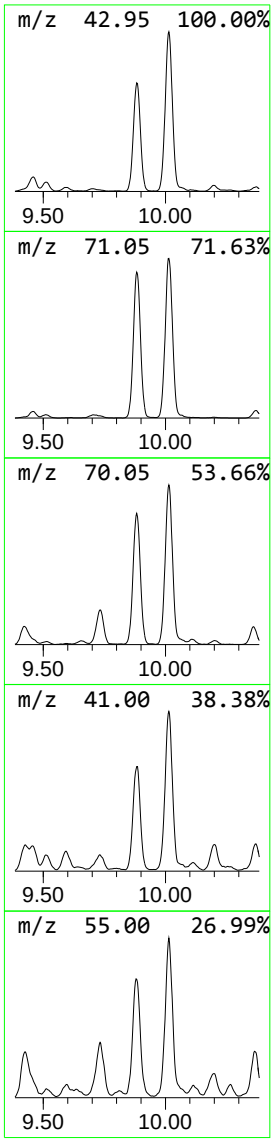
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	21.80 ug/l	2530560	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	78
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5	Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	64





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Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

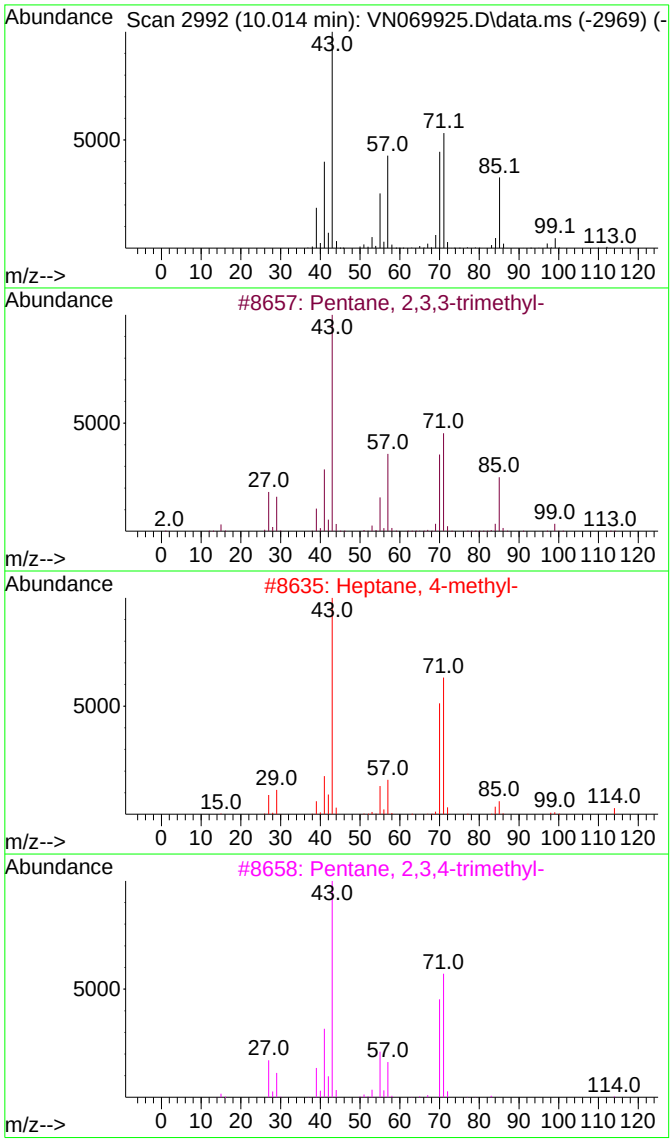
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

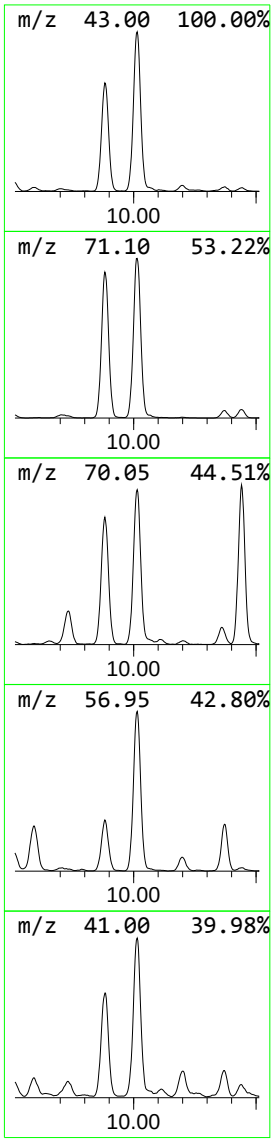
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	35.93 ug/l	4171130	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59





