LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
Acq On : 13 Jun 2023 14:48
Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

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\82N060623W.M
Title : SW846 8260

Signal : TIC: VN078185.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.489	86	91	99	rBV2	21851	44076	1.87%	0.190%
2	2.842	139	151	156	rBV2	48124	134794	5.71%	0.582%
3	3.259	220	222	232	rVB5	10715	26556	1.12%	0.115%
4	4.436	410	422	446	rBV	358981	1075065	45.54%	4.641%
5	7.447	922	934	940	rBV2	8425	24460	1.04%	0.106%
6	8.177	1047	1058	1062	rBV	305570	756664	32.05%	3.266%
7	8.236	1062	1068	1079	rVB	546733	1233327	52.24%	5.324%
8	8.459	1098	1106	1113	rVB4	19276	46654	1.98%	0.201%
9	8.583	1116	1127	1139	rBV	310797	711632	30.14%	3.072%
10	8.971	1187	1193	1203	rVB3	16971	36456	1.54%	0.157%
11	9.106	1208	1216	1225	rBV	782879	1597731	67.68%	6.897%
12	9.600	1295	1300	1309	rBV3	12084	27186	1.15%	0.117%
13	10.453	1438	1445	1450	rBV3	18496	36720	1.56%	0.159%
14	10.571	1456	1465	1471	rBV	1174325	2191334	92.82%	9.459%
15	10.635	1471	1476	1487	rVB	797187	1445432	61.22%	6.239%
16	11.871	1677	1686	1698	rBV	1027813	1854996	78.57%	8.007%
17	12.076	1713	1721	1731	rBV4	38328	84560	3.58%	0.365%
18	12.400	1763	1776	1783	rBV3	25447	66373	2.81%	0.287%
19	12.494	1783	1792	1795	rVV7	10179	25036	1.06%	0.108%
20	12.853	1846	1853	1864	rVB	696202	1242606	52.63%	5.364%
21	13.035	1879	1884	1889	rBV	16969	29946	1.27%	0.129%
22	13.100	1889	1895	1899	rVV2	47187	92084	3.90%	0.397%
23	13.165	1902	1906	1913	rVB3	84706	168409	7.13%	0.727%
24	13.265	1915	1923	1931	rBV	1528100	2360877	100.00%	10.191%
25	13.341	1932	1936	1940	rVV2	28608	55987	2.37%	0.242%
26	13.400	1942	1946	1953	rVB7	20517	36583	1.55%	0.158%
27	13.506	1955	1964	1972	rBV2	530177	1028757	43.58%	4.441%
28	13.612	1978	1982	1987	rVB7	32957	57020	2.42%	0.246%
29	13.676	1989	1993	1997	rBV7	30309	59287	2.51%	0.256%
30	13.729	1998	2002	2007	rVB6	26178	47433	2.01%	0.205%
31	13.794	2007	2013	2021	rBV	693929	1253506	53.09%	5.411%
32	13.876	2021	2027	2034	rVB3	73284	168196	7.12%	0.726%
33	13.953	2036	2040	2042	rBV5	18292	27073	1.15%	0.117%
34	13.988	2042	2046	2050	rBV3	45062	83190	3.52%	0.359%
35	14.023	2050	2052	2062	rVB4	66476	130840	5.54%	0.565%
36	14.112	2062	2067	2074	rBV2	142771	251746	10.66%	1.087%

LSC Area Percent Report

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Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BUR-1578DL

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\82N060623W.M
Title : SW846 8260

37	14.188	2077	2080	2085	rVB	21428	26613	1.13%	0.115%
38	14.253	2086	2091	2093	rBV3	60418	98151	4.16%	0.424%
39	14.329	2100	2104	2110	rBV2	63395	102135	4.33%	0.441%
40	14.447	2119	2124	2130	rVB5	65650	110755	4.69%	0.478%
41	14.576	2142	2146	2150	rVV7	38527	62694	2.66%	0.271%
42	14.629	2151	2155	2158	rVV6	68762	105941	4.49%	0.457%
43	14.659	2158	2160	2164	rVV4	46752	70897	3.00%	0.306%
44	14.700	2164	2167	2170	rVB	53389	68268	2.89%	0.295%
45	14.735	2170	2173	2175	rBV3	62639	79916	3.39%	0.345%
46	14.770	2175	2179	2188	rVB	183279	334890	14.18%	1.446%
47	14.882	2189	2198	2202	rBV6	120747	223347	9.46%	0.964%
48	14.935	2202	2207	2208	rBV2	67782	88851	3.76%	0.384%
49	14.959	2209	2211	2218	rVB3	123287	203293	8.61%	0.878%
50	15.059	2218	2228	2234	rBV5	140129	427691	18.12%	1.846%
51	15.217	2250	2255	2262	rVB	81353	159152	6.74%	0.687%
52	15.282	2262	2266	2268	rBV4	20947	29266	1.24%	0.126%
53	15.323	2268	2273	2278	rBV5	62801	120937	5.12%	0.522%
54	15.453	2286	2295	2302	rBV8	91190	276781	11.72%	1.195%
55	15.600	2316	2320	2323	rBV6	36056	61778	2.62%	0.267%
56	15.706	2333	2338	2342	rBV3	41273	74529	3.16%	0.322%
57	15.753	2342	2346	2350	rBV6	36880	66194	2.80%	0.286%
58	15.841	2357	2361	2371	rVB9	80062	178902	7.58%	0.772%
59	15.953	2373	2380	2386	rBV4	59170	137830	5.84%	0.595%
60	16.029	2390	2393	2398	rBV7	18444	32058	1.36%	0.138%
61	16.123	2404	2409	2410	rBV3	28192	40136	1.70%	0.173%
62	16.170	2413	2417	2425	rVB3	94728	174646	7.40%	0.754%
63	16.341	2440	2446	2454	rVB4	28512	72833	3.08%	0.314%
64	16.482	2463	2470	2482	rBV	441914	1073238	45.46%	4.633%
65	16.717	2502	2510	2517	rBV4	62333	151988	6.44%	0.656%

