LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

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\82N091024W.M
Title : SW846 8260

Signal : TIC: VN083972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.218	1058	1065	1075	rVB3	631381	1522130	1.14%	0.164%
2	8.753	1140	1156	1168	rBV	2818087	7387804	5.53%	0.794%
3	9.094	1205	1214	1221	rBV2	828505	2025570	1.52%	0.218%
4	9.588	1283	1298	1303	rBV3	1588705	3827745	2.87%	0.411%
5	9.641	1303	1307	1314	rVB	954955	1771073	1.33%	0.190%
6	10.012	1362	1370	1379	rVB	3476608	6860165	5.14%	0.737%
7	10.147	1386	1393	1399	rVB	4879575	8976066	6.72%	0.964%
8	10.335	1416	1425	1438	rBV2	1083416	2808617	2.10%	0.302%
9	10.494	1445	1452	1458	rVB	3673161	6691505	5.01%	0.719%
10	10.565	1458	1464	1469	rBV2	923106	1726856	1.29%	0.186%
11	10.629	1469	1475	1484	rVV	2157534	4254815	3.19%	0.457%
12	10.741	1487	1494	1501	rVB2	1290632	2546211	1.91%	0.274%
13	11.012	1530	1540	1547	rVB4	862210	2155712	1.61%	0.232%
14	11.271	1574	1584	1592	rVV	629312	1543958	1.16%	0.166%
15	11.641	1639	1647	1659	rVB2	1369738	3350929	2.51%	0.360%
16	11.741	1659	1664	1674	rBV	1049722	1909383	1.43%	0.205%
17	11.865	1674	1685	1689	rBV3	1050526	2964732	2.22%	0.319%
18	11.965	1689	1702	1711	rVV	10682647	19234393	14.40%	2.067%
19	12.070	1711	1720	1731	rVV3	62690841	133572692	99.99%	14.351%
20	12.400	1766	1776	1784	rVV	39167553	69104016	51.73%	7.425%
21	12.694	1819	1826	1833	rBV	8257655	13942703	10.44%	1.498%
22	12.823	1841	1848	1855	rVB	2322920	4368266	3.27%	0.469%
23	13.035	1878	1884	1889	rVV	11743978	19535294	14.62%	2.099%
24	13.100	1889	1895	1899	rVV2	51703420	96791471	72.46%	10.399%
25	13.135	1899	1901	1904	rVV	26053955	33860806	25.35%	3.638%
26	13.176	1904	1908	1916	rVB	29998243	49871987	37.33%	5.358%
27	13.335	1927	1935	1943	rBV	23566064	39930129	29.89%	4.290%
28	13.423	1943	1950	1954	rBV	1942243	3293962	2.47%	0.354%
29	13.488	1954	1961	1968	rBV2	69224667	133582656	100.00%	14.352%
30	13.617	1974	1983	1984	rBV3	1622157	3359179	2.51%	0.361%
31	13.647	1985	1988	1990	rVV	1915023	2912867	2.18%	0.313%
32	13.670	1990	1992	1997	rVB	1739927	2412037	1.81%	0.259%
33	13.823	2009	2018	2034	rVB	24102338	46365220	34.71%	4.982%
34	13.953	2034	2040	2041	rBV	3379057	4734314	3.54%	0.509%
35	13.994	2041	2047	2062	rVV3	17129588	58608672	43.87%	6.297%
36	14.112	2062	2067	2073	rVV2	927923	2227651	1.67%	0.239%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

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\82N091024W.M
Title : SW846 8260

37	14.182	2073	2079	2084	rVV2	3492035	5883449	4.40%	0.632%
38	14.241	2084	2089	2092	rVV	5780346	9653713	7.23%	1.037%
39	14.270	2092	2094	2099	rVV	5377334	7666937	5.74%	0.824%
40	14.329	2099	2104	2111	rVV	9855754	15685793	11.74%	1.685%
41	14.441	2118	2123	2129	rVB3	2753551	4869798	3.65%	0.523%
42	14.570	2140	2145	2151	rVB	2219465	3490694	2.61%	0.375%
43	14.653	2151	2159	2162	rBV	6326843	10293089	7.71%	1.106%
44	14.694	2162	2166	2170	rVV	8189538	12626372	9.45%	1.357%
45	14.735	2170	2173	2177	rVB2	1438072	1922436	1.44%	0.207%
46	14.923	2200	2205	2210	rBV	3610611	6509993	4.87%	0.699%
47	15.053	2216	2227	2232	rBV4	5633243	15919633	11.92%	1.710%
48	15.100	2232	2235	2245	rVB2	805634	1817109	1.36%	0.195%
49	15.206	2248	2253	2261	rVB2	801298	1554165	1.16%	0.167%
50	15.317	2261	2272	2284	rBV3	1387842	4075262	3.05%	0.438%
51	15.435	2285	2292	2300	rVB4	866822	2185991	1.64%	0.235%
52	15.641	2313	2327	2335	rBV	8776187	17446993	13.06%	1.875%
53	15.823	2350	2358	2370	rVB4	518628	1762670	1.32%	0.189%
54	15.941	2370	2378	2386	rBV	653146	1498016	1.12%	0.161%
55	16.782	2512	2521	2522	rBV	3340307	5852400	4.38%	0.629%

