LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010925\
Data File : VN085407.D
Acq On : 09 Jan 2025 14:28
Operator : JC\MD
Sample : Q1033-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
28612

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\82N122724W.M
Title : SW846 8260

Signal : TIC: VN085407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	16	22	29	rVB	92385	127780	7.27%	0.935%
2	2.295	50	58	67	rBV2	97602	178664	10.16%	1.307%
3	4.418	409	419	438	rBV	71296	218799	12.44%	1.601%
4	7.477	928	939	951	rBV	52997	135468	7.70%	0.991%
5	7.836	990	1000	1013	rBV2	131073	336561	19.14%	2.462%
6	7.959	1013	1021	1032	rVB	28605	68453	3.89%	0.501%
7	8.159	1045	1055	1060	rBV	153106	366840	20.86%	2.684%
8	8.218	1060	1065	1080	rVB	273932	603891	34.34%	4.418%
9	8.594	1116	1129	1142	rBV2	253498	865234	49.20%	6.329%
10	9.094	1205	1214	1225	rBV	408428	817005	46.46%	5.977%
11	10.500	1445	1453	1456	rBV2	15863	26951	1.53%	0.197%
12	10.565	1456	1464	1469	rVV	584667	1081409	61.49%	7.911%
13	10.624	1469	1474	1486	rVB	445601	815120	46.35%	5.963%
14	11.859	1676	1684	1695	rBV	529938	944443	53.70%	6.909%
15	11.959	1695	1701	1707	rVV	140028	235372	13.38%	1.722%
16	12.023	1707	1712	1714	rVV2	12510	21221	1.21%	0.155%
17	12.065	1714	1719	1729	rVB	81199	164596	9.36%	1.204%
18	12.400	1767	1776	1788	rBV3	248092	502656	28.58%	3.677%
19	12.847	1844	1852	1862	rBV	391624	666707	37.91%	4.877%
20	13.094	1887	1894	1896	rBV2	15329	24969	1.42%	0.183%
21	13.123	1896	1899	1903	rVV	20315	34341	1.95%	0.251%
22	13.170	1903	1907	1913	rVB	26702	41362	2.35%	0.303%
23	13.341	1928	1936	1941	rVB4	15075	27818	1.58%	0.203%
24	13.529	1963	1968	1972	rVV2	45179	71387	4.06%	0.522%
25	13.576	1972	1976	1985	rVB	26008	41818	2.38%	0.306%
26	13.788	2005	2012	2021	rBV2	511528	936655	53.26%	6.852%
27	13.853	2021	2023	2032	rVB4	13041	19459	1.11%	0.142%
28	13.994	2040	2047	2054	rVB	83675	153810	8.75%	1.125%
29	14.170	2069	2077	2085	rBV	1018604	1653678	94.03%	12.097%
30	14.459	2118	2126	2132	rVB2	14635	26532	1.51%	0.194%
31	14.688	2161	2165	2170	rVV4	16297	24740	1.41%	0.181%
32	15.035	2216	2224	2231	rBV5	15380	33051	1.88%	0.242%
33	15.112	2231	2237	2245	rVV	74233	126316	7.18%	0.924%
34	15.200	2245	2252	2264	rVV	140632	252354	14.35%	1.846%
35	15.306	2264	2270	2278	rVV3	12747	25102	1.43%	0.184%
36	15.635	2316	2326	2337	rBV	940231	1758657	100.00%	12.865%

LSC Area Percent Report

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Title : SW846 8260

37	15.741	2337	2344	2352	rVB	27618	54468	3.10%	0.398%
38	16.776	2512	2520	2522	rBV2	103687	186497	10.60%	1.364%