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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

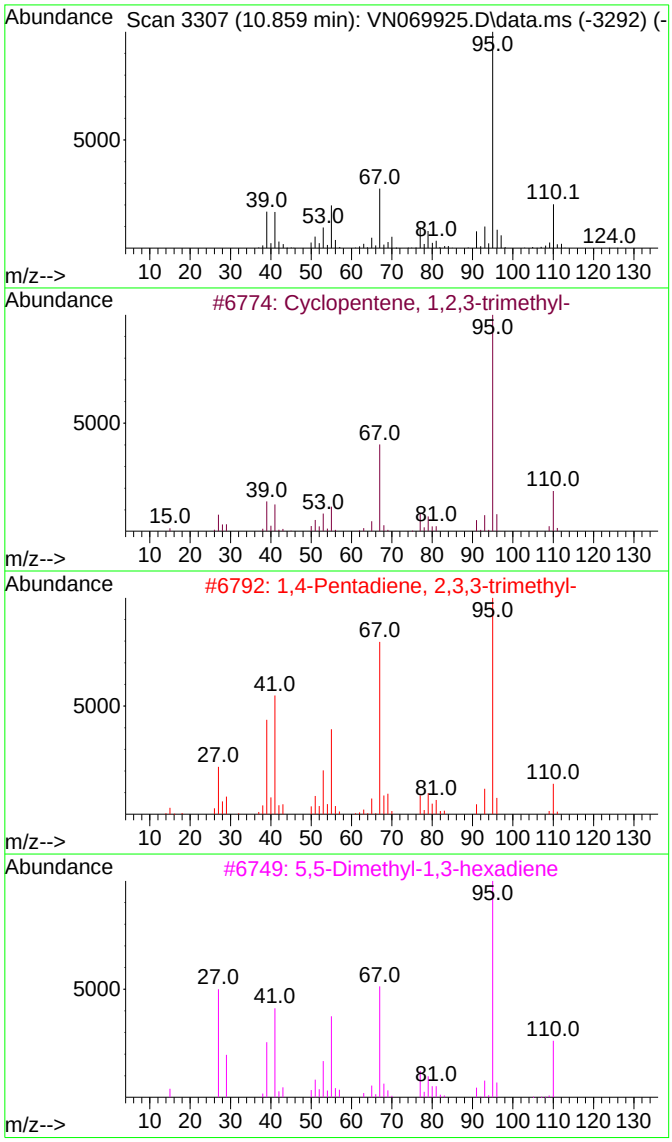
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

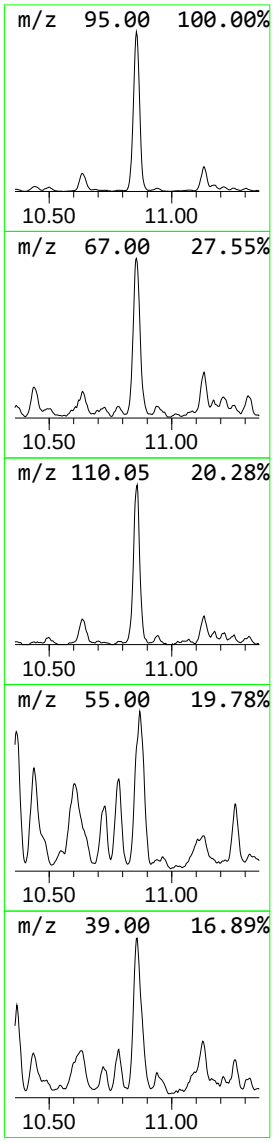
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.859	6.96 ug/l	1208210	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	81
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	80
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	78
4	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	72
5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