Sum of corrected areas: 930746099

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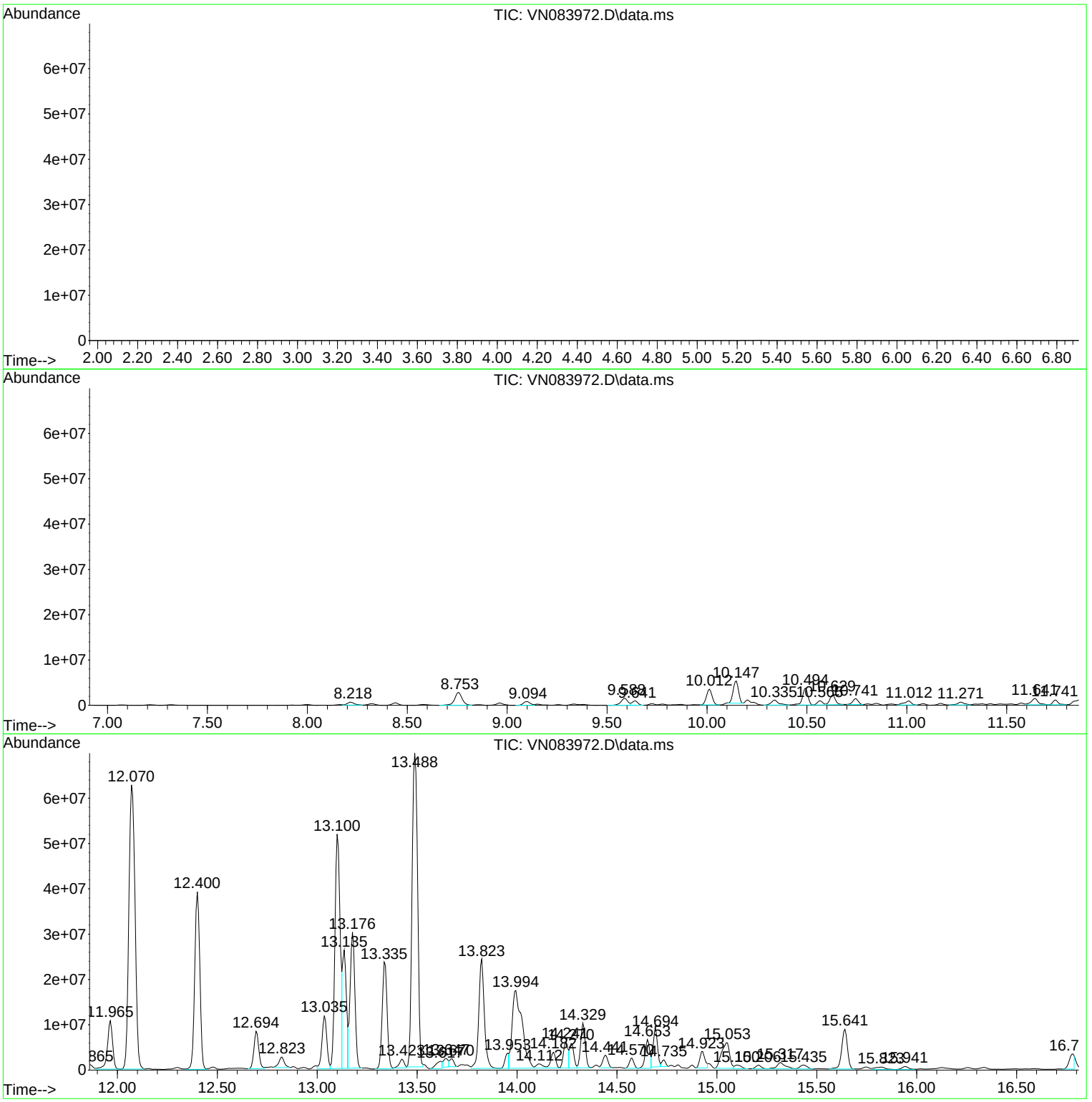
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
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MSVOA_N
ClientSampleId :
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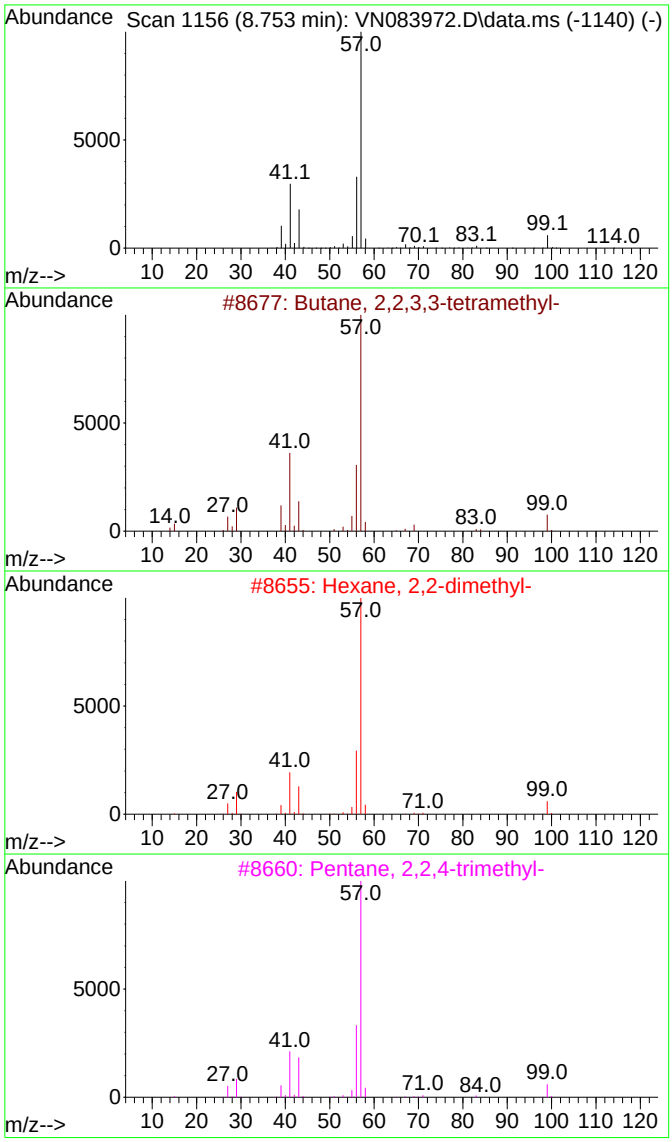
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

