LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 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: VN069971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.253	817	844	883	rBV2	365163	1315080	16.76%	1.716%
2	4.591	950	970	992	rBV	27802	85717	1.09%	0.112%
3	5.076	1116	1151	1190	rBV2	1556408	5839097	74.40%	7.617%
4	5.377	1240	1263	1292	rVB3	52744	187557	2.39%	0.245%
5	5.616	1327	1352	1380	rBV4	47728	169177	2.16%	0.221%
6	6.892	1807	1828	1846	rBV4	44199	149061	1.90%	0.194%
7	7.048	1862	1886	1912	rBV	724124	2152900	27.43%	2.808%
8	7.324	1973	1989	2021	rVB5	82499	285845	3.64%	0.373%
9	7.785	2141	2161	2167	rBV5	36783	87795	1.12%	0.115%
10	7.847	2169	2184	2205	rVB4	128004	355957	4.54%	0.464%
11	8.024	2226	2250	2261	rBV2	870047	2121043	27.03%	2.767%
12	8.086	2261	2273	2289	rVV	1465167	3341568	42.58%	4.359%
13	8.174	2289	2306	2333	rVB	2027839	5045543	64.29%	6.582%
14	8.357	2357	2374	2388	rBV4	99450	240228	3.06%	0.313%
15	8.440	2388	2405	2430	rVV	981426	2319190	29.55%	3.025%
16	8.552	2430	2447	2454	rVV5	149129	344682	4.39%	0.450%
17	8.617	2455	2471	2493	rVV	1786760	4439575	56.57%	5.791%
18	8.708	2495	2505	2522	rVB4	143707	325403	4.15%	0.424%
19	8.968	2583	2602	2628	rBV	2468257	5198081	66.24%	6.781%
20	9.199	2673	2688	2707	rBV2	183100	377924	4.82%	0.493%
21	9.427	2751	2773	2779	rBV3	254695	539303	6.87%	0.704%
22	9.515	2796	2806	2822	rVB6	138296	292297	3.72%	0.381%
23	9.593	2823	2835	2848	rBV2	155899	308377	3.93%	0.402%
24	9.732	2867	2887	2902	rVB3	188694	462138	5.89%	0.603%
25	9.883	2927	2943	2967	rVB2	1222754	2491539	31.75%	3.250%
26	10.014	2968	2992	3020	rBV	1881753	4090948	52.13%	5.337%
27	10.119	3021	3031	3045	rVB10	60131	140311	1.79%	0.183%
28	10.202	3046	3062	3075	rBV4	219678	473389	6.03%	0.618%
29	10.371	3099	3125	3136	rBV5	268367	565274	7.20%	0.737%
30	10.443	3136	3152	3183	rVB	4073118	7659053	97.59%	9.991%
31	10.609	3202	3214	3215	rBV4	67340	93168	1.19%	0.122%
32	10.725	3244	3257	3267	rVB4	63521	119386	1.52%	0.156%
33	10.781	3268	3278	3292	rVV3	121337	223636	2.85%	0.292%
34	10.859	3292	3307	3329	rVV4	497079	1164768	14.84%	1.519%
35	10.945	3331	3339	3359	rVB7	63757	149716	1.91%	0.195%
36	11.132	3402	3409	3420	rVB4	98206	165118	2.10%	0.215%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 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	11.258	3447	3456	3467	rVB5	87917	150273	1.91%	0.196%
38	11.317	3467	3478	3496	rVB4	46910	89504	1.14%	0.117%
39	11.403	3499	3510	3519	rBV6	55924	100848	1.29%	0.132%
40	11.452	3520	3528	3544	rVB6	76069	131368	1.67%	0.171%
41	11.744	3621	3637	3655	rBV	4280886	7847868	100.00%	10.238%
42	12.734	3989	4006	4027	rBV	3463291	6183248	78.79%	8.066%
43	13.495	4278	4290	4304	rVB5	72526	175545	2.24%	0.229%
44	13.675	4340	4357	4384	rBV	3897422	6792997	86.56%	8.862%
45	13.838	4406	4418	4431	rBV	742581	1175455	14.98%	1.533%
46	14.311	4584	4594	4611	rVB6	43229	101081	1.29%	0.132%
47	14.396	4612	4626	4640	rVB6	48712	108551	1.38%	0.142%
48	14.466	4640	4652	4662	rBV3	75024	130128	1.66%	0.170%
49	14.622	4700	4710	4717	rBV	58637	93246	1.19%	0.122%
50	14.659	4717	4724	4736	rVB3	57473	87510	1.12%	0.114%
51	14.823	4771	4785	4800	rBV4	87933	169732	2.16%	0.221%