Sum of corrected areas: 13670184

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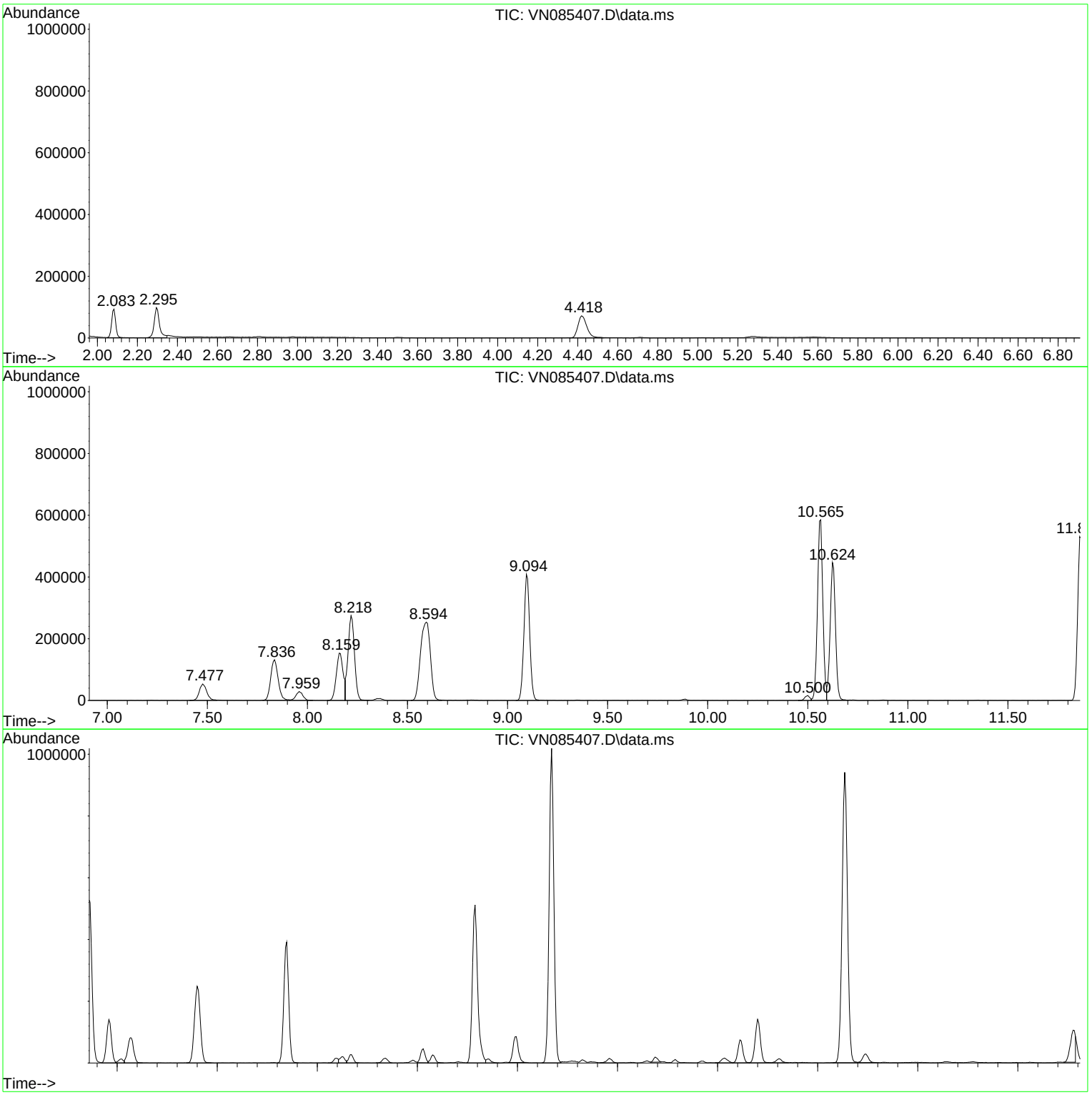
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

