LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086878.D
Acq On : 06 Jun 2025 19:51
Operator : JC\MD
Sample : Q2216-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3864

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\82N060625W.M
Title : SW846 8260

Signal : TIC: VN086878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.112	21	27	35	rBV	63543	99680	7.17%	0.849%
2	2.524	89	97	109	rBV	72397	143089	10.30%	1.219%
3	2.706	123	128	136	rVB	27457	54997	3.96%	0.468%
4	4.312	391	401	409	rBV	8623	24533	1.77%	0.209%
5	4.447	412	424	439	rBV	73878	232840	16.76%	1.983%
6	5.536	596	609	629	rBV	112011	408976	29.43%	3.483%
7	5.747	636	645	653	rBV	8081	25155	1.81%	0.214%
8	7.241	889	899	909	rBV4	19624	56597	4.07%	0.482%
9	7.494	934	942	953	rBV	22543	60054	4.32%	0.511%
10	8.177	1047	1058	1062	rBV	166349	395873	28.49%	3.371%
11	8.235	1062	1068	1081	rVB	334139	792750	57.05%	6.751%
12	8.588	1118	1128	1137	rBV	190025	433838	31.22%	3.695%
13	8.818	1160	1167	1177	rVB3	15391	35244	2.54%	0.300%
14	8.977	1186	1194	1201	rBV3	17355	41550	2.99%	0.354%
15	9.106	1207	1216	1225	rBV	487307	1000073	71.96%	8.517%
16	9.465	1272	1277	1284	rVV6	6316	19082	1.37%	0.163%
17	9.535	1284	1289	1295	rVV2	13568	28639	2.06%	0.244%
18	9.659	1304	1310	1322	rVB3	26958	60669	4.37%	0.517%
19	9.912	1347	1353	1364	rVB	72665	151991	10.94%	1.294%
20	10.453	1440	1445	1452	rBV3	10298	24238	1.74%	0.206%
21	10.571	1456	1465	1472	rVV	740612	1389674	100.00%	11.835%
22	10.635	1472	1476	1487	rVV2	22850	56598	4.07%	0.482%
23	10.735	1488	1493	1502	rVB4	9075	22785	1.64%	0.194%
24	10.865	1507	1515	1523	rBV5	17158	49355	3.55%	0.420%
25	11.065	1542	1549	1565	rBV3	13173	36887	2.65%	0.314%
26	11.312	1585	1591	1600	rBV5	12559	28225	2.03%	0.240%
27	11.865	1676	1685	1696	rBV	622241	1116827	80.37%	9.511%
28	11.965	1697	1702	1709	rBV4	8264	20797	1.50%	0.177%
29	12.070	1713	1720	1724	rBV2	22309	42557	3.06%	0.362%
30	12.400	1772	1776	1781	rVB2	14548	25149	1.81%	0.214%
31	12.588	1802	1808	1812	rBV7	7754	17240	1.24%	0.147%
32	12.847	1845	1852	1862	rVB	457515	809974	58.29%	6.898%
33	13.094	1890	1894	1898	rBV4	10885	18385	1.32%	0.157%
34	13.170	1902	1907	1916	rVB5	47298	113551	8.17%	0.967%
35	13.312	1926	1931	1940	rBV10	10047	32190	2.32%	0.274%
36	13.482	1955	1960	1965	rVB	24634	40548	2.92%	0.345%

LSC Area Percent Report

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Sample : Q2216-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3864

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\82N060625W.M
Title : SW846 8260

37	13.788	2006	2012	2021	rBV	601159	1055593	75.96%	8.990%
38	14.117	2061	2068	2080	rBV9	50472	158438	11.40%	1.349%
39	14.435	2118	2122	2126	rBV4	16727	30942	2.23%	0.264%
40	14.506	2130	2134	2140	rVB6	18463	34439	2.48%	0.293%
41	14.570	2142	2145	2150	rBV6	18591	32097	2.31%	0.273%
42	14.623	2150	2154	2158	rBV2	58378	99434	7.16%	0.847%
43	14.764	2168	2178	2187	rBV9	72793	298021	21.45%	2.538%
44	14.847	2188	2192	2202	rVB9	35793	89483	6.44%	0.762%
45	14.959	2207	2211	2218	rBV4	34725	78763	5.67%	0.671%
46	15.035	2221	2224	2228	rBV5	26117	49436	3.56%	0.421%
47	15.217	2251	2255	2259	rBV4	46194	84392	6.07%	0.719%
48	15.264	2260	2263	2267	rVB4	52338	71773	5.16%	0.611%
49	15.323	2268	2273	2279	rVB5	48782	104326	7.51%	0.888%
50	15.588	2315	2318	2320	rBV3	36383	50994	3.67%	0.434%
51	15.641	2321	2327	2334	rVV	399811	789911	56.84%	6.727%
52	15.941	2370	2378	2379	rBV5	68340	157064	11.30%	1.338%
53	16.170	2413	2417	2423	rBV5	68014	138265	9.95%	1.178%
54	16.782	2515	2521	2522	rBV	308914	508254	36.57%	4.328%