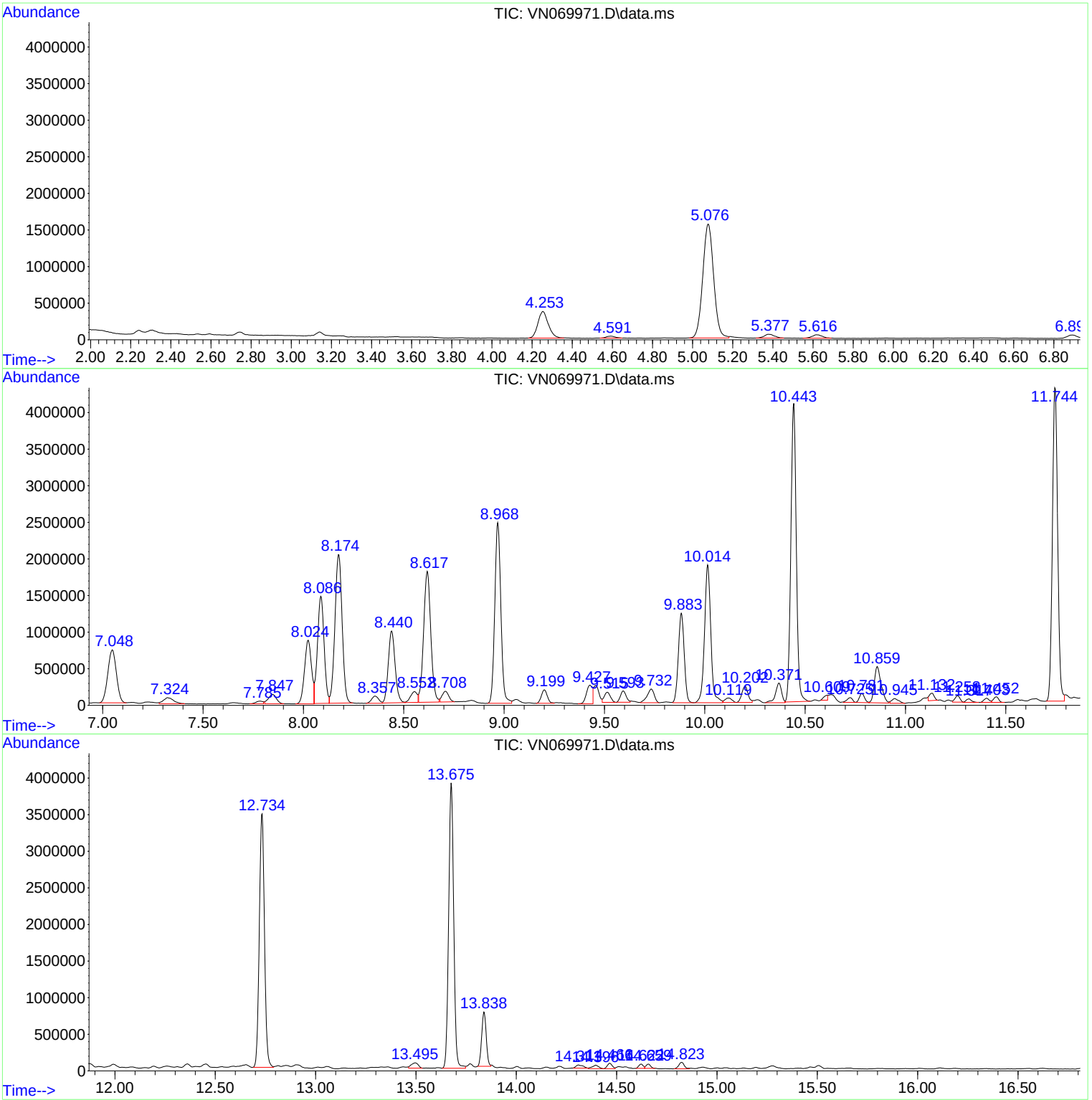
Sum of corrected areas: 76657198

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 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\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

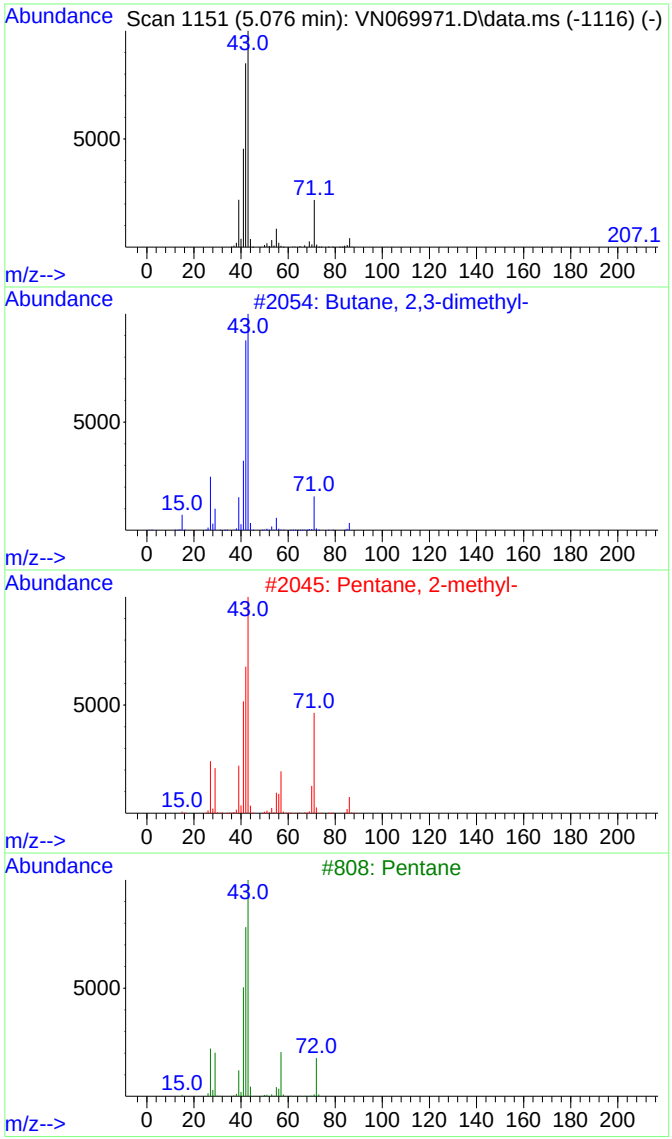
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