Sum of corrected areas: 23166302

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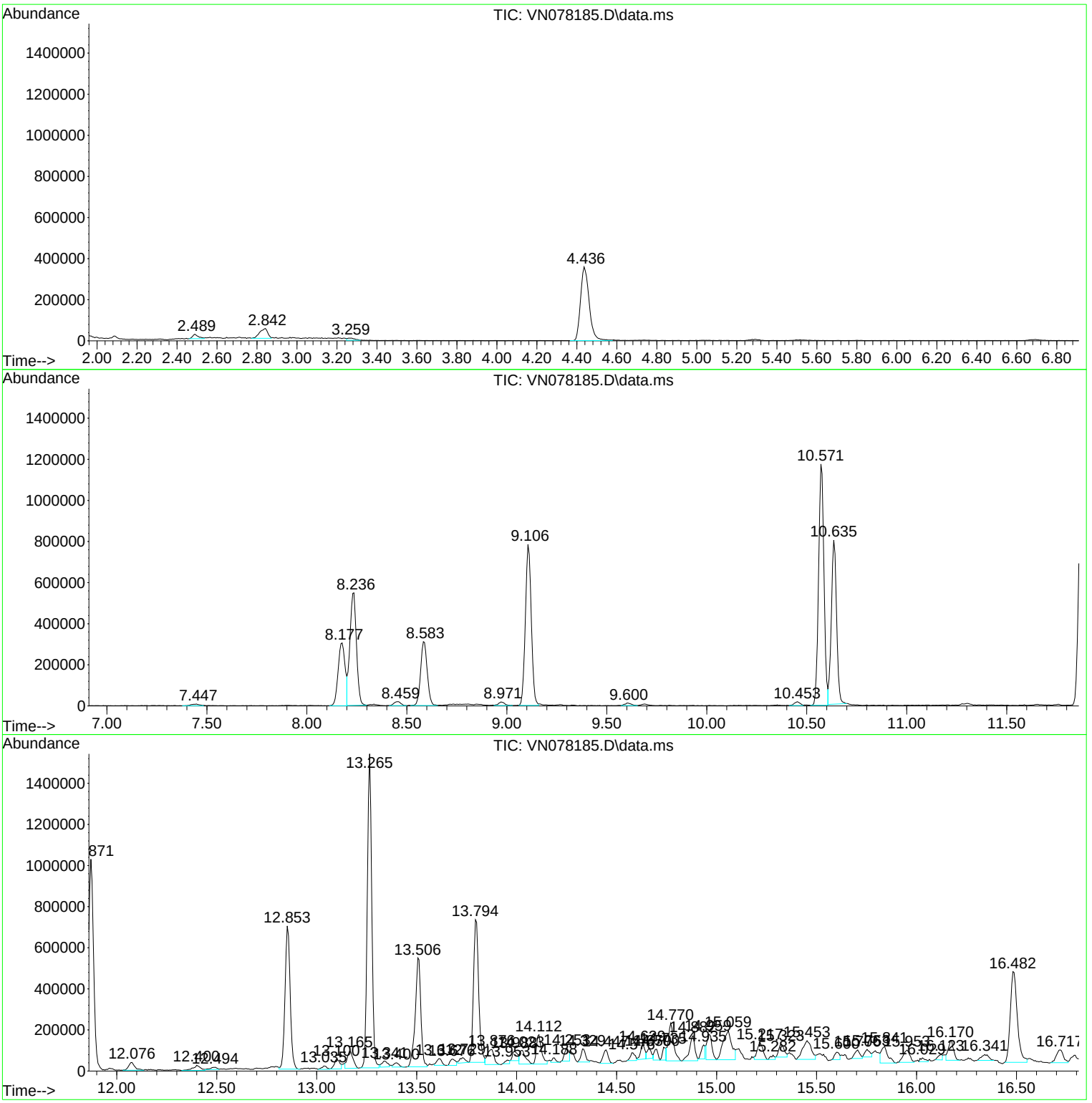
Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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



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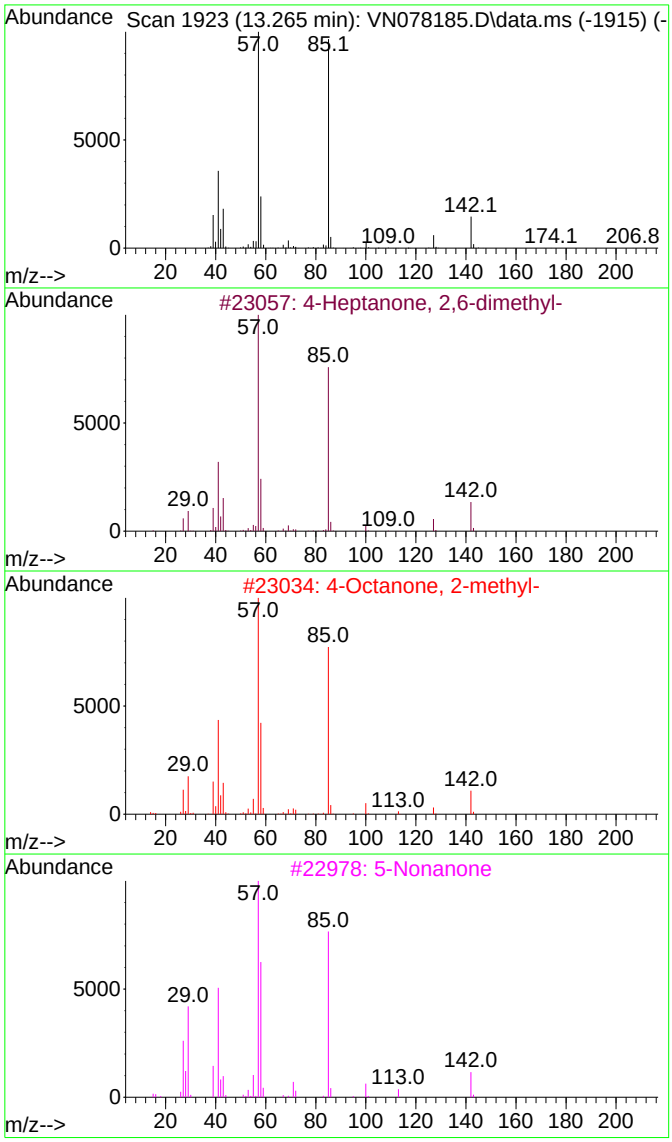
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