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



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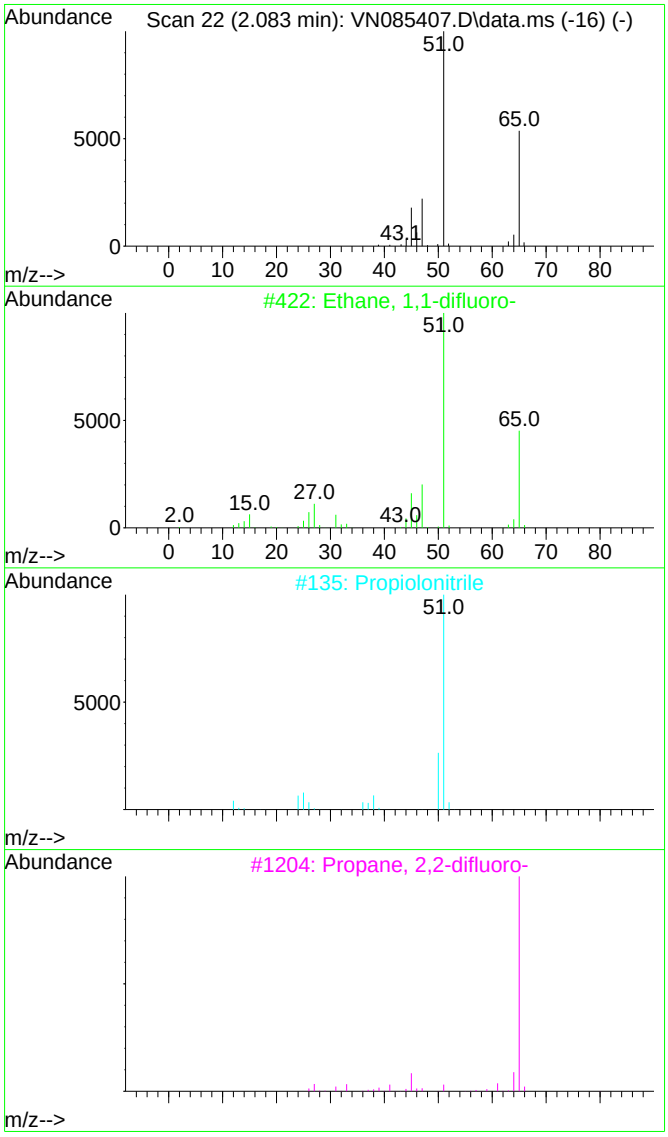
Quant Title : SW846 8260

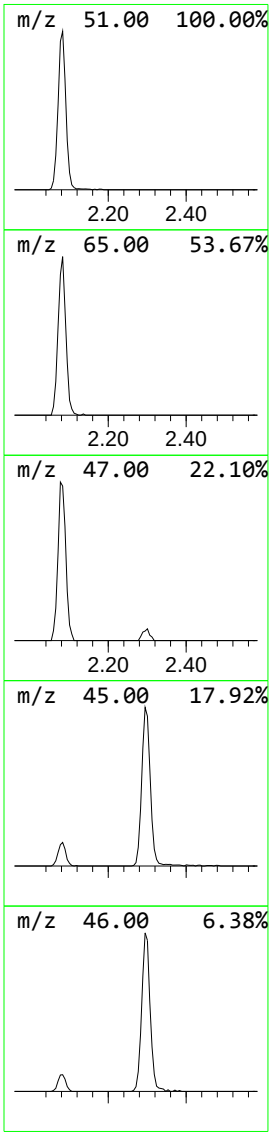
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	10.58 ug/l	127780	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2	Propiolonitrile	51	C3HN	001070-71-9	3
3	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2
4	Difluoromethane	52	CH2F2	000075-10-5	1
5	2-Chloroethanol	80	C2H5ClO	000107-07-3	1





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Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
28612

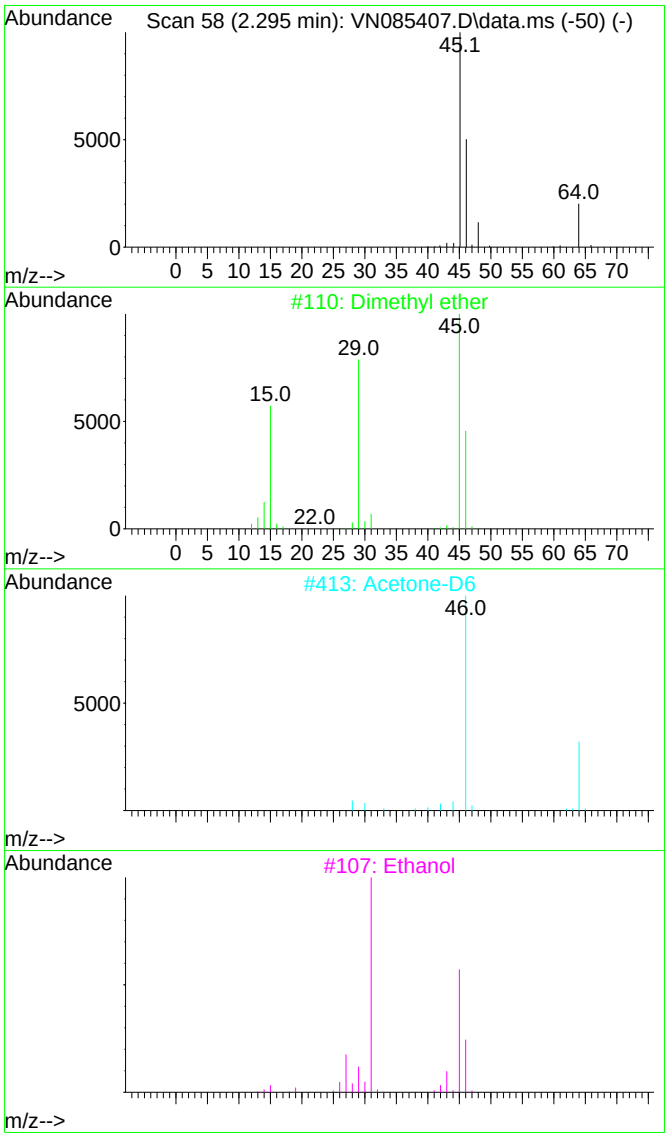
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