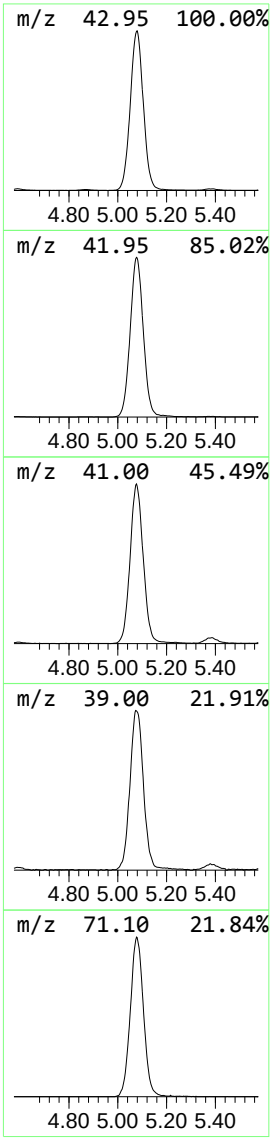
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.076	87.37 ug/l	5839100	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	Pentane	72	C5H12	000109-66-0	38
4	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	16
5	Pyrrolidine	71	C4H9N	000123-75-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

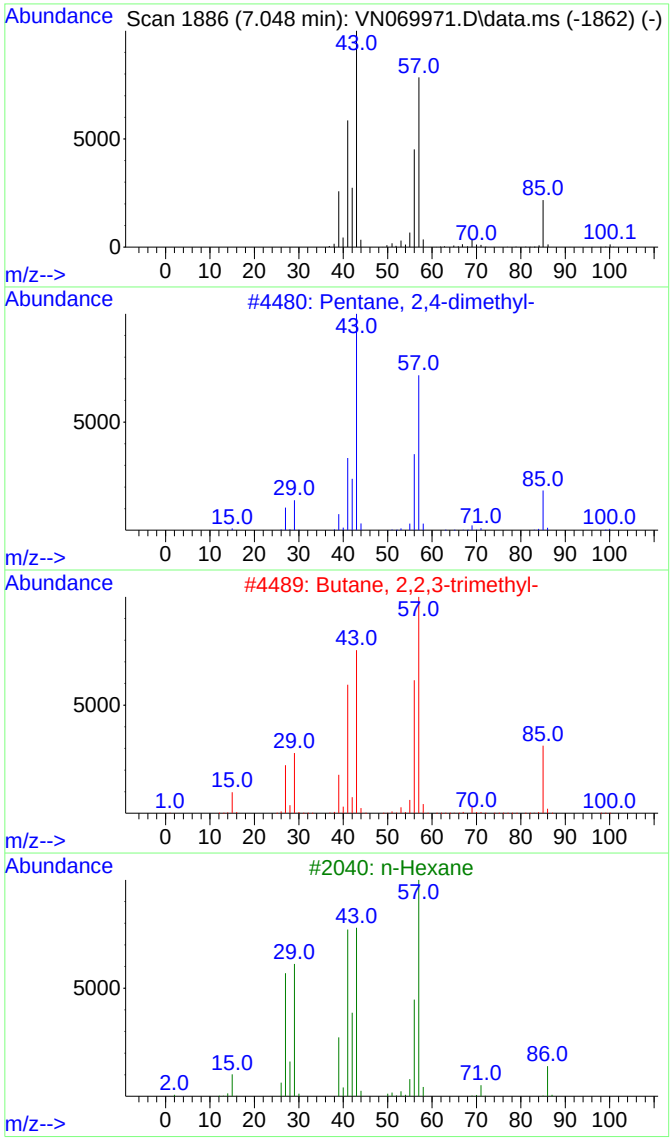
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

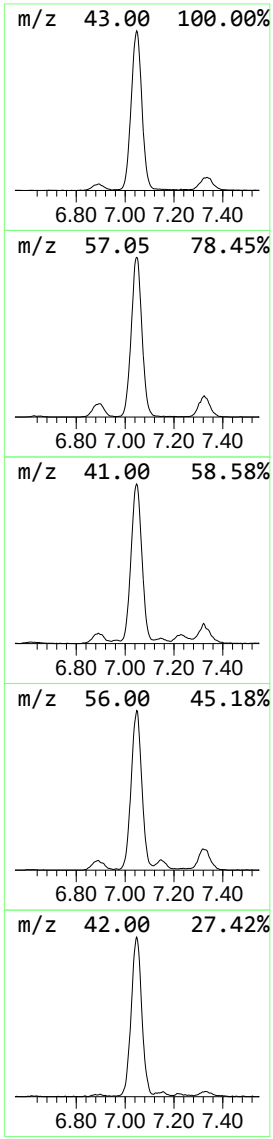
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.048	32.21 ug/l	2152900	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	n-Hexane	86	C6H14	000110-54-3	53
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
5	2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

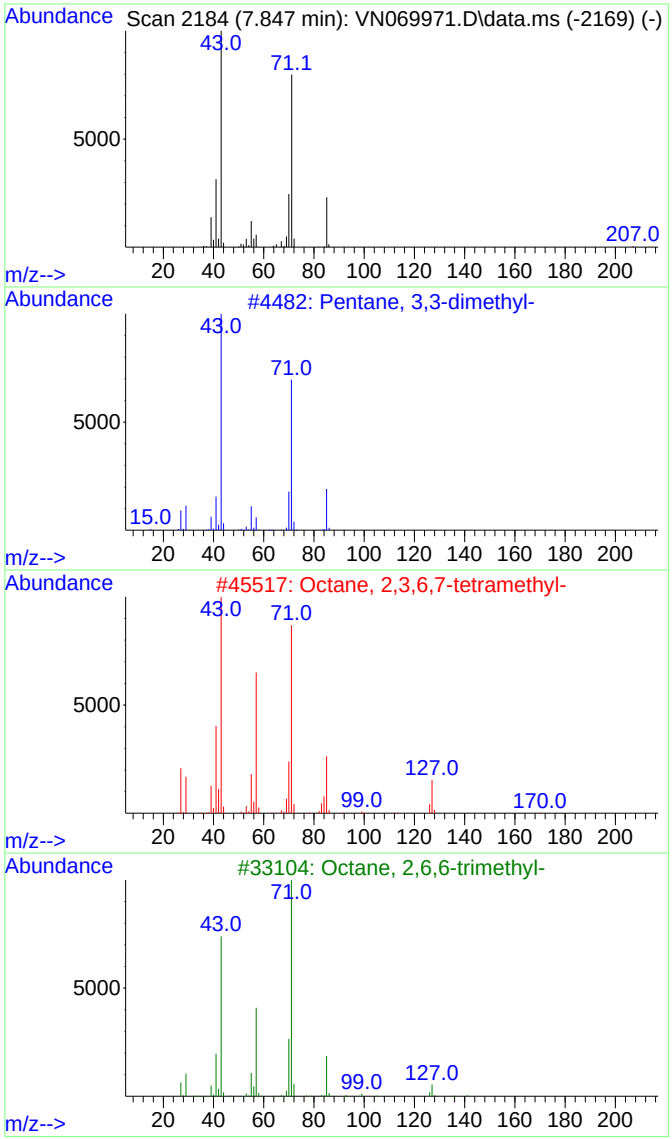
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