Sum of corrected areas: 11742235

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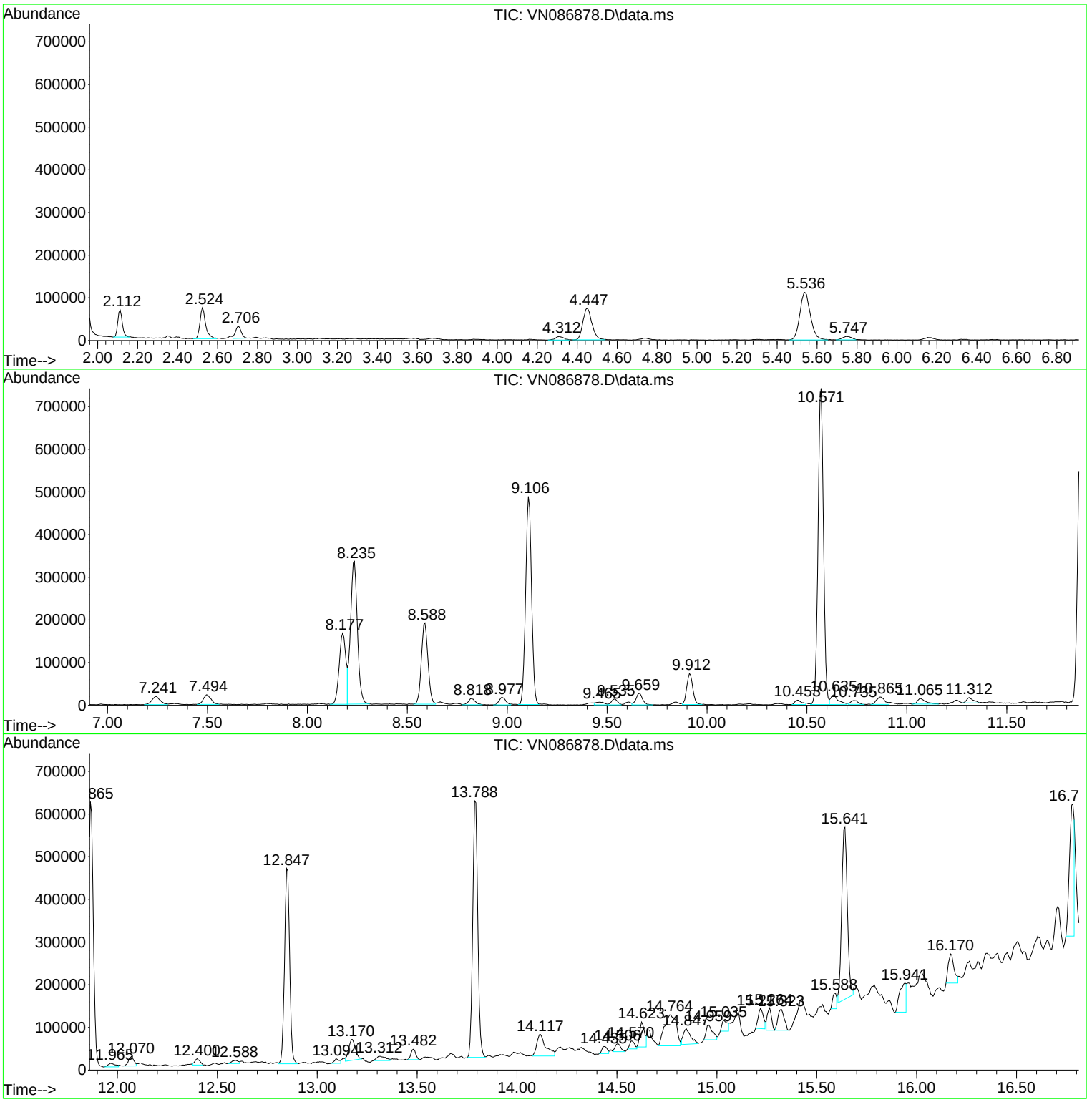
MSVOA_N
ClientSampleId :
3864