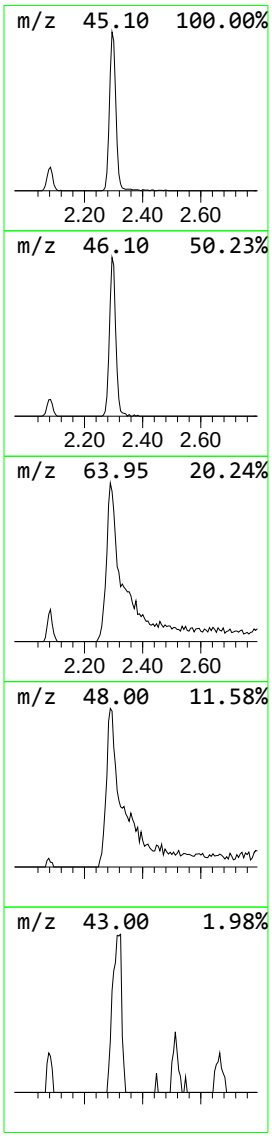
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown2.295 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	14.79 ug/l	178664	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	45
2	Acetone-D6	64	C3D6O	000666-52-4	9
3	Ethanol	46	C2H6O	000064-17-5	9
4	Hydrazine, methyl-	46	CH6N2	000060-34-4	7
5	Formic acid	46	CH2O2	000064-18-6	5





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Operator : JC\MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
28612

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

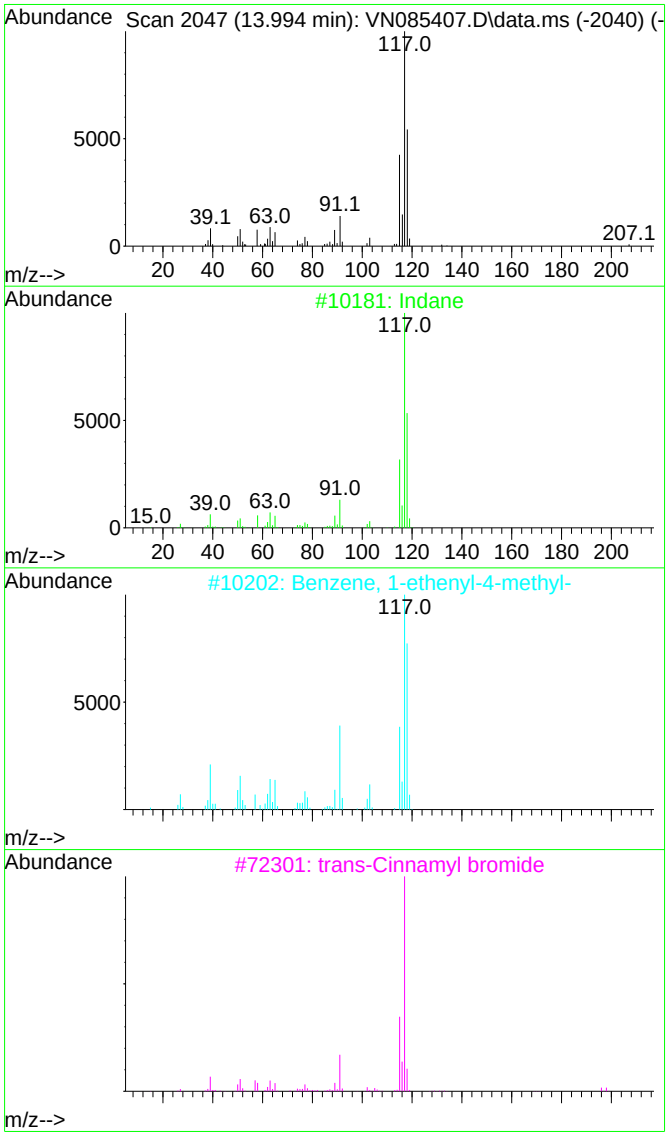
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