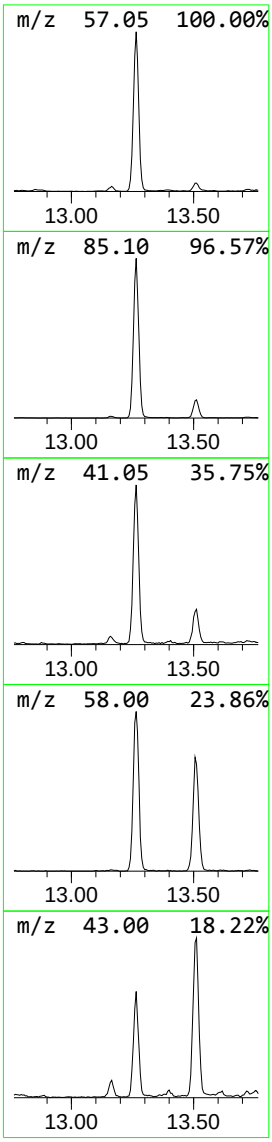
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	94.17 ug/l	2360880	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	72
3	5-Nonanone	142	C9H18O	000502-56-7	59
4	2,4-Heptanedione, 6-methyl-	142	C8H14O2	003002-23-1	53
5	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53





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Data File : VN078185.D
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Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

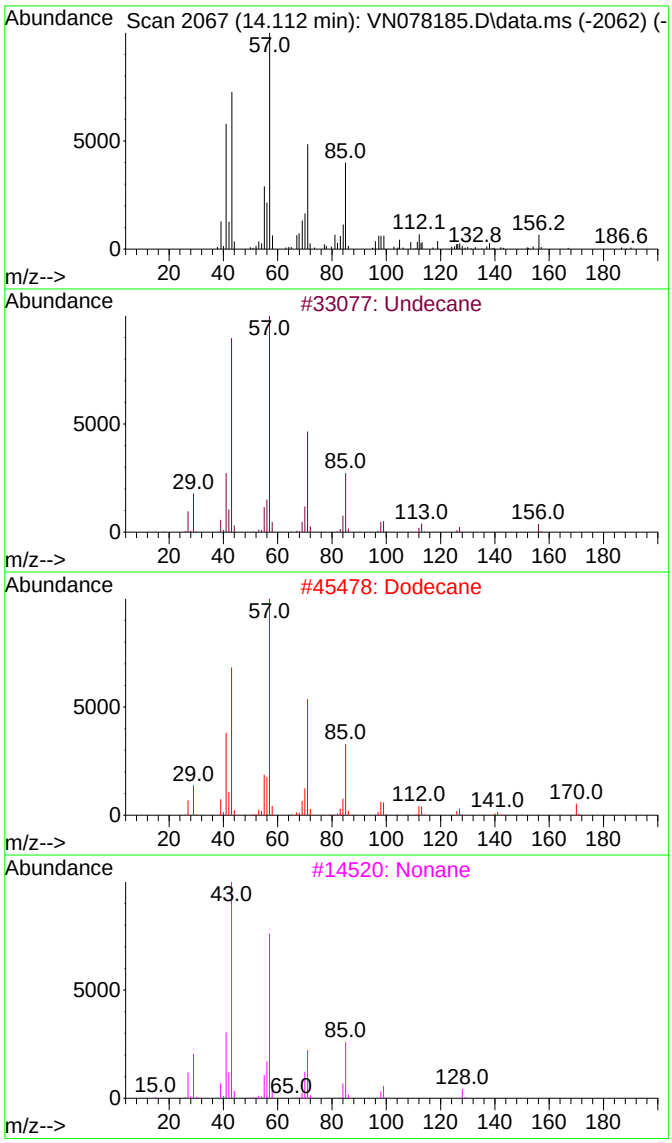
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

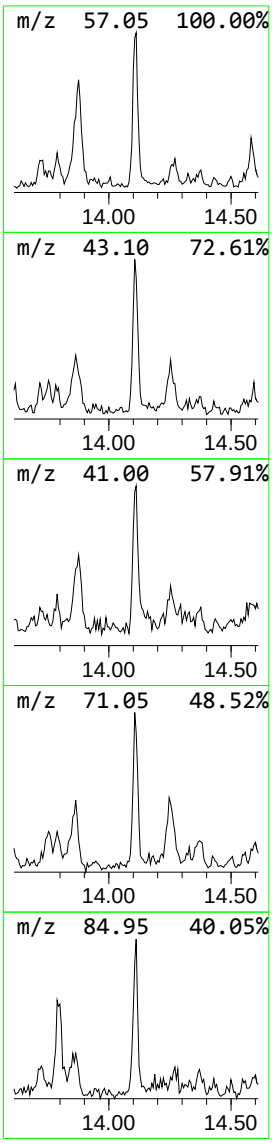
****

Peak Number 2 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.112	10.04 ug/l	251746	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Dodecane	170	C12H26	000112-40-3	86
3	Nonane	128	C9H20	000111-84-2	53
4	Nonadecane	268	C19H40	000629-92-5	53
5	Tetradecane	198	C14H30	000629-59-4	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
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Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