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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Data File : VN086878.D
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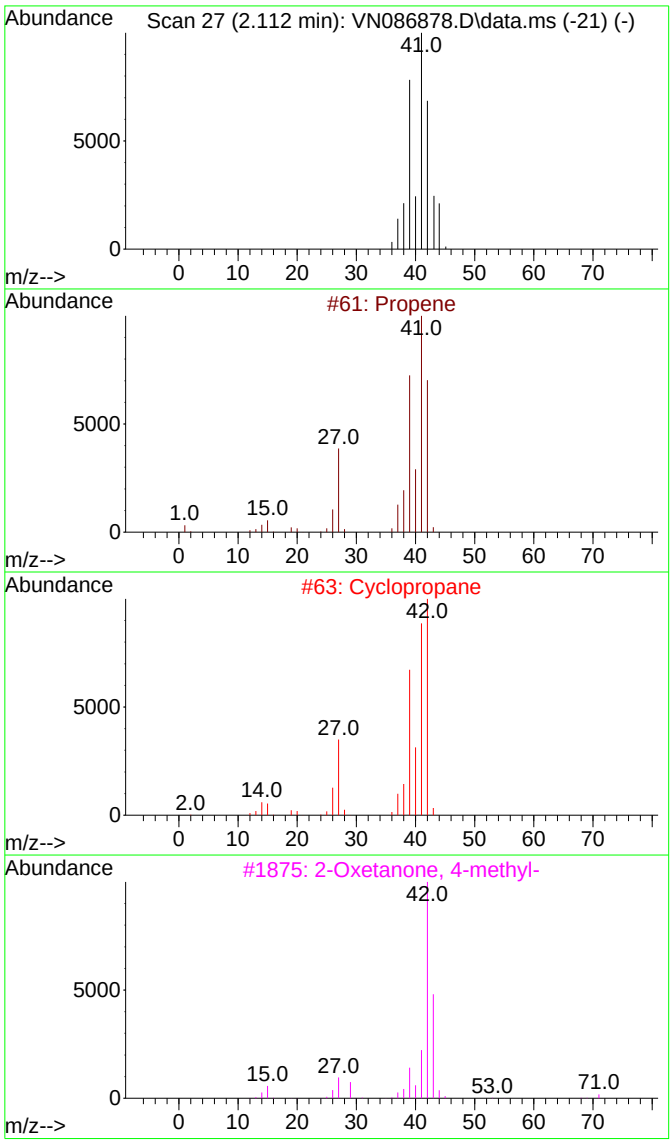
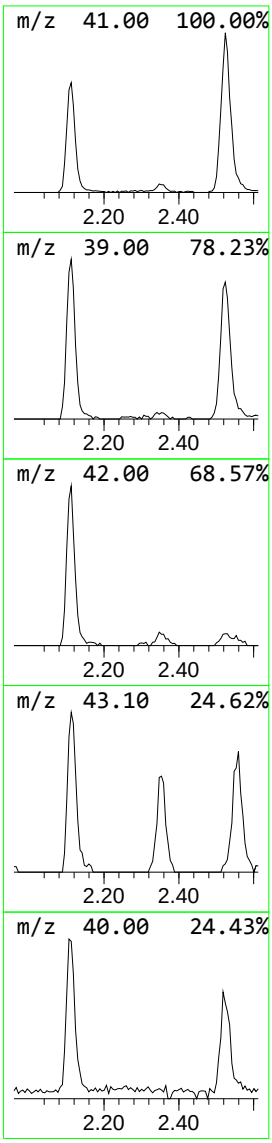
****

Peak Number 1 Propene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.112	6.29 ug/l	99680	Pentafluorobenzene	8.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Cyclopropane	42	C3H6	000075-19-4	64
3	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
4	Cyclopropene	40	C3H4	002781-85-3	9
5	4-Amino-1-butanol	89	C4H11NO	013325-10-5	1





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Data File : VN086878.D
Acq On : 06 Jun 2025 19:51
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3864

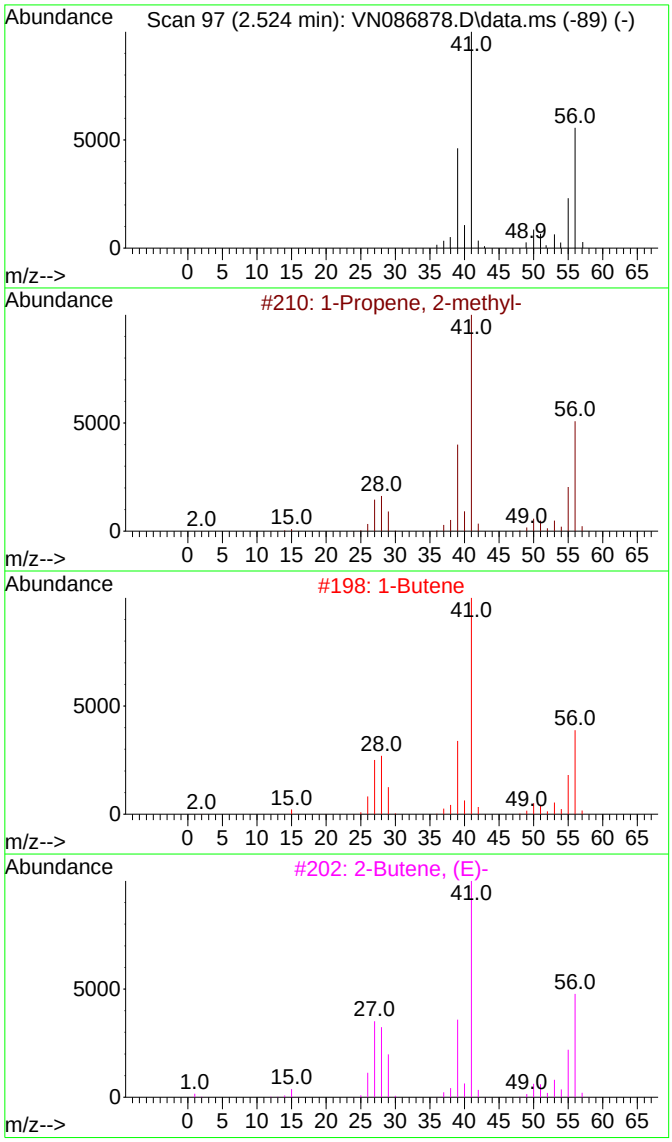
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