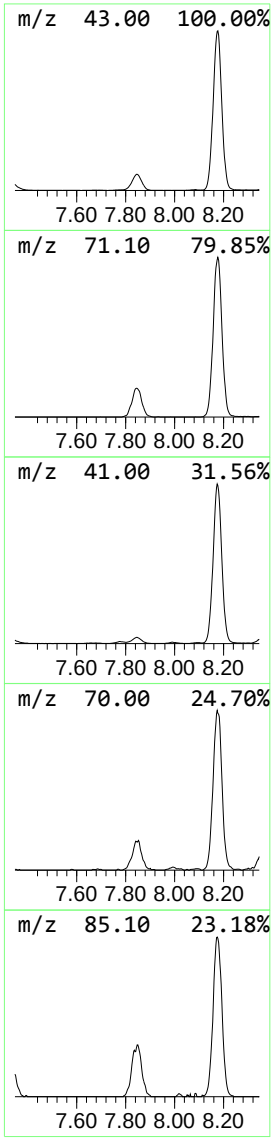
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.847	5.33 ug/l	355957	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	83
2	Octane, 2,3,6,7-tetramethyl-	170	C12H26	052670-34-5	78
3	Octane, 2,6,6-trimethyl-	156	C11H24	054166-32-4	72
4	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	64
5	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

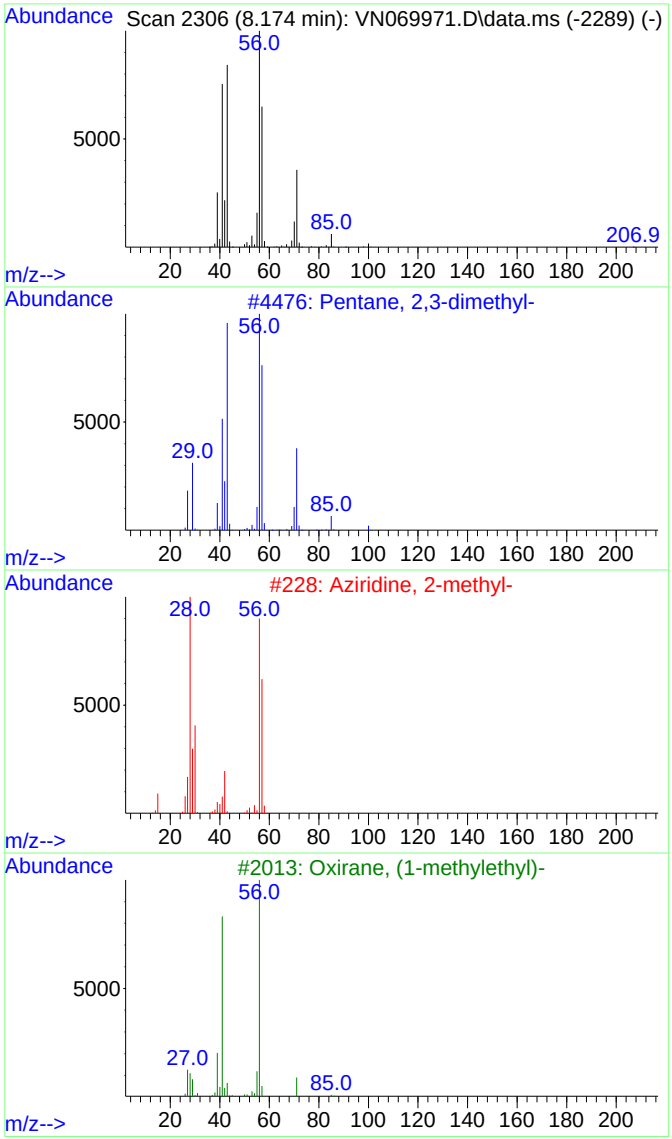
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

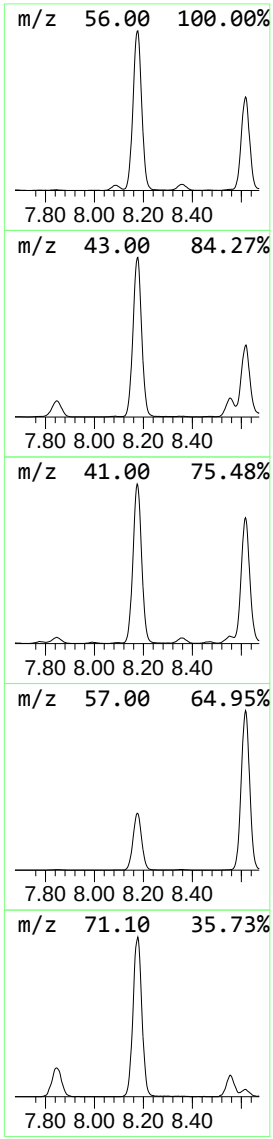
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	75.50 ug/l	5045540	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	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	40
4	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38
5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