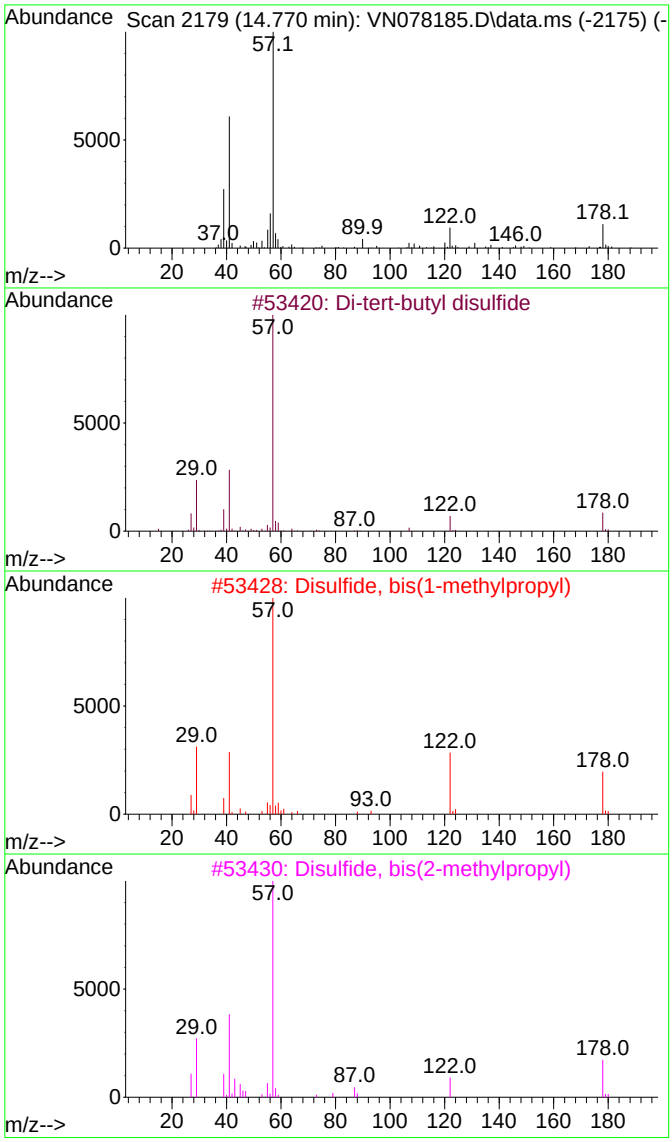
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

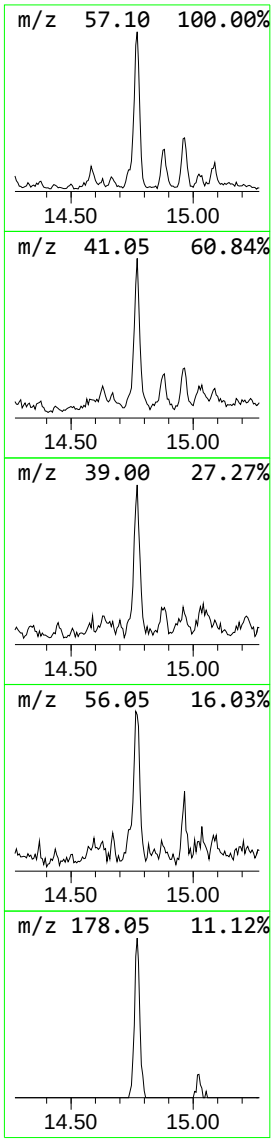
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Di-tert-butyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.770	13.36 ug/l	334890	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	64
2	Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	53
3	Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	50
4	Zinc, bis(1-methylpropyl)-	178	C8H18Zn	007446-94-8	47
5	Di-tert-butyl sulfide	146	C8H18S	000107-47-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

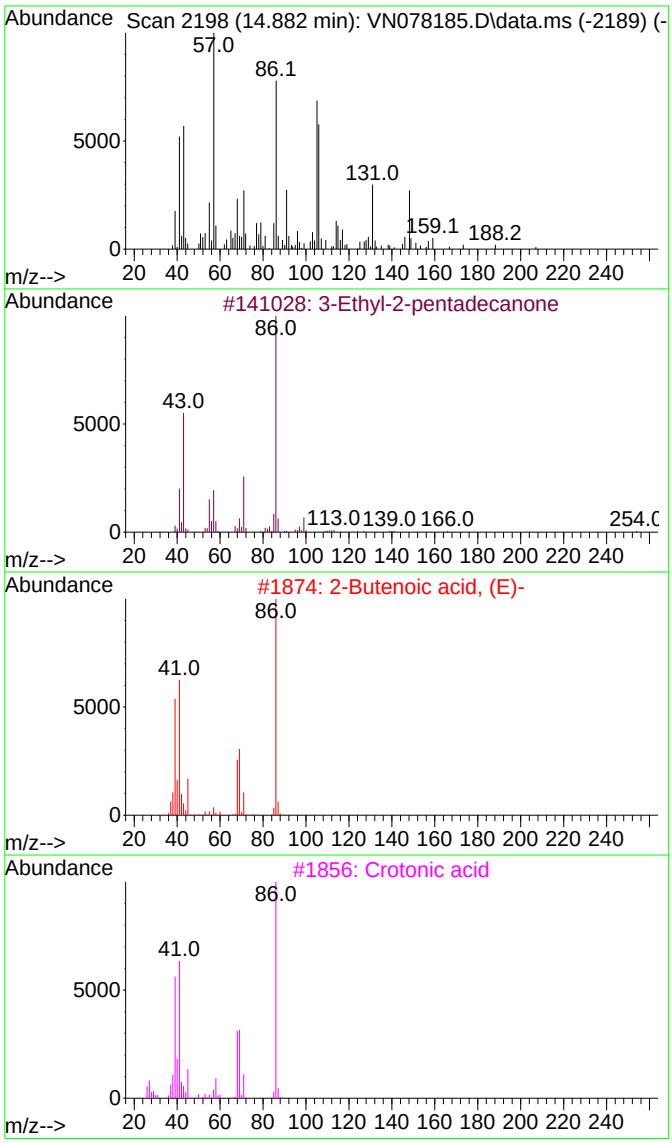
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