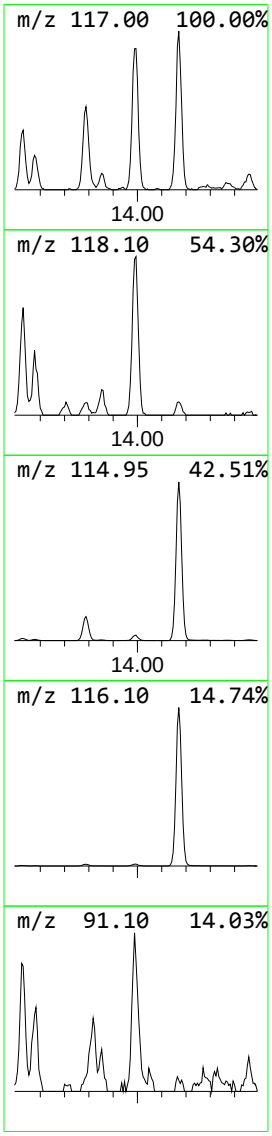
****

Peak Number 3 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	8.21 ug/l	153810	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	62
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	58
5	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	53





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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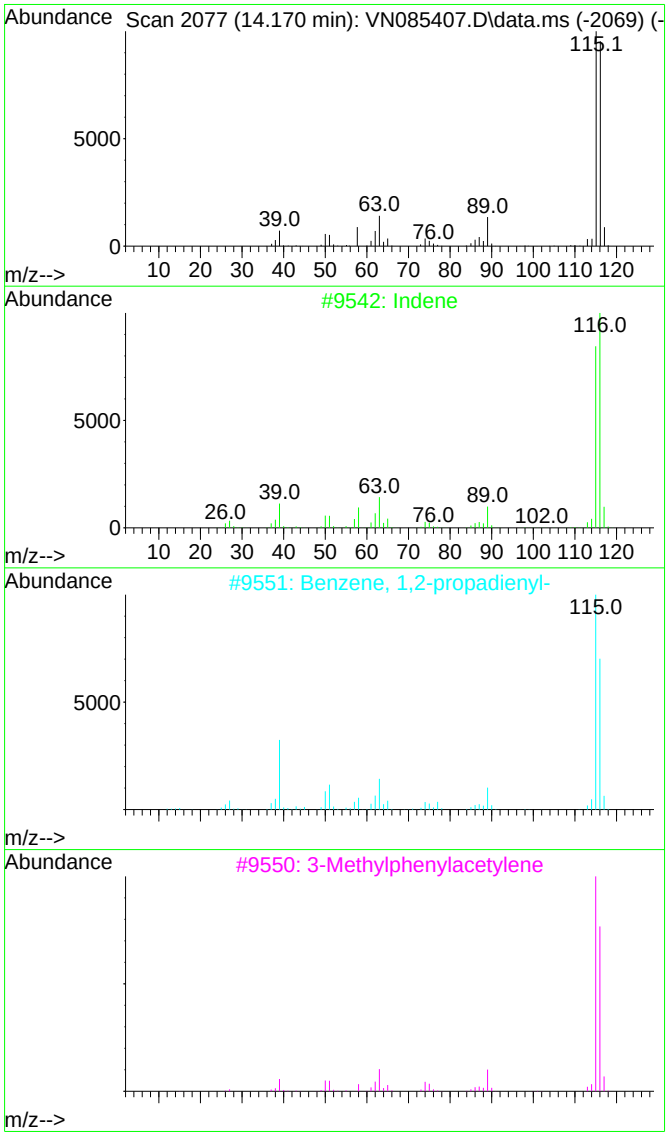
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