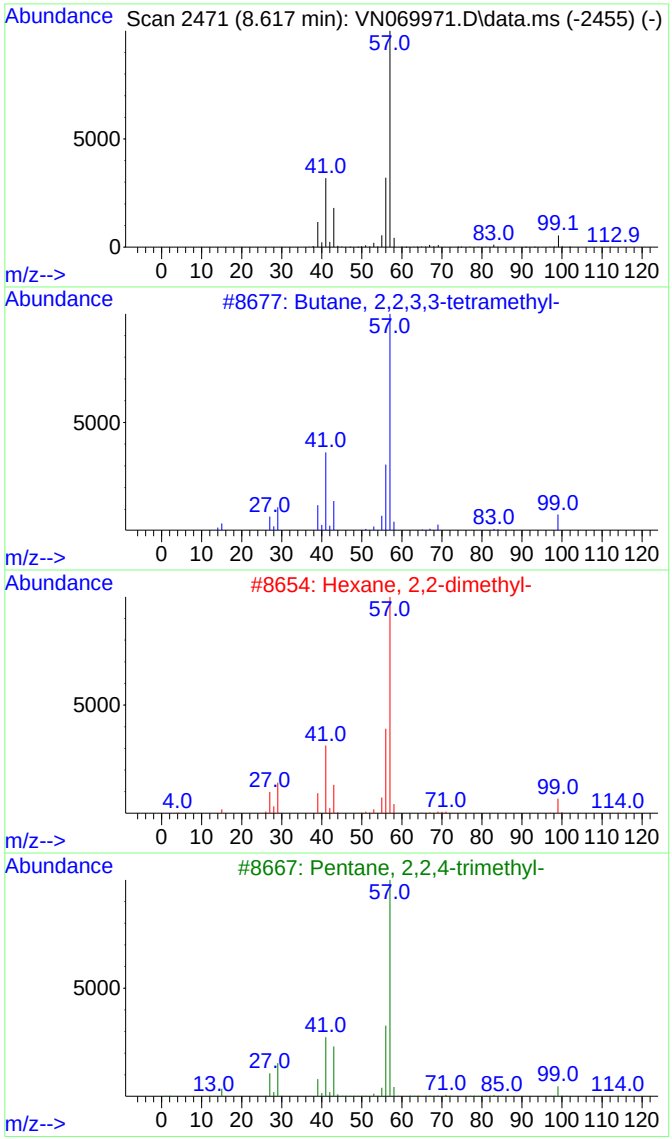
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

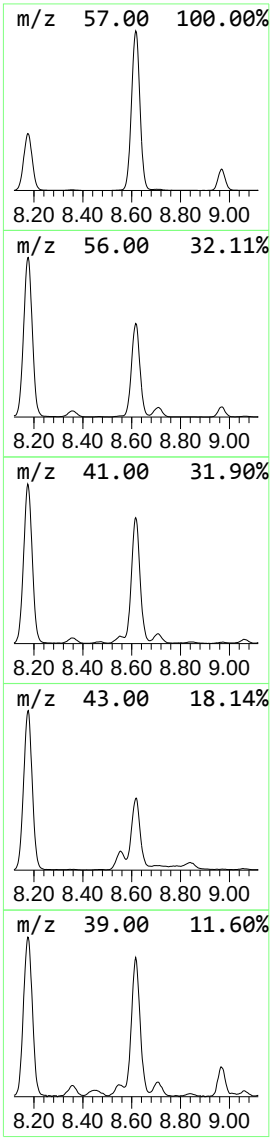
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,2,3,3-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	42.70 ug/l	4439580	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	78
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

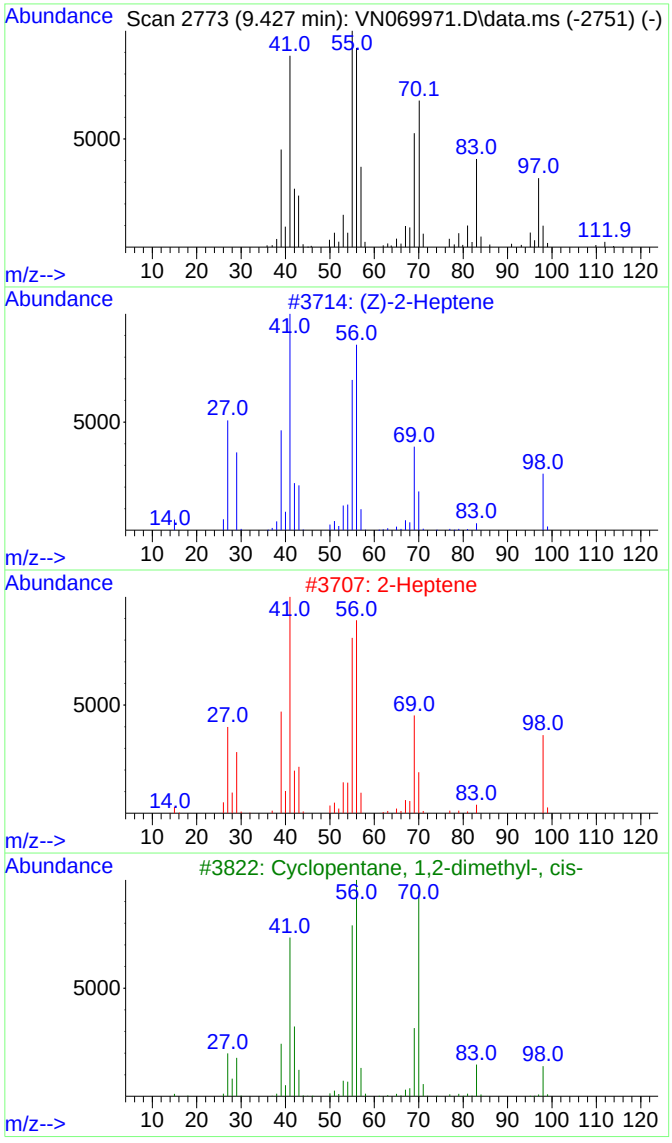
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