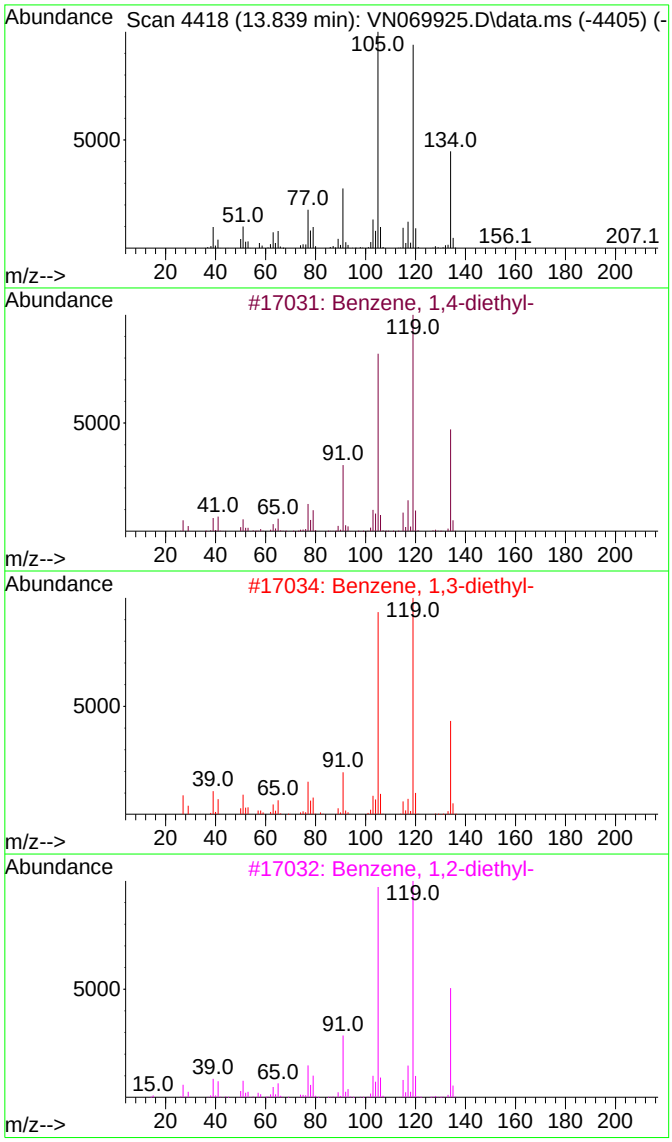
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

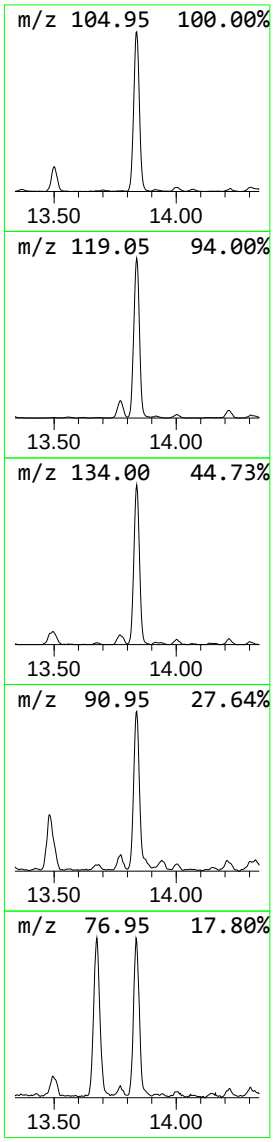
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,4-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	8.57 ug/l	1210110	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069925.D
Acq On : 9 Dec 2021 21:01
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

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, 2,3-dim...	5.079	77.2	ug/l	5863510	1	8.088	3799050	50.0
Pentane, 2,4-di...	7.045	27.9	ug/l	2117970	1	8.088	3799050	50.0
Pentane, 2,3-di...	8.174	66.1	ug/l	5022140	1	8.088	3799050	50.0
Butane, 2,2,3,3...	8.617	38.4	ug/l	4454750	2	8.968	5803850	50.0
Pentane, 2,3,4-...	9.883	21.8	ug/l	2530560	2	8.968	5803850	50.0
Pentane, 2,3,3-...	10.014	35.9	ug/l	4171130	2	8.968	5803850	50.0
Cyclopentene, 1...	10.859	7.0	ug/l	1208210	3	11.744	8681990	50.0
Benzene, 1,4-di...	13.839	8.6	ug/l	1210110	4	13.675	7058210	50.0