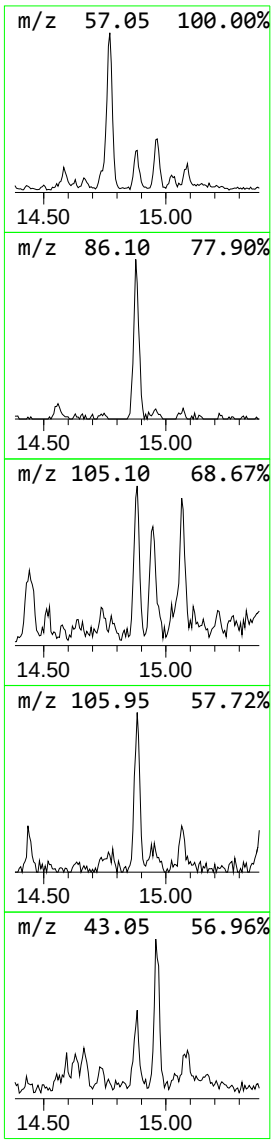
****

Peak Number 4 unknown14.882 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.882	8.91 ug/l	223347	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethyl-2-pentadecanone	254	C17H34O	1000374-11-2	35
2	2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	35
3	Crotonic acid	86	C4H6O2	003724-65-0	27
4	Isobutyramide, N-(2-butyl)-N-pro...	185	C11H23NO	1000458-83-3	27
5	.alpha.((1,1-Dimethylethyl)amino...	193	C12H19NO	018366-40-0	22





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

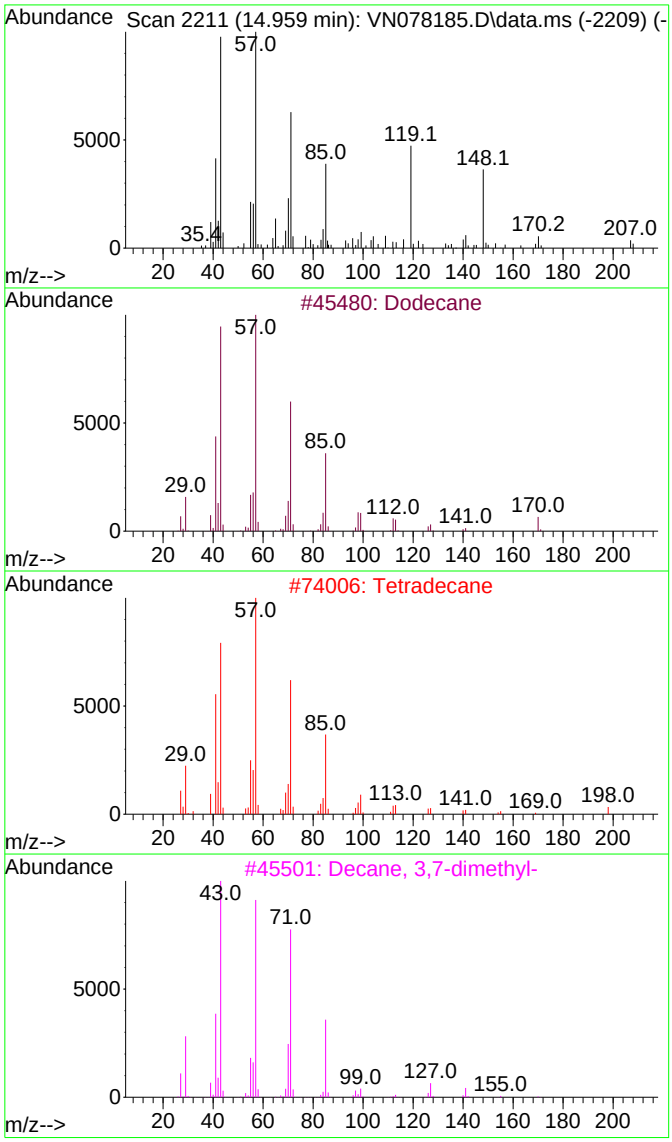
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

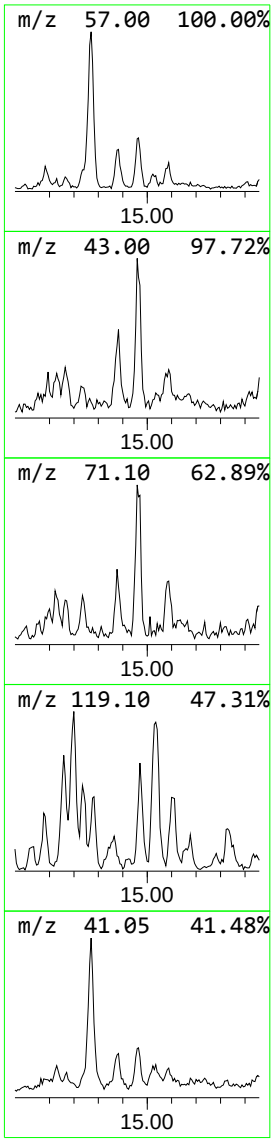
****

Peak Number 5 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	8.11 ug/l	203293	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	52
2	Tetradecane	198	C14H30	000629-59-4	49
3	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	47
4	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	43
5	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	43





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MSVOA_N
ClientSampleId :
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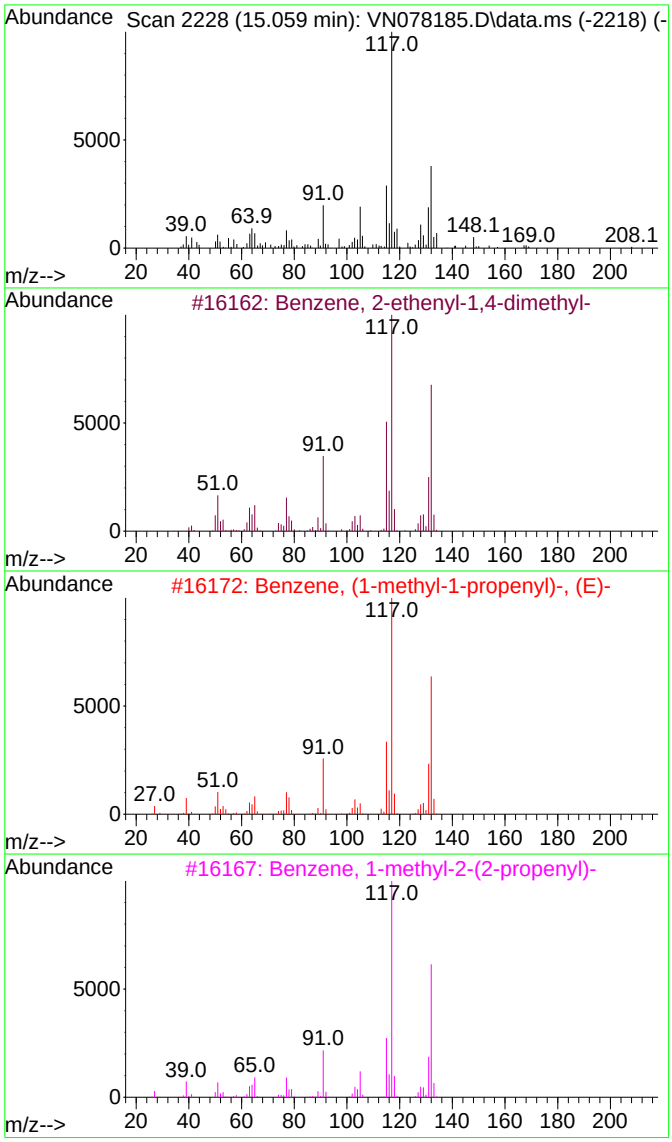
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