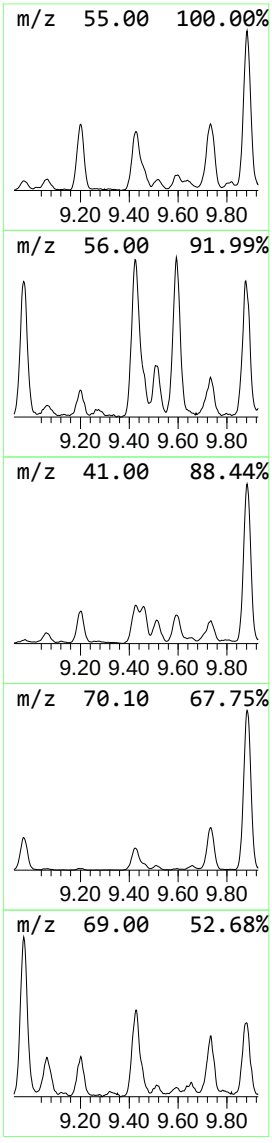
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (Z)-2-Heptene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.427	5.19 ug/l	539303	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-2-Heptene	98	C7H14	006443-92-1	52
2	2-Heptene	98	C7H14	000592-77-8	52
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	49
4	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	49
5	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

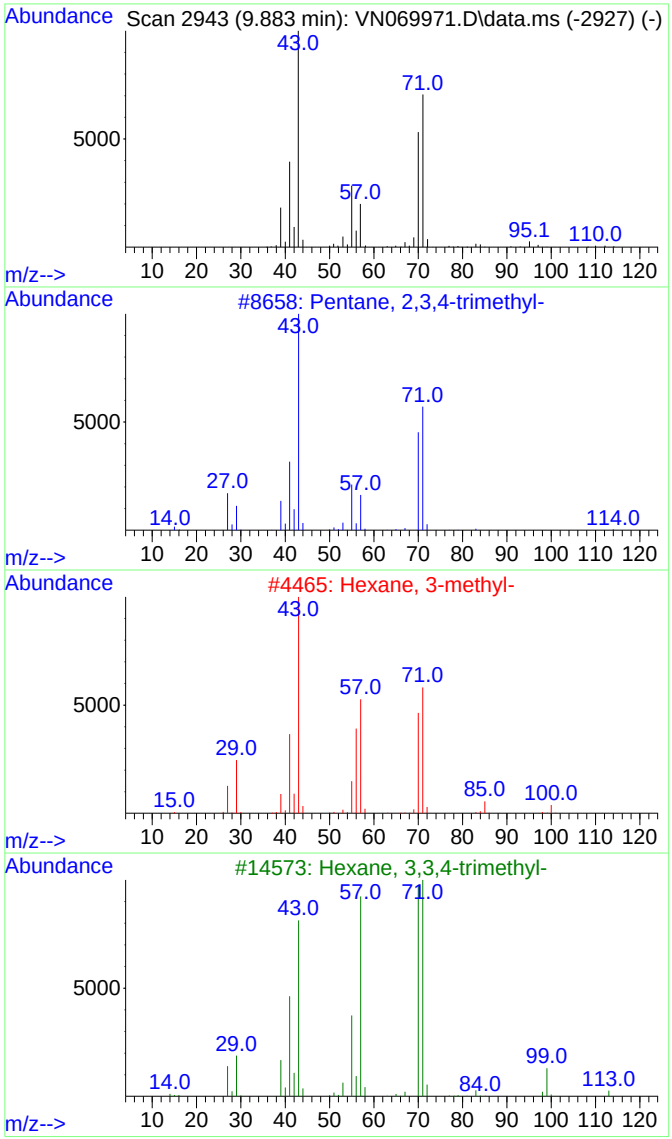
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

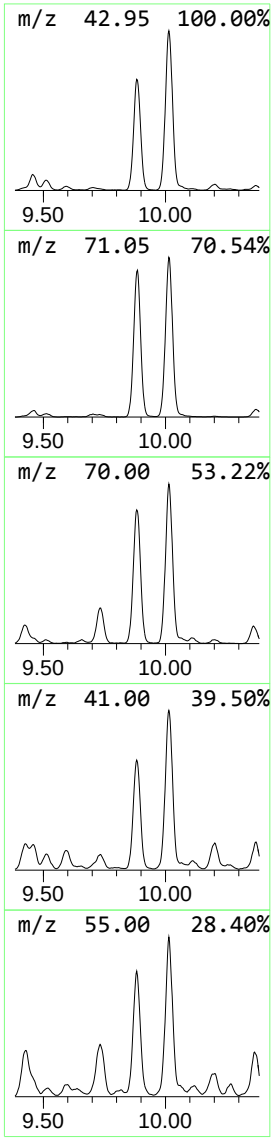
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	23.97 ug/l	2491540	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	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	72
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72
5	Heptane, 4-methyl-	114	C8H18	000589-53-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