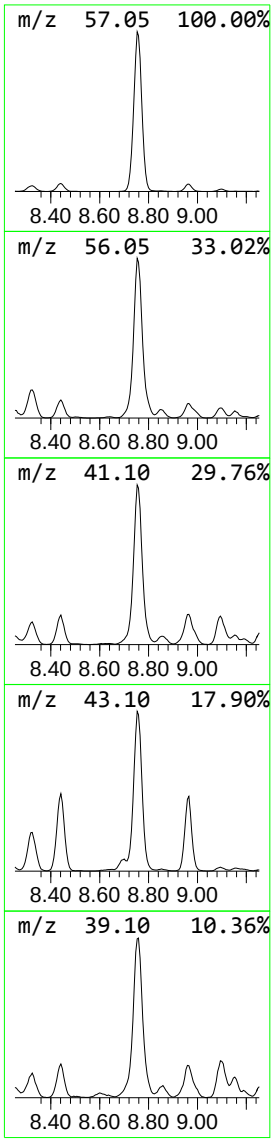
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	182.36 ug/l	7387800	1,4-Difluorobenzene	9.100

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	64
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

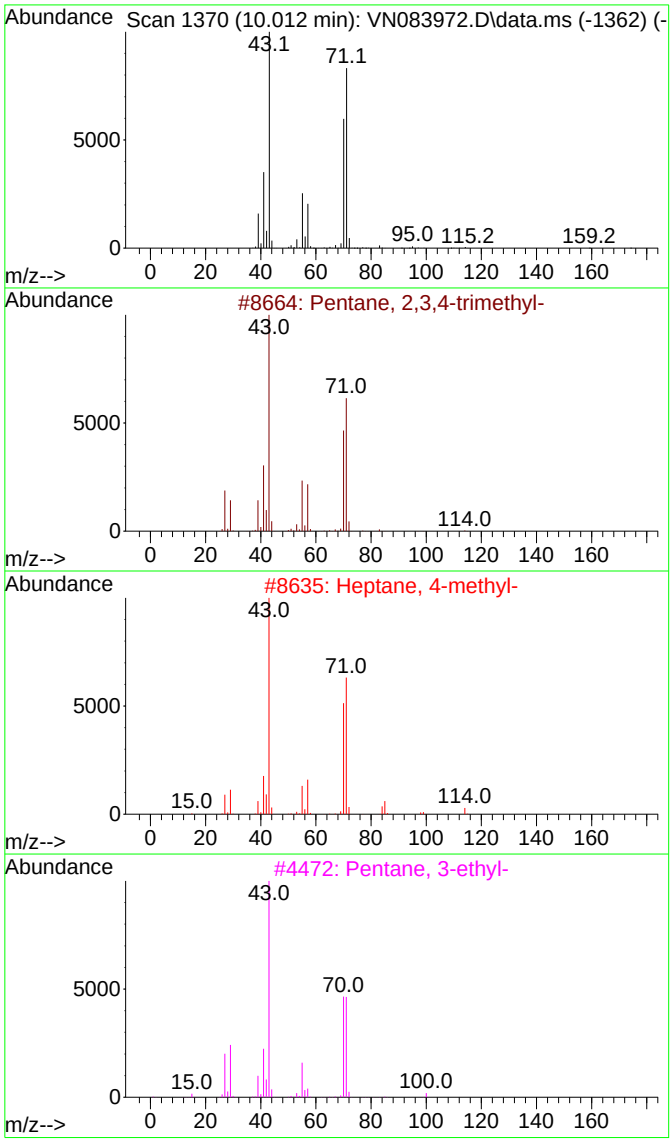
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

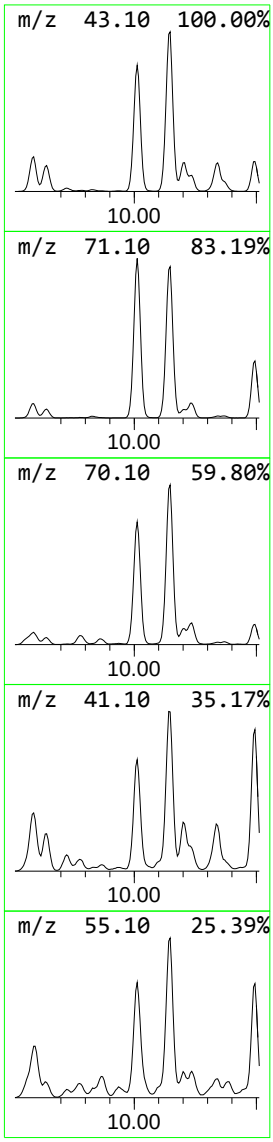
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.012	169.34 ug/l	6860170	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