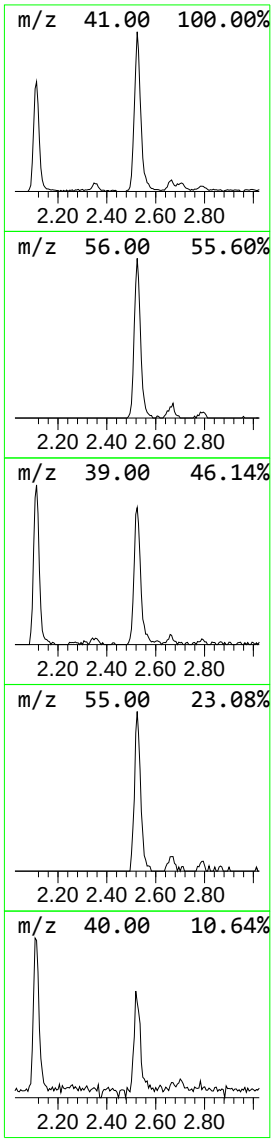
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.524	9.02 ug/l	143089	Pentafluorobenzene	8.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2	1-Butene	56	C4H8	000106-98-9	87
3	2-Butene, (E)-	56	C4H8	000624-64-6	80
4	2-Butene, (Z)-	56	C4H8	000590-18-1	80
5	2-Butene	56	C4H8	000107-01-7	72





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3864

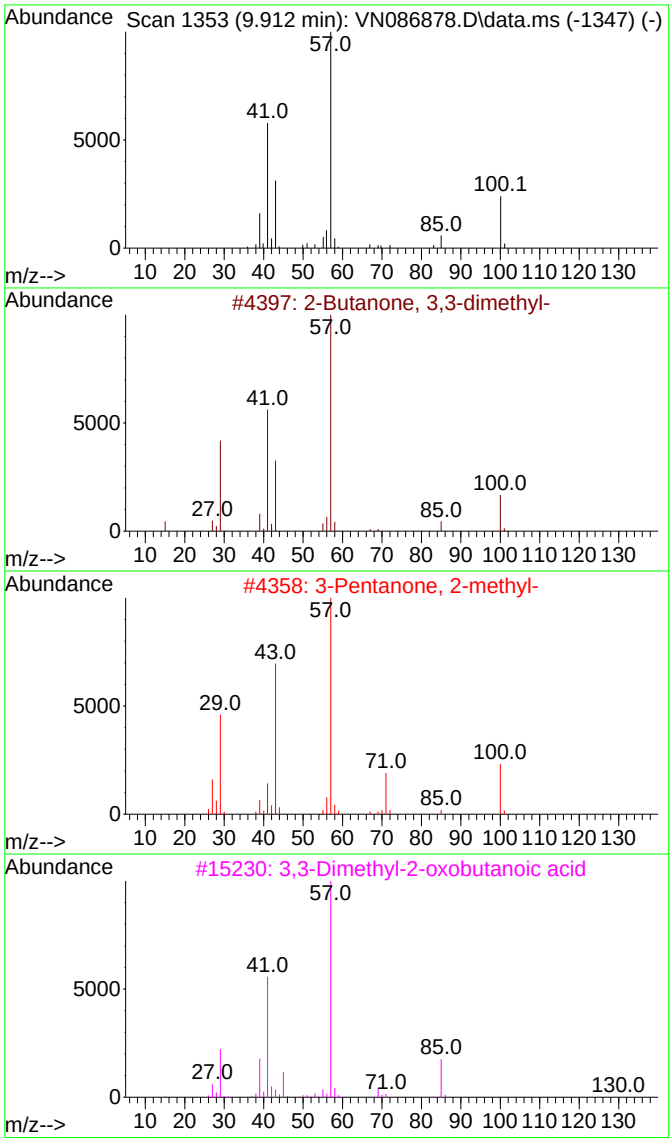
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

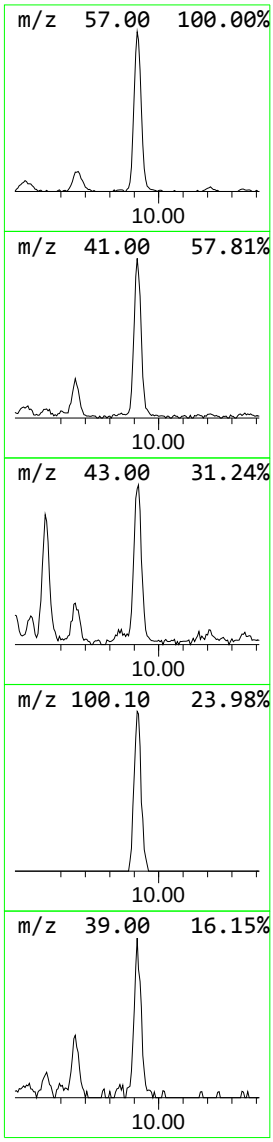
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.912	7.60 ug/l	151991	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
3	3,3-Dimethyl-2-oxobutanoic acid	130	C6H10O3	000815-17-8	40
4	cis-1-Ethoxy-1-butene	100	C6H12O	1000139-43-8	40
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38