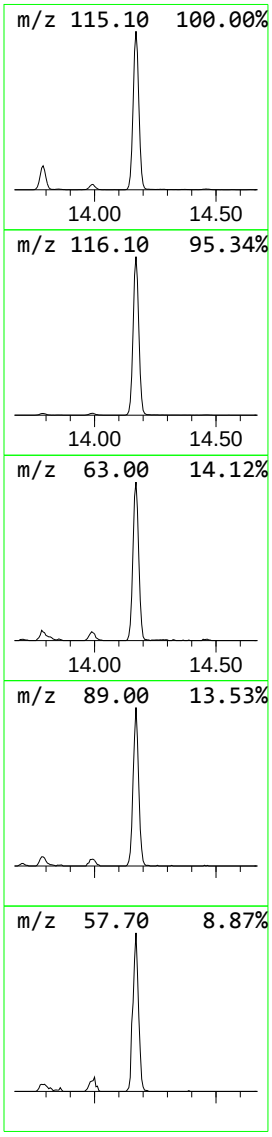
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.170	88.28 ug/l	1653680	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	96
2	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90





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Instrument :
MSVOA_N
ClientSampleId :
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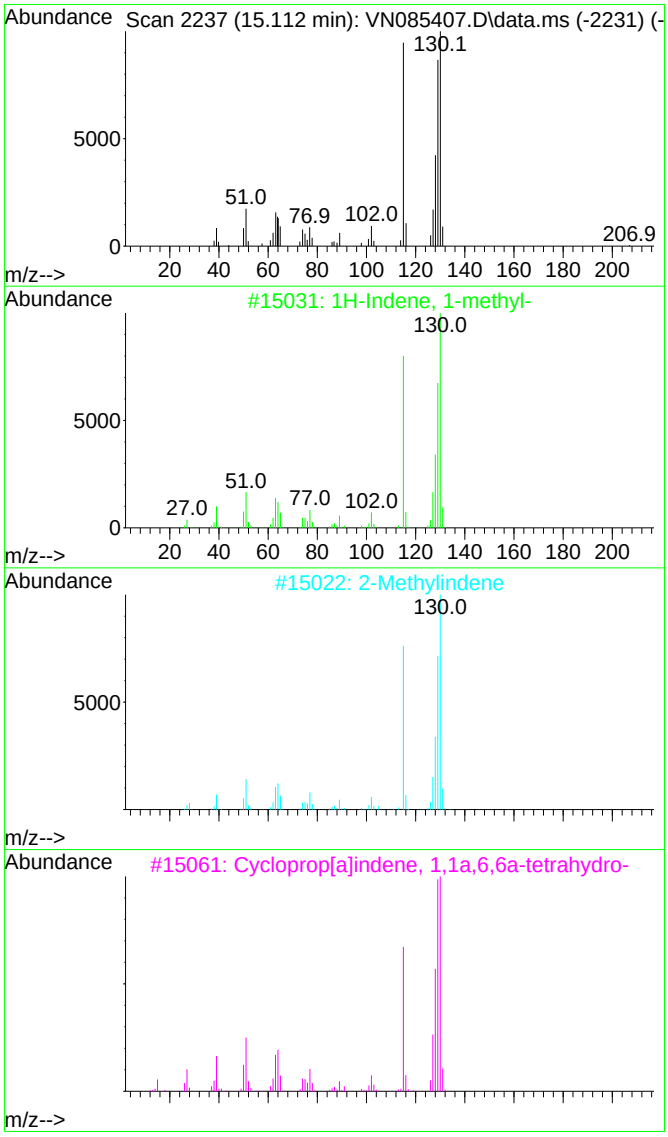
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

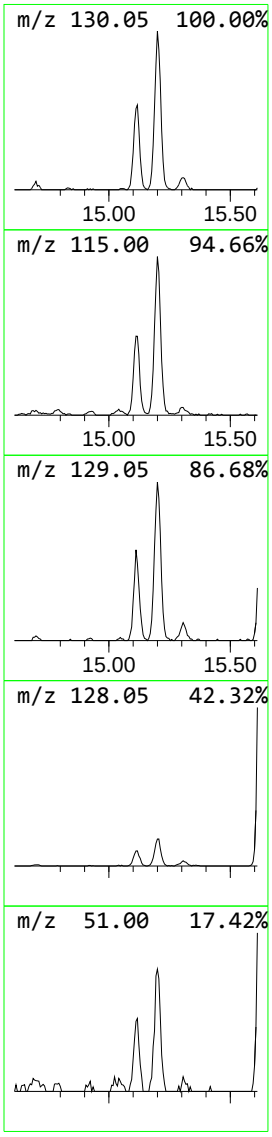
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Indene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.111	6.74 ug/l	126316	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
2	2-Methylindene	130	C10H10	002177-47-1	95
3	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
4	Benzene, 1-butynyl-	130	C10H10	000622-76-4	91
5	Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	91