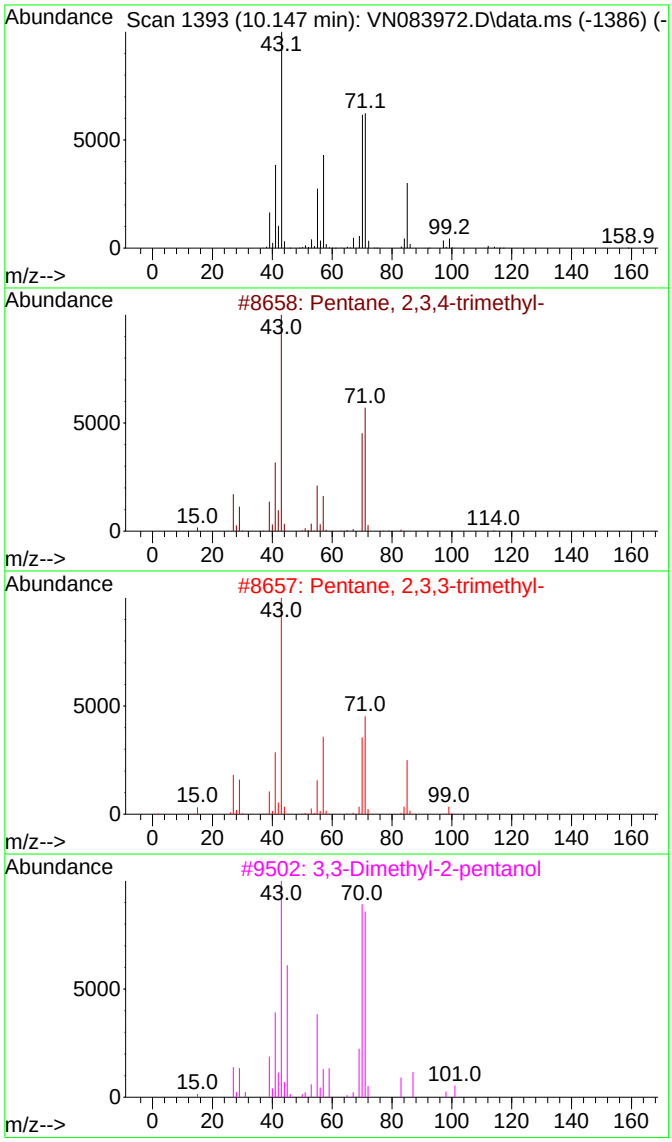
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

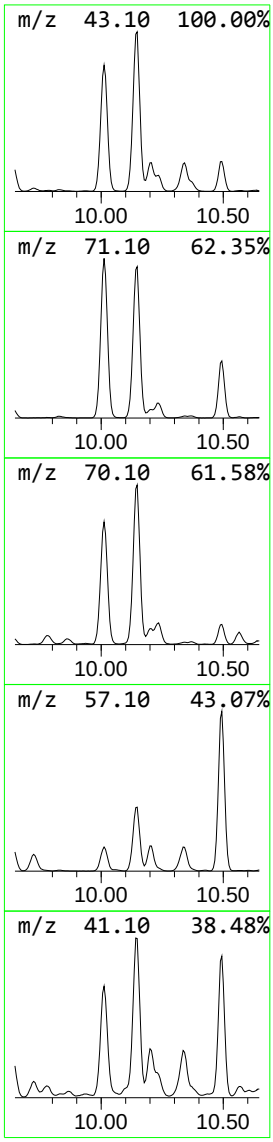
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.147	221.57 ug/l	8976070	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	76
2	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3	3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	59
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

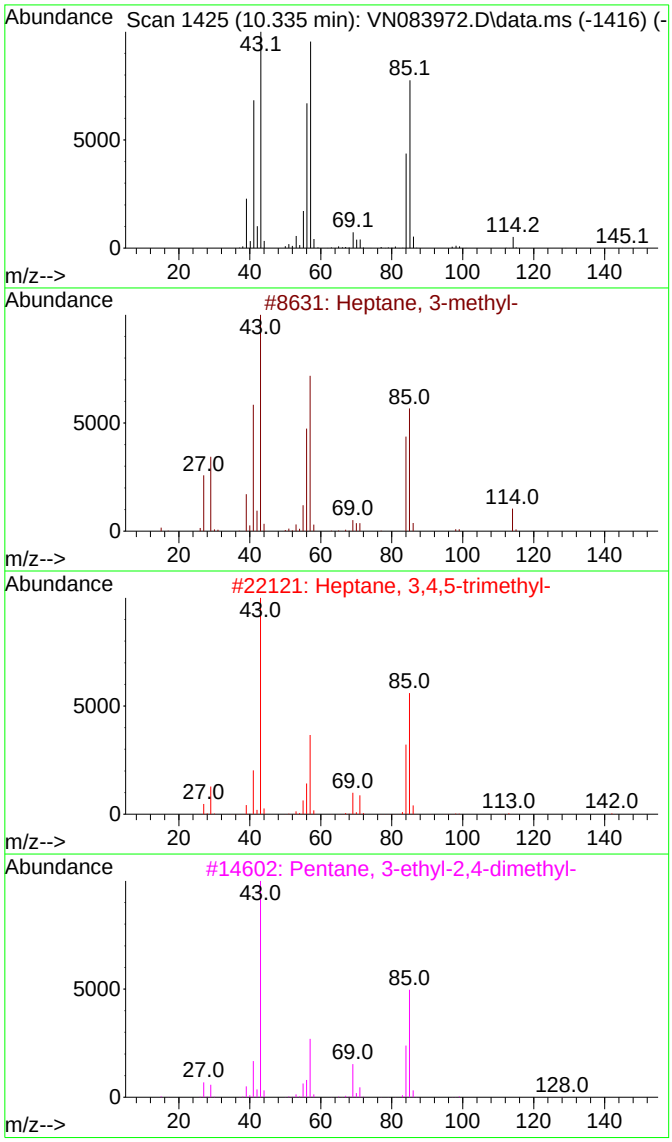
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

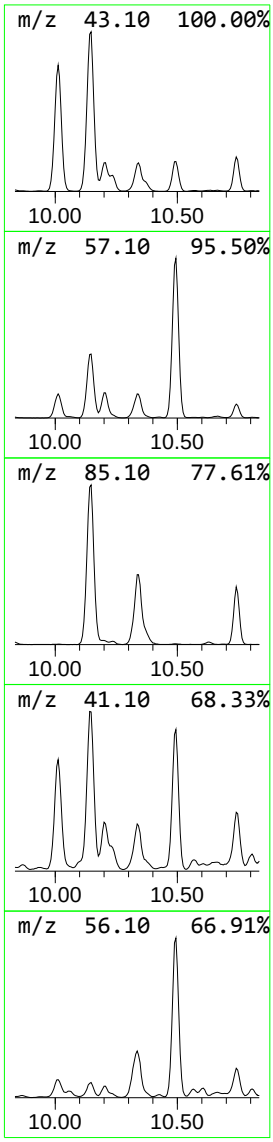
****

Peak Number 4 Heptane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.335	69.33 ug/l	2808620	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	90
2	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	64
3	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
4	Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	53
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