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Operator : JC\MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3864

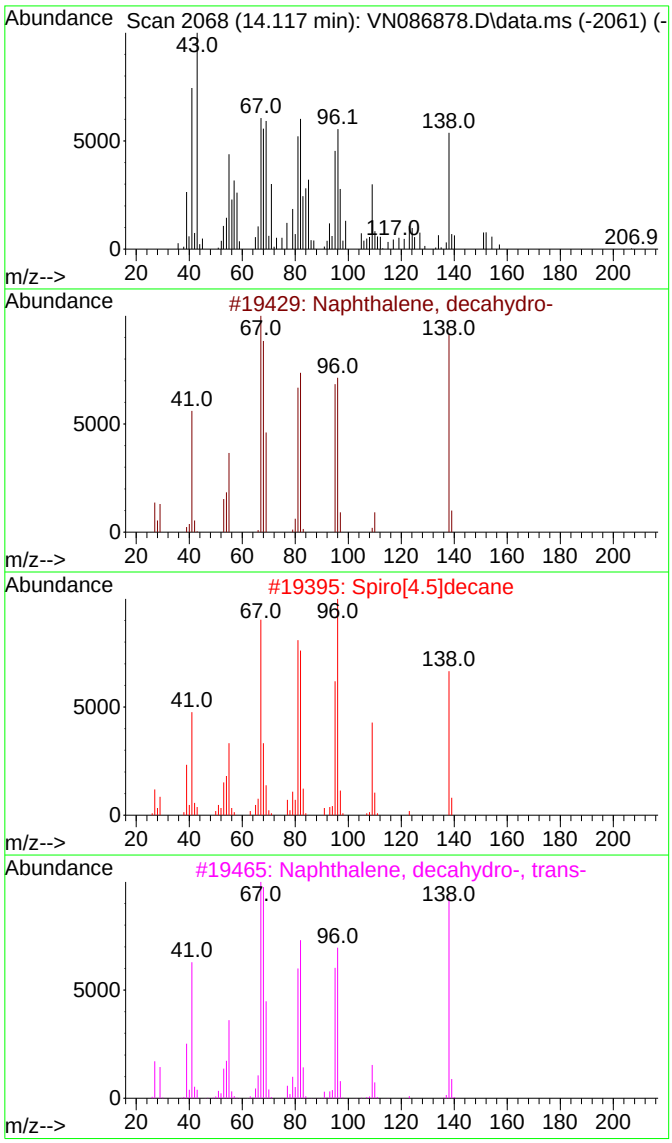
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

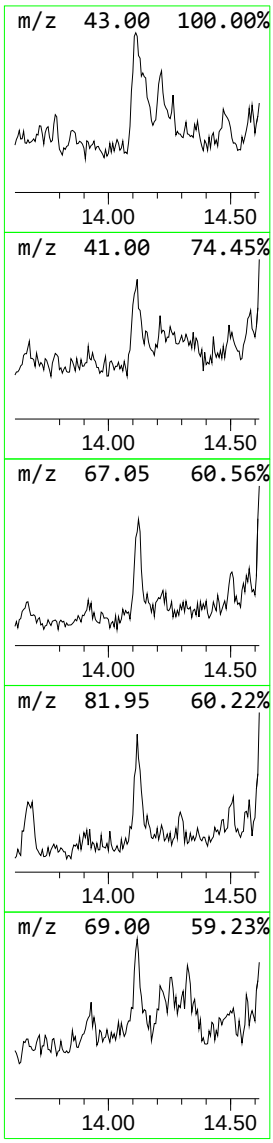
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, decahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.117	7.50 ug/l	158438	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2	Spiro[4.5]decane	138	C10H18	000176-63-6	93
3	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
4	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	64
5	1,1'-Bicyclopentyl	138	C10H18	001636-39-1	64