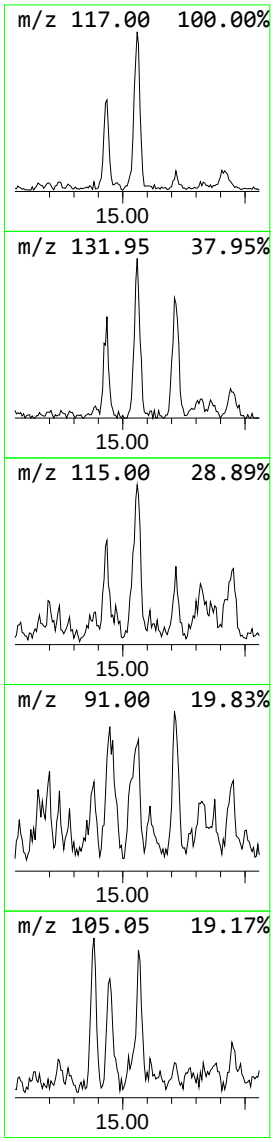
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	17.06 ug/l	427691	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
4	Indan, 1-methyl-	132	C10H12	000767-58-8	76
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
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ClientSampleId :
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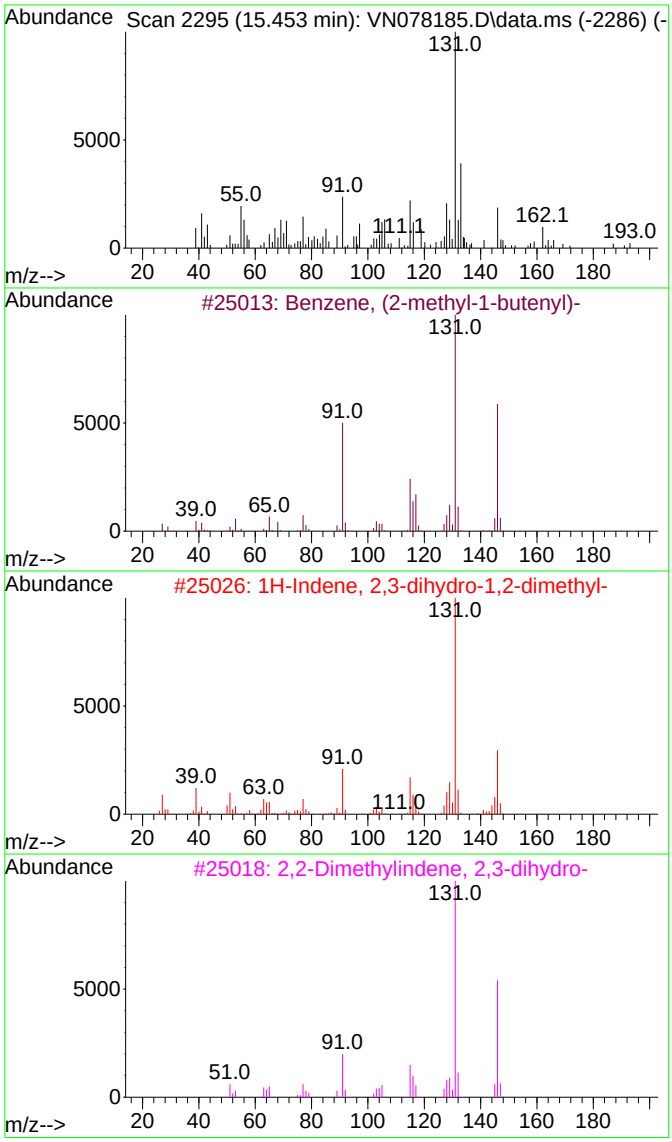
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