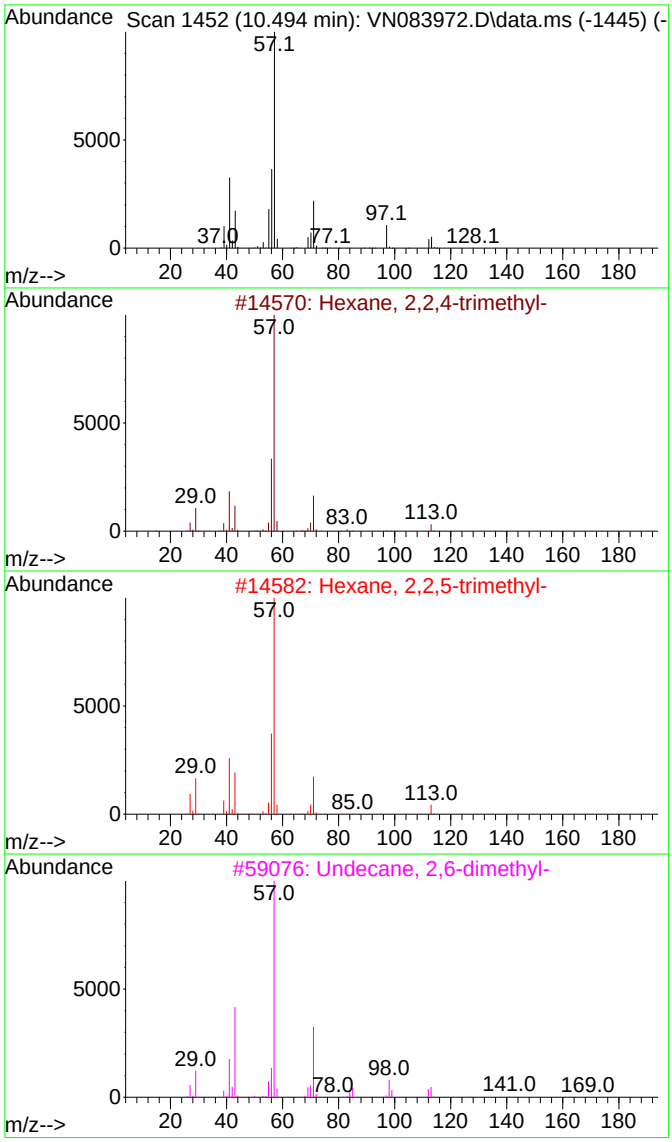
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

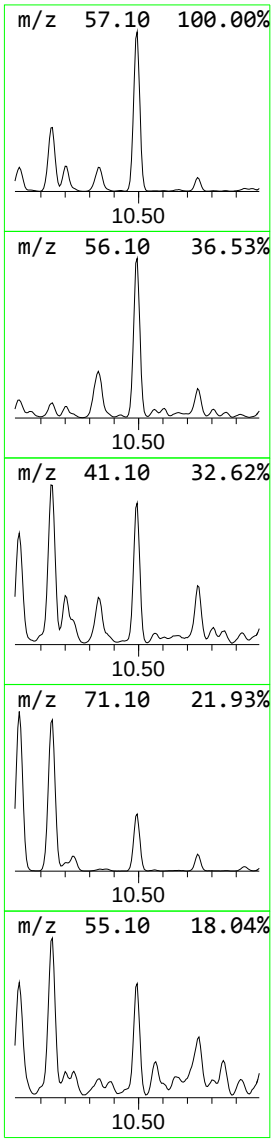
****

Peak Number 5 Hexane, 2,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.494	112.85 ug/l	6691510	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
2	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
4	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	53
5	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50





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Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

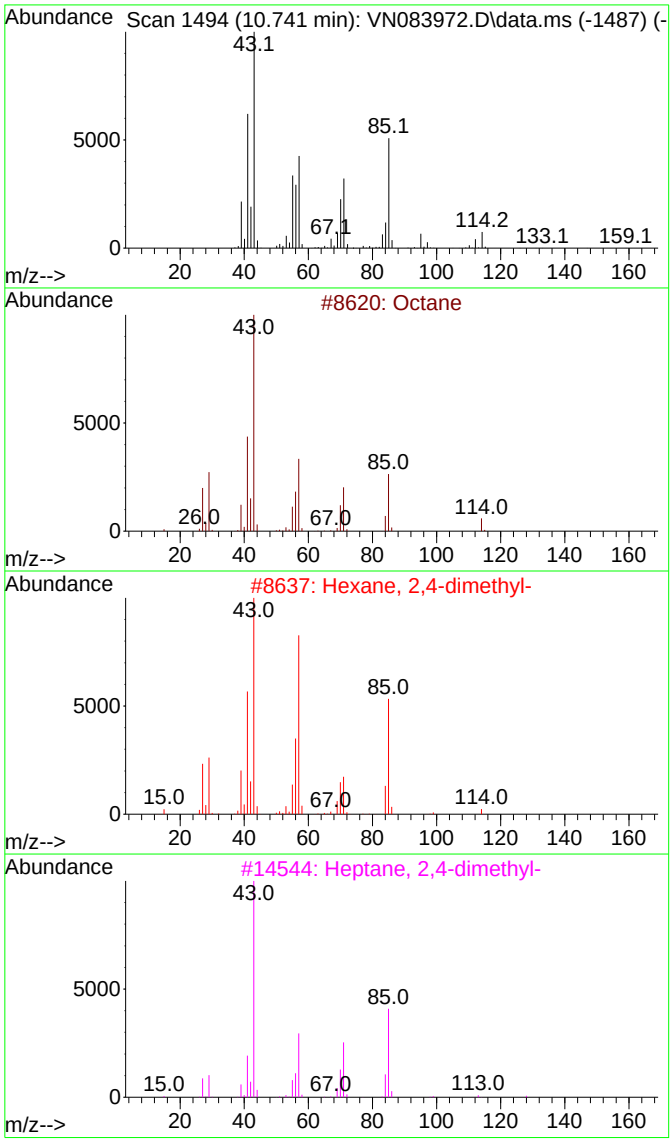
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