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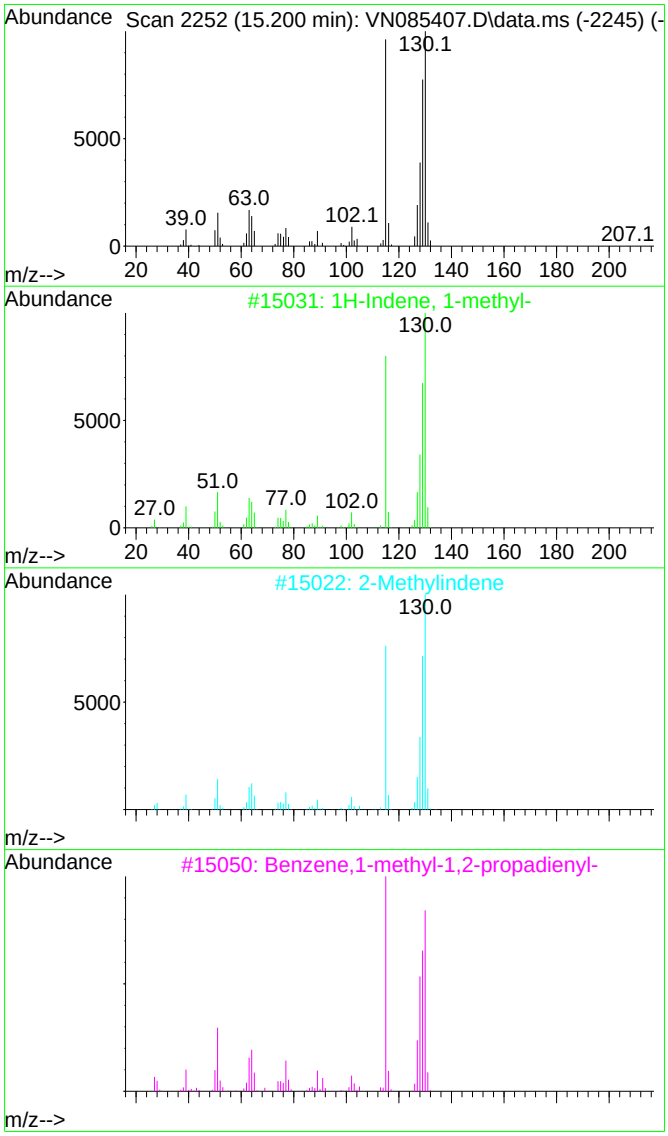
Quant Title : SW846 8260

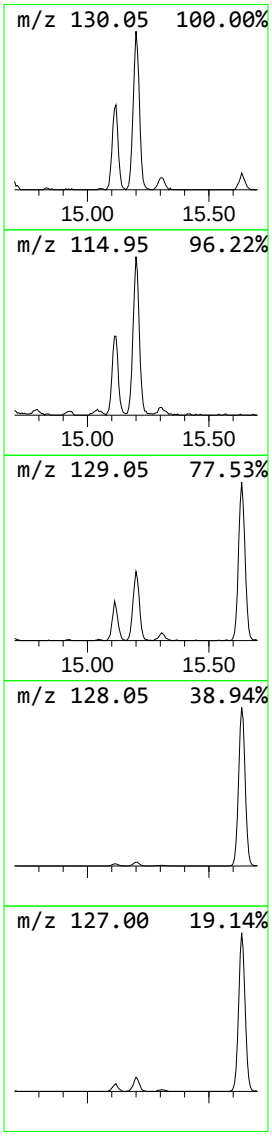
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Methylindene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.200	13.47 ug/l	252354	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2	2-Methylindene	130	C10H10	002177-47-1	96
3	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
4	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95





Tentatively Identified Compound (LSC) summary

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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
Ethane, 1,1-dif...	2.083	10.6	ug/l	127780	1	8.218	603891	50.0
unknown2.295	2.295	14.8	ug/l	178664	1	8.218	603891	50.0
Indane	13.994	8.2	ug/l	153810	4	13.788	936655	50.0
Indene	14.170	88.3	ug/l	1653680	4	13.788	936655	50.0
1H-Indene, 1-me...	15.111	6.7	ug/l	126316	4	13.788	936655	50.0
2-Methylindene	15.200	13.5	ug/l	252354	4	13.788	936655	50.0