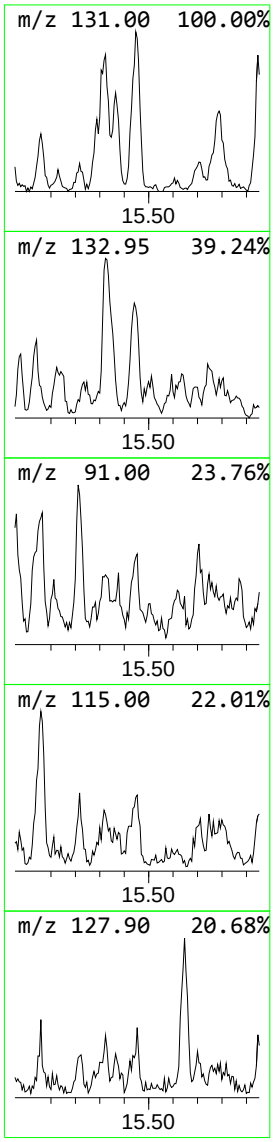
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-butenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.453	11.04 ug/l	276781	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	64
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	64
3	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	64
4	2-Butene, 3-chloro-1-phenyl-, (Z)-	166	C10H11Cl	016608-68-7	60
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
Acq On : 13 Jun 2023 14:48
Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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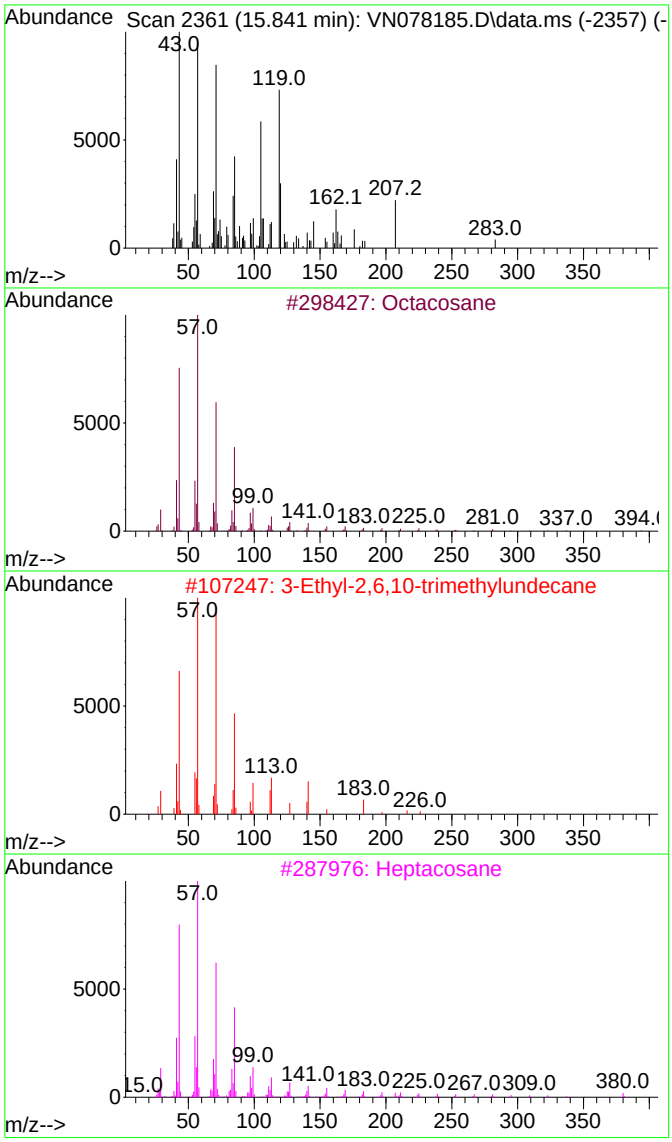
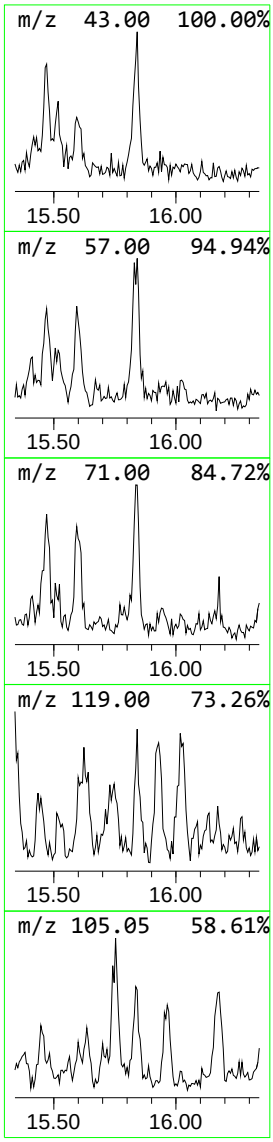
Peak Number 8 unknown15.841 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	7.14 ug/l	178902	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	38
2	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	38
3	Heptacosane	380	C27H56	000593-49-7	38
4	Hexadecane	226	C16H34	000544-76-3	35
5	Tetracosane	338	C24H50	000646-31-1	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
Acq On : 13 Jun 2023 14:48
Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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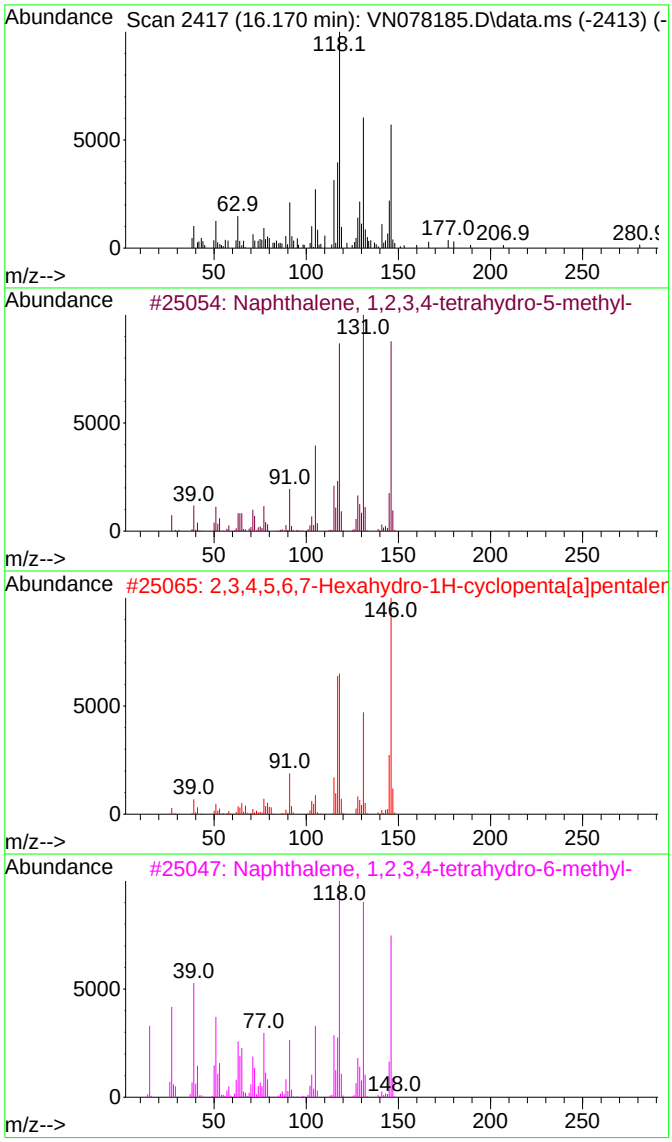
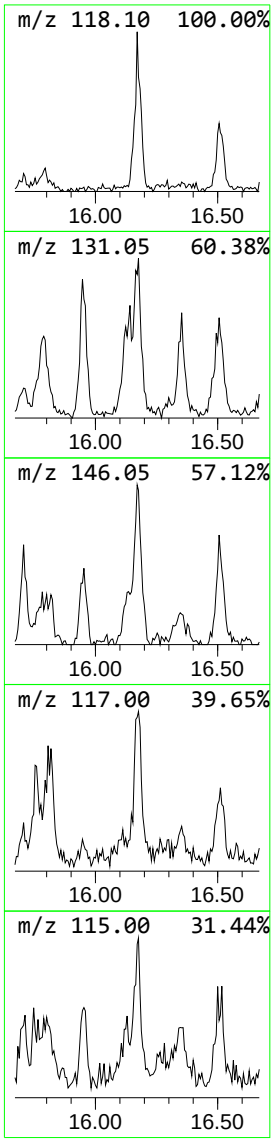
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	6.97 ug/l	174646	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
2	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	62
4	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	52