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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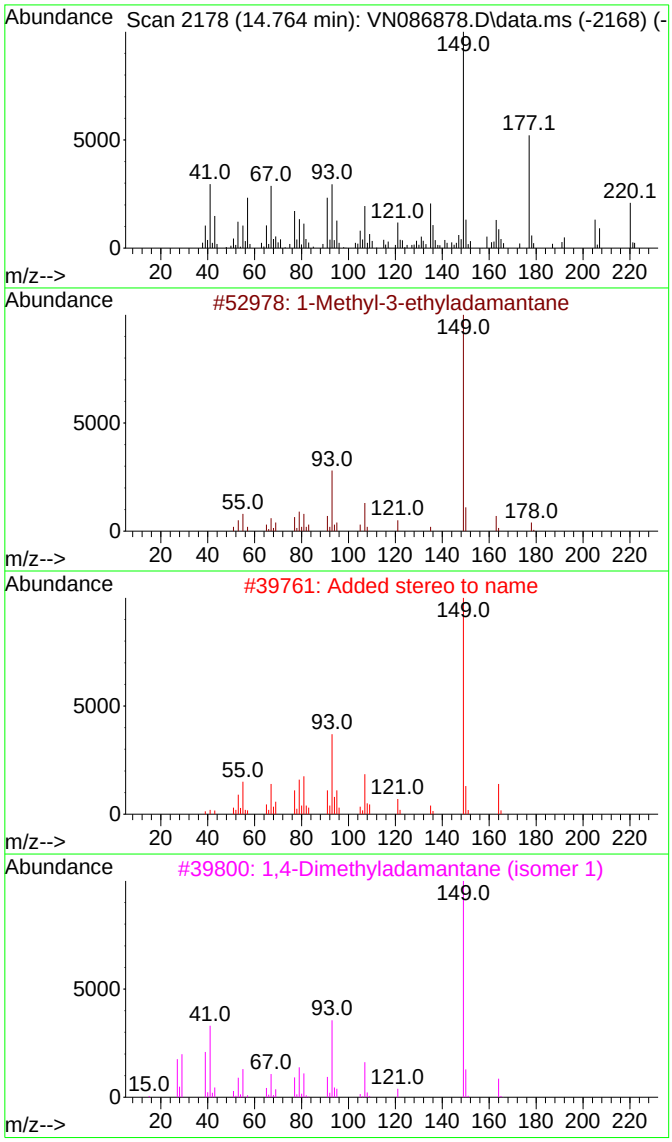
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

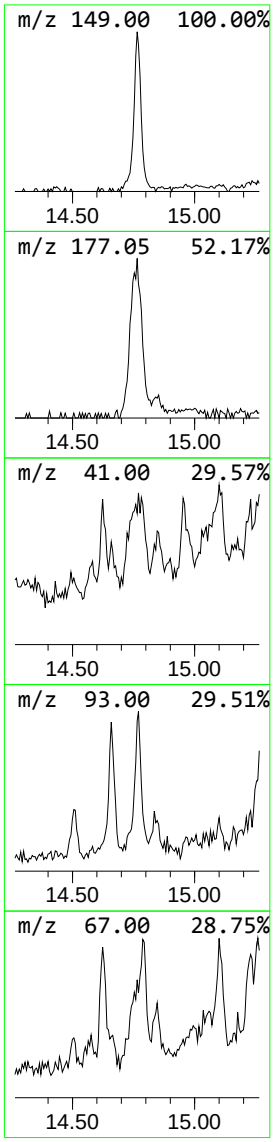
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Methyl-3-ethyladamantane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.764	14.12 ug/l	298021	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	55
2	Added stereo to name	164	C12H20	024145-89-9	50
3	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	46
4	Diethyl Phthalate	222	C12H14O4	000084-66-2	46
5	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	46





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

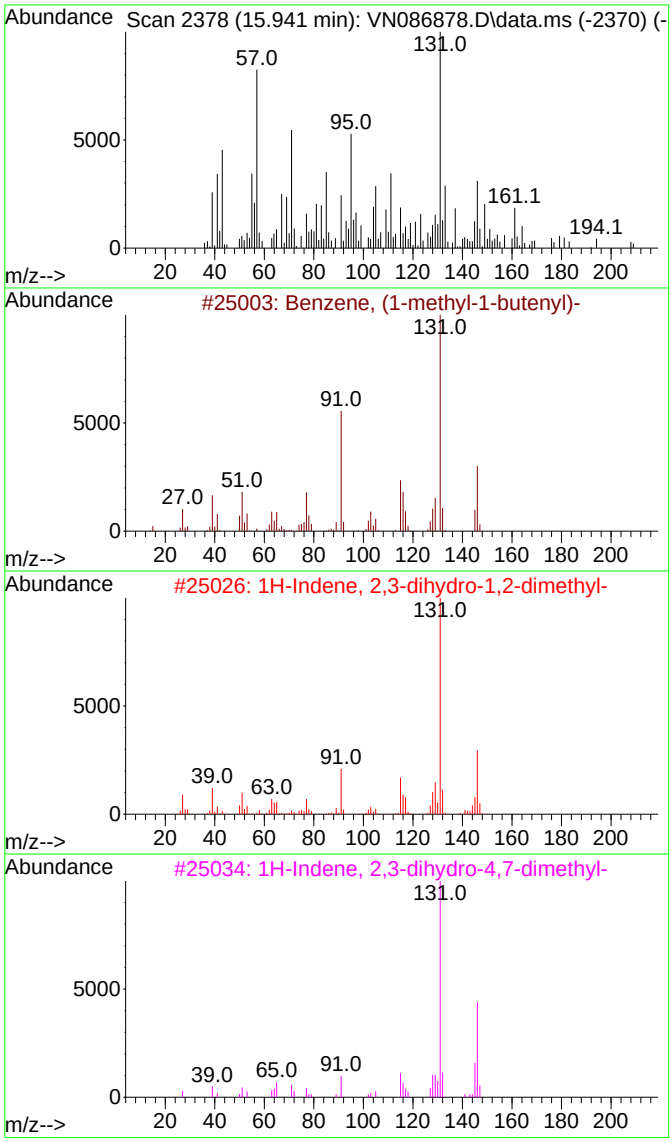
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