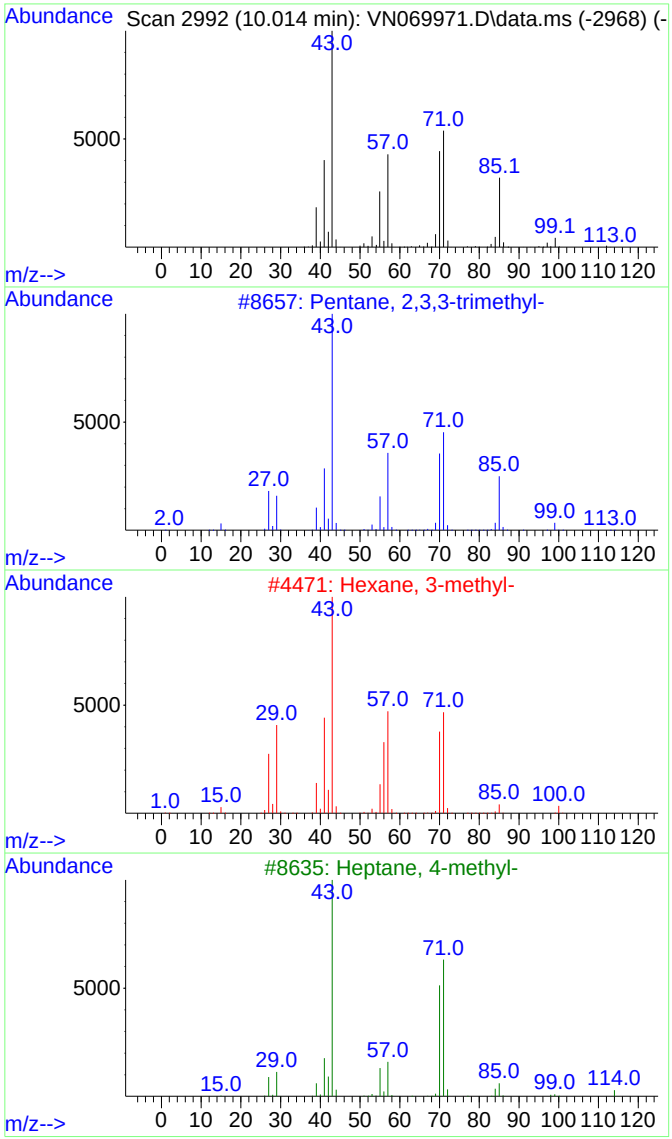
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

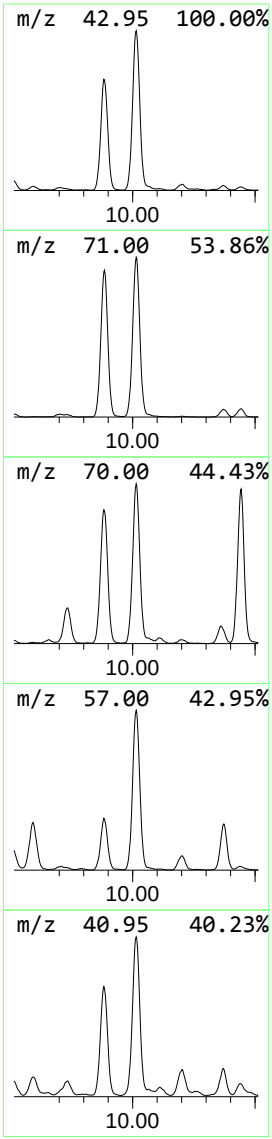
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	39.35 ug/l	4090950	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	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

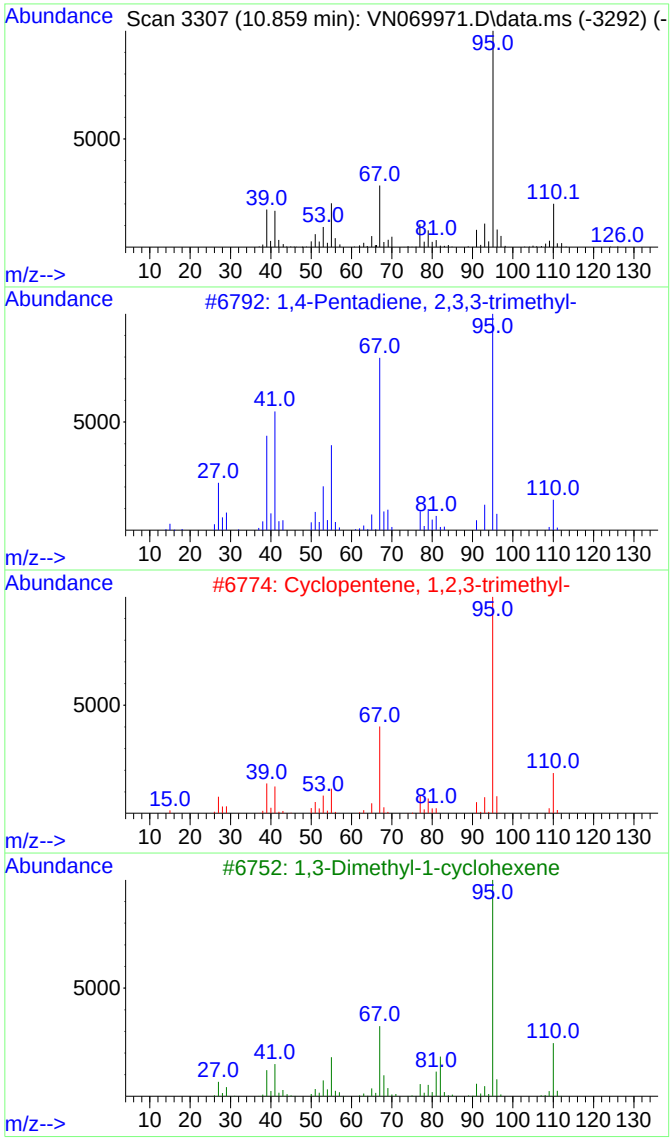
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