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
Acq On : 13 Jun 2023 14:48
Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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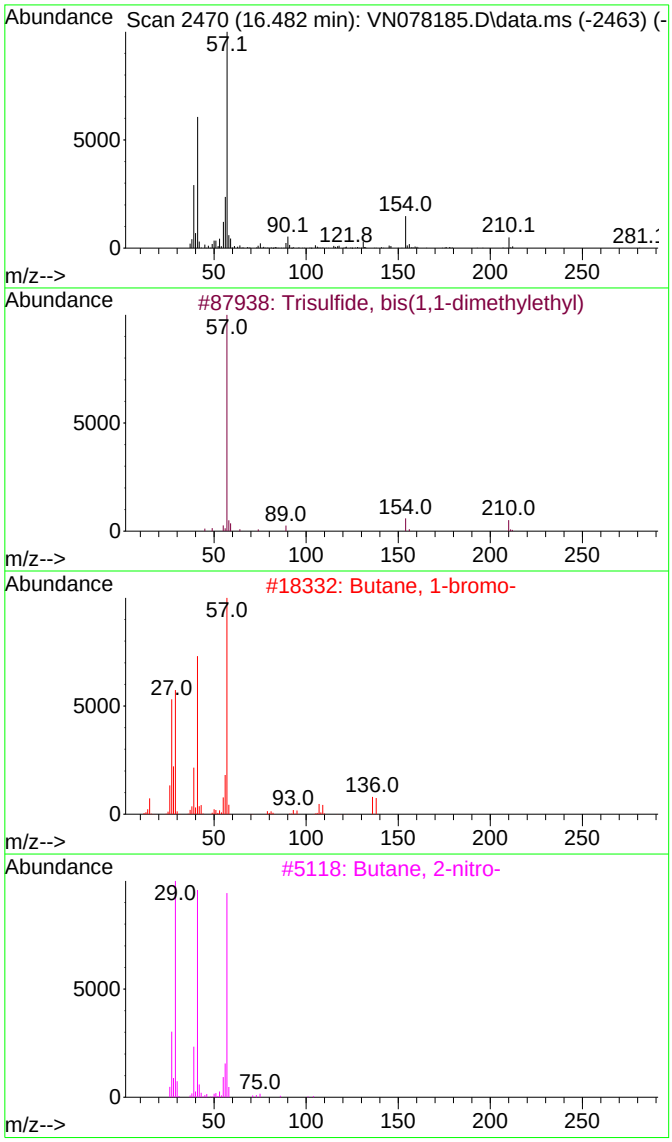
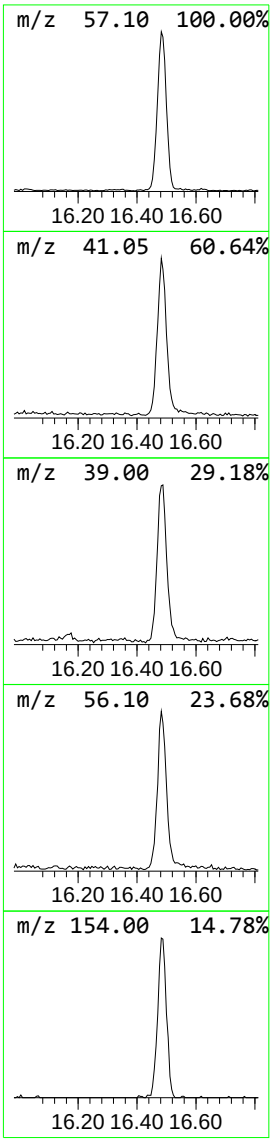
Peak Number 10 unknown16.482 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	42.81 ug/l	1073240	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	46
2	Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
3	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	32
4	Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	23
5	1-[(chloromethyl)sulfonyl]butane	170	C5H11ClO2S	1000404-59-5	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078185.D
Acq On : 13 Jun 2023 14:48
Operator : JC\MD
Sample : 03172-01 20X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.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
4-Heptanone, 2,...	13.265	94.2	ug/l	2360880	4	13.794	1253510	50.0
Undecane	14.112	10.0	ug/l	251746	4	13.794	1253510	50.0
Di-tert-butyl d...	14.770	13.4	ug/l	334890	4	13.794	1253510	50.0
unknown14.882	14.882	8.9	ug/l	223347	4	13.794	1253510	50.0
Dodecane	14.959	8.1	ug/l	203293	4	13.794	1253510	50.0
Benzene, 2-ethe...	15.059	17.1	ug/l	427691	4	13.794	1253510	50.0
Benzene, (2-met...	15.453	11.0	ug/l	276781	4	13.794	1253510	50.0
unknown15.841	15.841	7.1	ug/l	178902	4	13.794	1253510	50.0
Naphthalene, 1,...	16.170	7.0	ug/l	174646	4	13.794	1253510	50.0
unknown16.482	16.482	42.8	ug/l	1073240	4	13.794	1253510	50.0