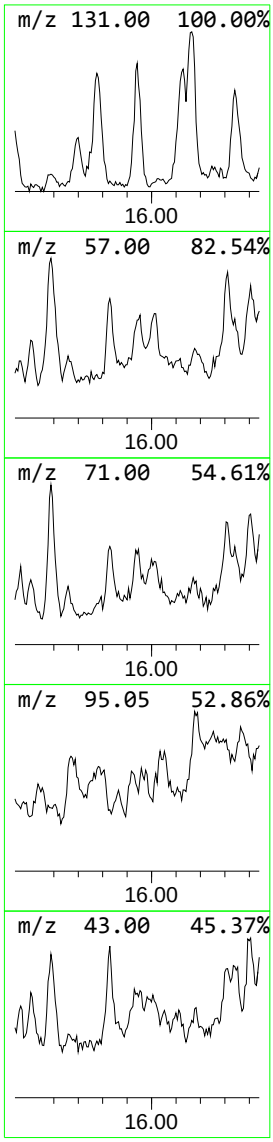
****

Peak Number 6 unknown15.491 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.941	7.44 ug/l	157064	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	49
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	49
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	38
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	38
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	38





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MSVOA_N
ClientSampleId :
3864

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

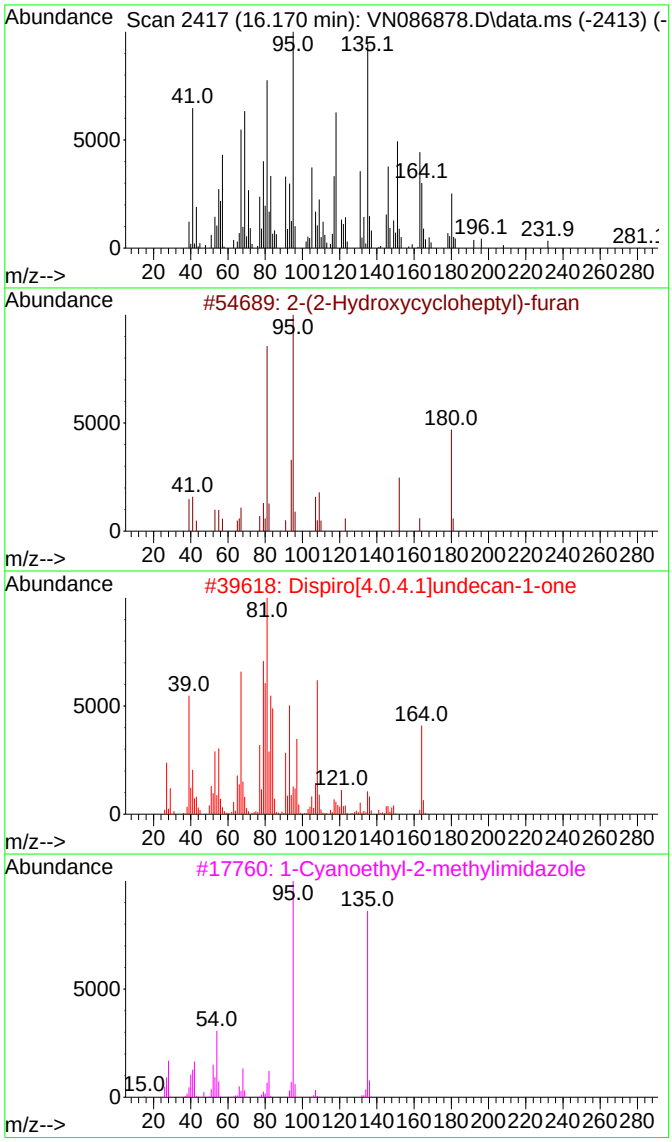
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

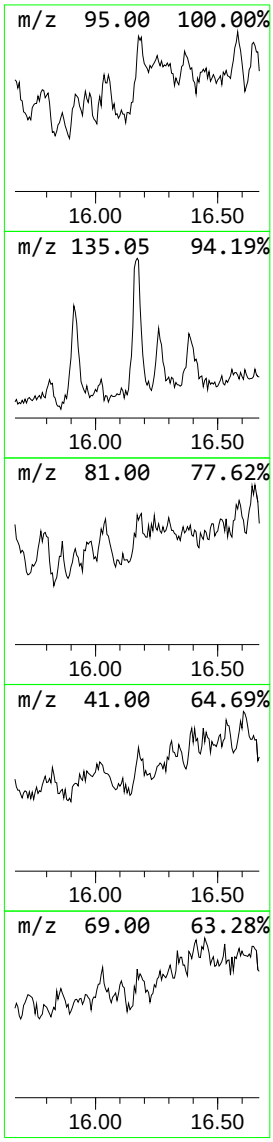
****

Peak Number 7 unknown16.170 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	6.55 ug/l	138265	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	27
2	Dispiro[4.0.4.1]undecan-1-one	164	C11H16O	1010186-37-7	25
3	1-Cyanoethyl-2-methylimidazole	135	C7H9N3	023996-55-6	25
4	4-(Ethoxymethyl)-2,6-dimethylphenol	180	C11H16O2	1000486-83-2	11
5	2-Ethoxyphenyl isocyanate	163	C9H9NO2	005395-71-1	11