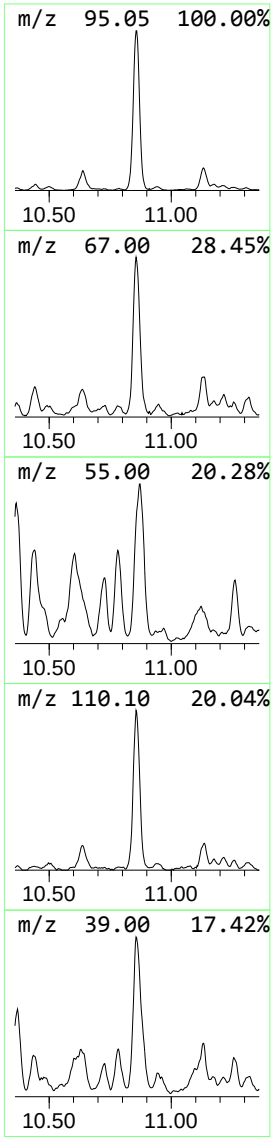
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.859	7.42 ug/l	1164770	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	86
2	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	81
3	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	68
4	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	64
5	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-11A

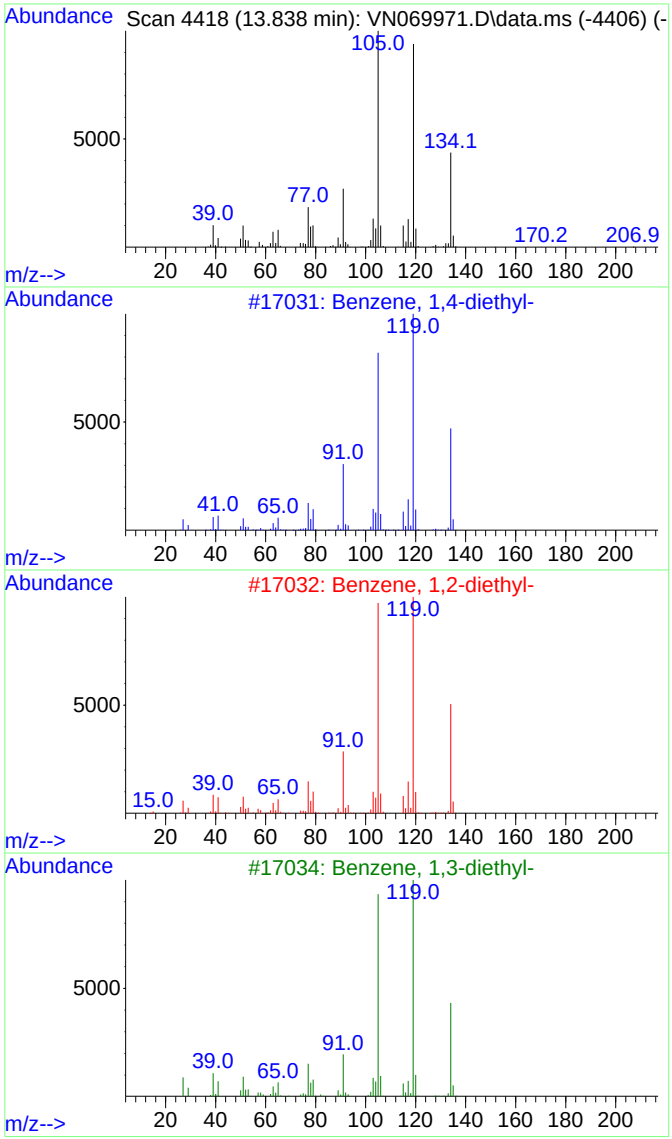
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

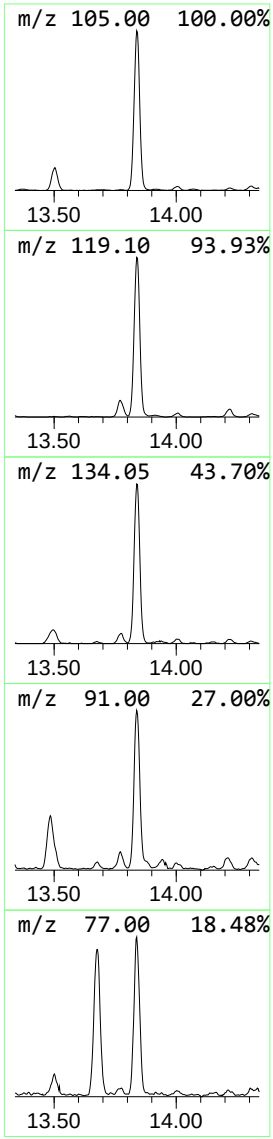
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,4-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	8.65 ug/l	1175460	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, 1,2-diethyl-	134	C10H14	000135-01-3	96
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
Data File : VN069971.D
Acq On : 10 Dec 2021 20:39
Operator : JC/MD
Sample : M4969-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 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...	5.076	87.4	ug/l	5839100	1	8.088	3341570	50.0
Pentane, 2,4-di...	7.048	32.2	ug/l	2152900	1	8.088	3341570	50.0
Pentane, 3,3-di...	7.847	5.3	ug/l	355957	1	8.088	3341570	50.0
Pentane, 2,3-di...	8.174	75.5	ug/l	5045540	1	8.088	3341570	50.0
Butane, 2,2,3,3...	8.617	42.7	ug/l	4439580	2	8.968	5198080	50.0
(Z)-2-Heptene	9.427	5.2	ug/l	539303	2	8.968	5198080	50.0
Pentane, 2,3,4-...	9.883	24.0	ug/l	2491540	2	8.968	5198080	50.0
Pentane, 2,3,3-...	10.014	39.4	ug/l	4090950	2	8.968	5198080	50.0
1,4-Pentadiene,...	10.859	7.4	ug/l	1164770	3	11.746	7847870	50.0
Benzene, 1,4-di...	13.839	8.7	ug/l	1175460	4	13.675	6793000	50.0