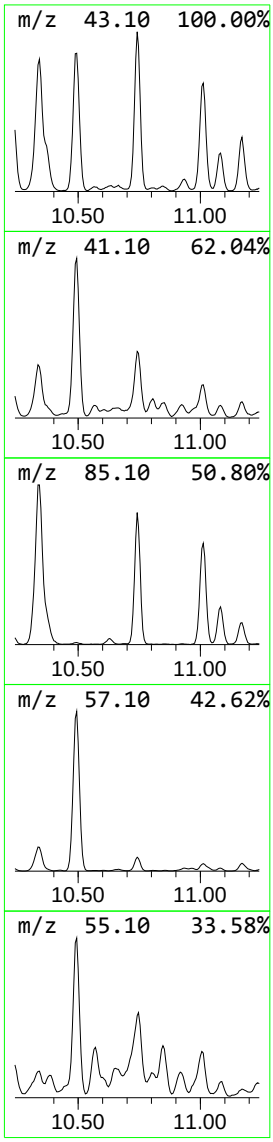
****

Peak Number 6 Octane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.741	42.94 ug/l	2546210	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	90
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	58
4	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	43
5	2-Pyrrolidinone	85	C4H7NO	000616-45-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

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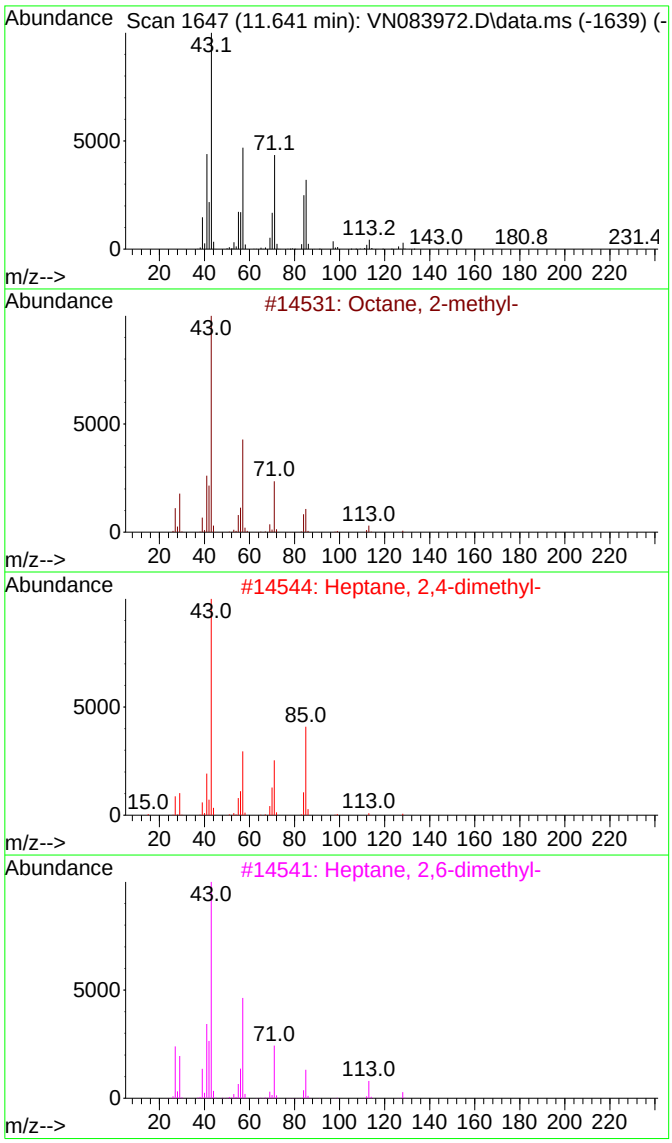
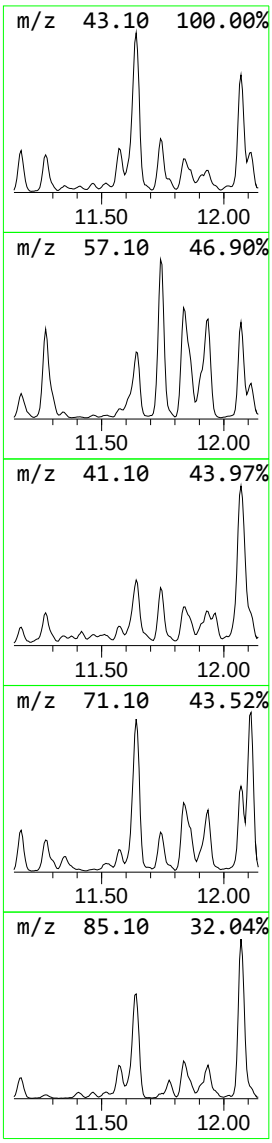
Peak Number 7 Octane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.641	56.51 ug/l	3350930	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	64
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
3	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	53
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	50
5	Octane	114	C8H18	000111-65-9	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