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ALS Vial : 18 Sample Multiplier: 1

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

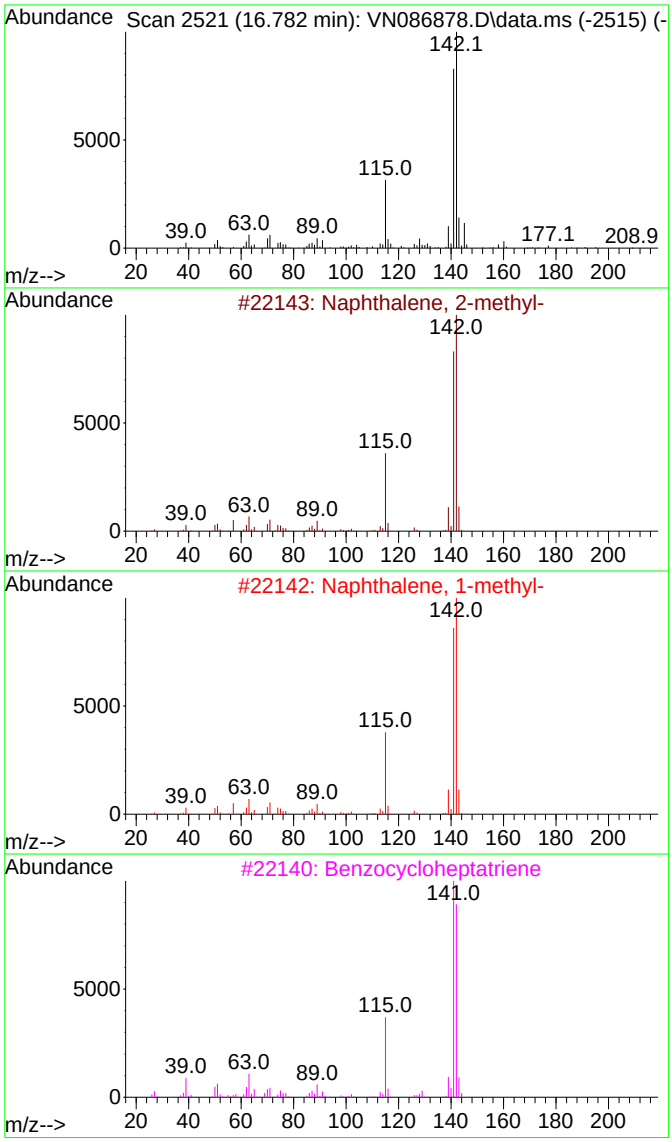
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

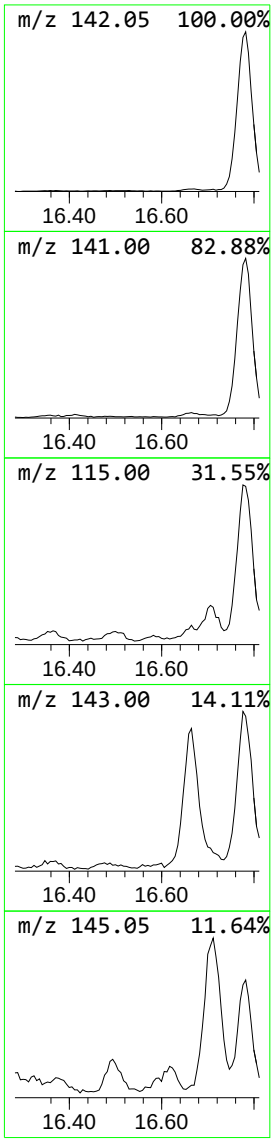
****

Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	24.07 ug/l	508254	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086878.D
Acq On : 06 Jun 2025 19:51
Operator : JC\MD
Sample : Q2216-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3864

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.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
Propene	2.112	6.3	ug/l	99680	1	8.235	792750	50.0
1-Propene, 2-me...	2.524	9.0	ug/l	143089	1	8.235	792750	50.0
2-Butanone, 3,3...	9.912	7.6	ug/l	151991	2	9.106	1000070	50.0
Naphthalene, de...	14.117	7.5	ug/l	158438	4	13.794	1055590	50.0
1-Methyl-3-ethy...	14.764	14.1	ug/l	298021	4	13.794	1055590	50.0
unknown15.491	15.941	7.4	ug/l	157064	4	13.794	1055590	50.0
unknown16.170	16.170	6.5	ug/l	138265	4	13.794	1055590	50.0
Naphthalene, 2-...	16.782	24.1	ug/l	508254	4	13.794	1055590	50.0