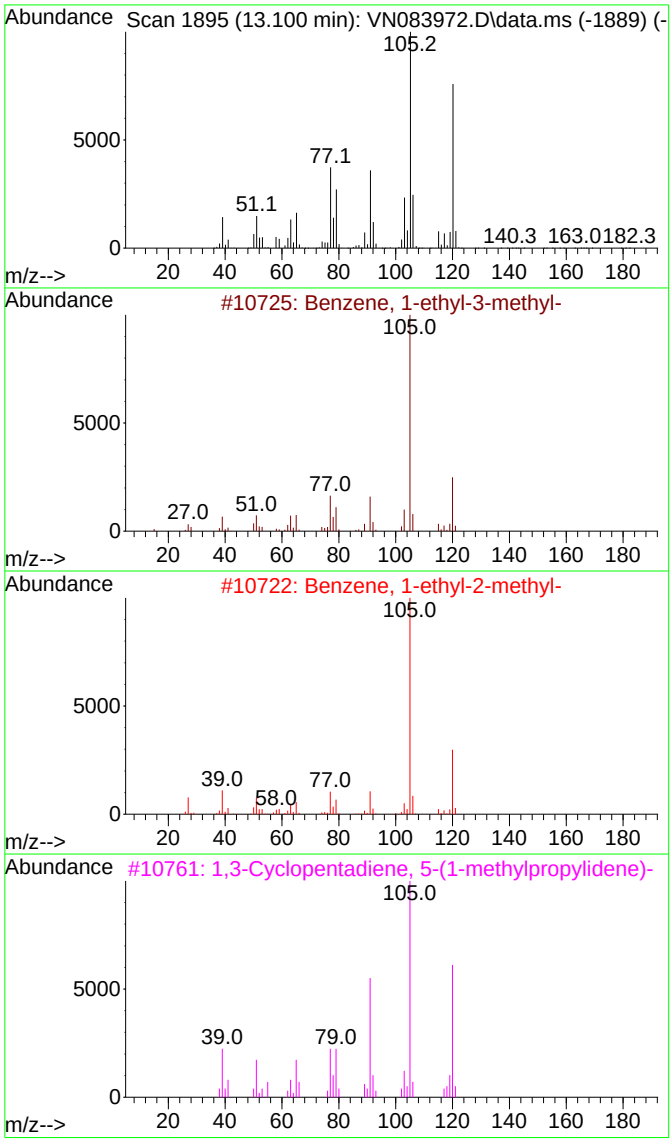
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

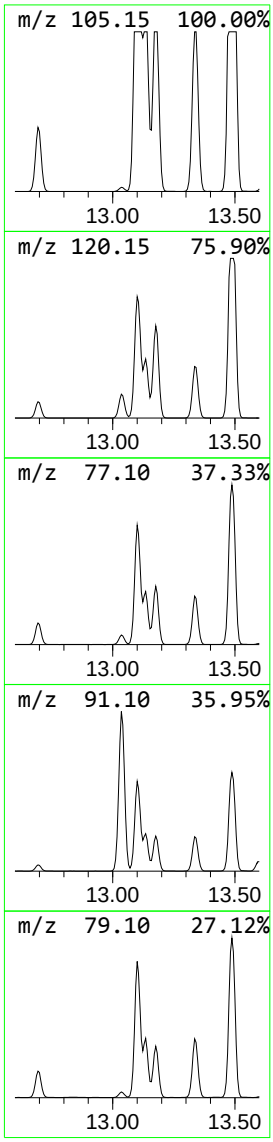
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	104.38 ug/l	96791500	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	81
3	1,3-Cyclopentadiene, 5-(1-methyl...	120	C9H12	003141-02-4	80
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	76
5	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

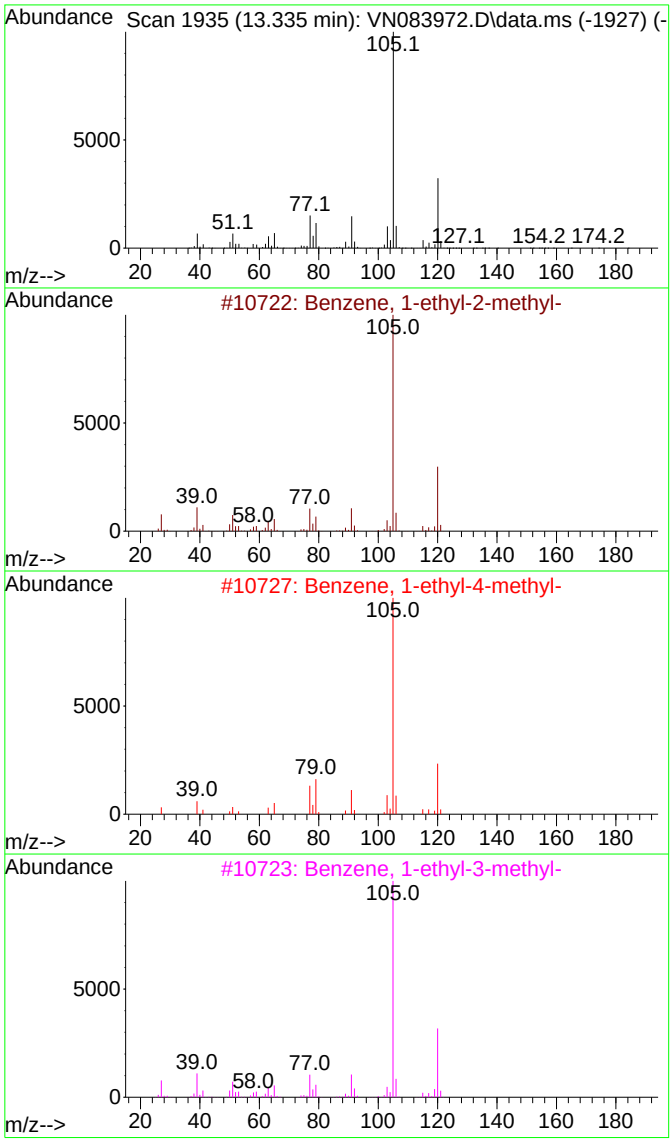
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

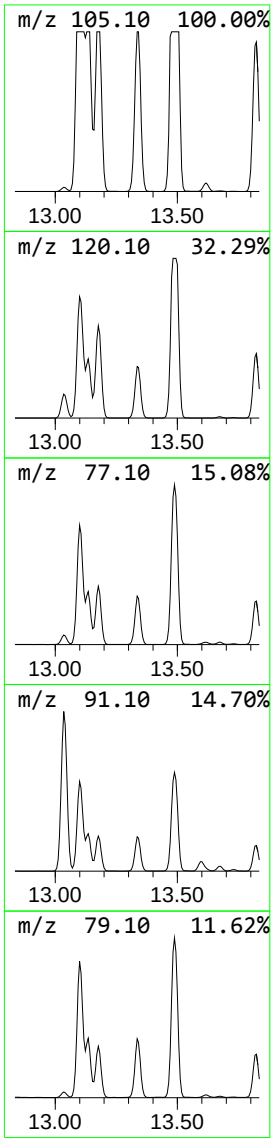
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	43.06 ug/l	39930100	1,4-Dichlorobenzene-d4	13.794

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	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

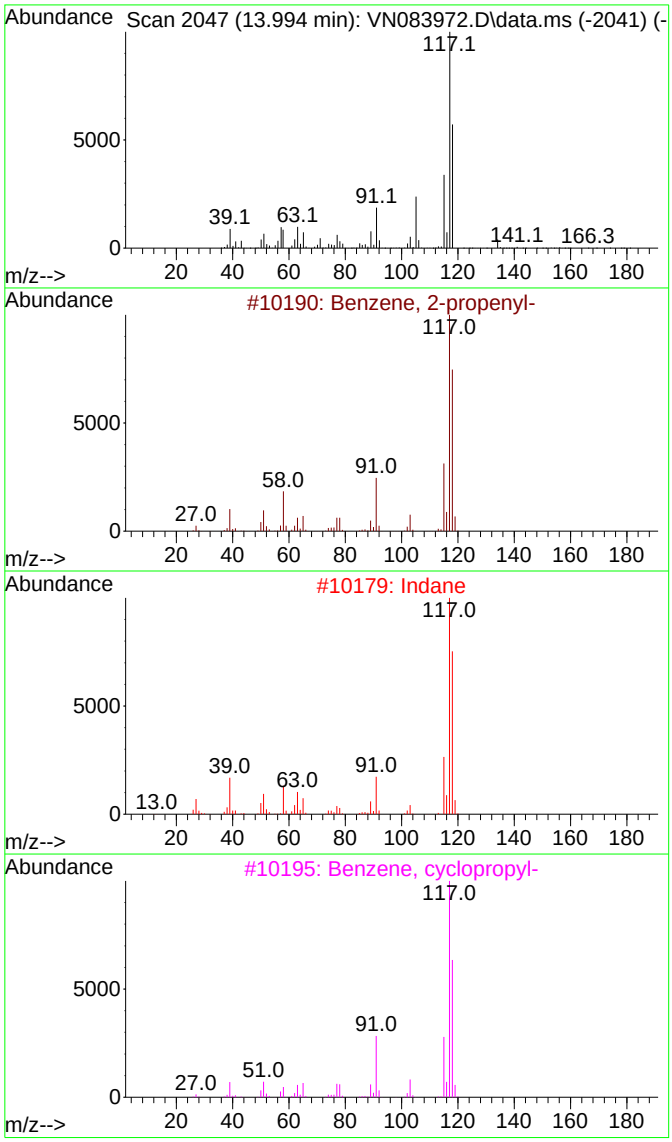
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

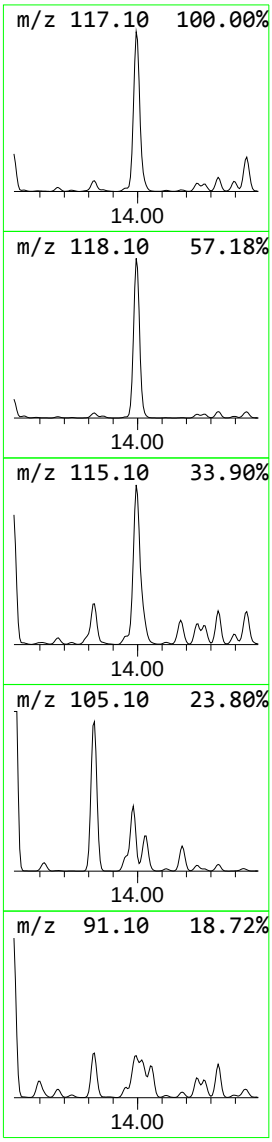
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-propenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	63.20 ug/l	58608700	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2	Indane	118	C9H10	000496-11-7	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083972.D
Acq On : 18 Sep 2024 09:08
Operator : JC\MD
Sample : P3964-02
Misc : 11.34g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.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, 2,2,3,3...	8.753	182.4	ug/l	7387800	2	9.100	2025570	50.0
Pentane, 2,3,4-...	10.012	169.3	ug/l	6860170	2	9.100	2025570	50.0
Pentane, 2,3,3-...	10.147	221.6	ug/l	8976070	2	9.100	2025570	50.0
Heptane, 3-methyl-	10.335	69.3	ug/l	2808620	2	9.100	2025570	50.0
Hexane, 2,2,4-t...	10.494	112.8	ug/l	6691510	3	11.865	2964730	50.0
Octane	10.741	42.9	ug/l	2546210	3	11.865	2964730	50.0
Octane, 2-methyl-	11.641	56.5	ug/l	3350930	3	11.865	2964730	50.0
Benzene, 1-ethy...	13.100	104.4	ug/l	96791500	4	13.794	46365200	50.0
Benzene, 1-ethy...	13.335	43.1	ug/l	39930100	4	13.794	46365200	50.0
Benzene, 2-prop...	13.994	63.2	ug/l	58608700	4	13.794	46365200	50.0