LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
Data File : VN073269.D
Acq On : 30 Jun 2022 16:37
Operator : JC\MD
Sample : N3554-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

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\82N062822W.M
Title : SW846 8260

Signal : TIC: VN073269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.005	15	20	27	rBV2	35289	50078	3.59%	0.383%
2	2.322	68	74	80	rBV	34065	108394	7.77%	0.829%
3	4.516	427	447	457	rBV3	12422	56318	4.03%	0.431%
4	7.245	902	911	922	rBV5	12381	36318	2.60%	0.278%
5	7.951	1021	1031	1036	rBV	208715	499530	35.79%	3.821%
6	8.016	1036	1042	1053	rVB	379980	885267	63.42%	6.772%
7	8.369	1090	1102	1119	rBV	214766	507291	36.34%	3.880%
8	8.904	1184	1193	1206	rBV	555392	1132435	81.13%	8.662%
9	10.381	1434	1444	1458	rBV	722141	1363148	97.66%	10.427%
10	11.680	1657	1665	1675	rBV	772238	1365700	97.85%	10.447%
11	12.669	1824	1833	1843	rBV	637209	1064822	76.29%	8.145%
12	13.439	1958	1964	1968	rVB2	14249	24093	1.73%	0.184%
13	13.551	1978	1983	1987	rBV	20671	31643	2.27%	0.242%
14	13.610	1987	1993	2006	rVB	814110	1395775	100.00%	10.677%
15	13.710	2006	2010	2014	rVB3	10775	16047	1.15%	0.123%
16	13.774	2014	2021	2026	rBV2	39625	68410	4.90%	0.523%
17	13.857	2031	2035	2042	rVB3	22460	37413	2.68%	0.286%
18	13.939	2043	2049	2054	rBV4	39669	68604	4.92%	0.525%
19	14.004	2054	2060	2066	rBV	26052	48928	3.51%	0.374%
20	14.098	2066	2076	2081	rVV	53507	115950	8.31%	0.887%
21	14.157	2081	2086	2090	rVV2	83369	130268	9.33%	0.996%
22	14.216	2090	2096	2098	rVV4	21291	40121	2.87%	0.307%
23	14.263	2098	2104	2110	rVB2	73796	139761	10.01%	1.069%
24	14.333	2110	2116	2122	rBV5	29849	62220	4.46%	0.476%
25	14.445	2130	2135	2136	rBV4	22107	29821	2.14%	0.228%
26	14.474	2137	2140	2143	rVV2	57413	87234	6.25%	0.667%
27	14.516	2143	2147	2151	rVV	88473	126538	9.07%	0.968%
28	14.557	2151	2154	2157	rVV3	32997	42690	3.06%	0.327%
29	14.598	2157	2161	2163	rVV4	23434	38463	2.76%	0.294%
30	14.627	2163	2166	2171	rVB	40967	56473	4.05%	0.432%
31	14.698	2173	2178	2182	rVV3	26815	41170	2.95%	0.315%
32	14.757	2182	2188	2191	rBV4	37458	76663	5.49%	0.586%
33	14.792	2191	2194	2199	rVB2	46221	64926	4.65%	0.497%
34	14.863	2199	2206	2210	rBV5	108327	269147	19.28%	2.059%
35	14.904	2210	2213	2221	rVB3	80719	180863	12.96%	1.383%
36	15.045	2233	2237	2240	rBV5	17499	32573	2.33%	0.249%

LSC Area Percent Report

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Operator : JC\MD
Sample : N3554-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

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\82N062822W.M
Title : SW846 8260

37	15.127	2241	2251	2262	rVV3	166847	486142	34.83%	3.719%
38	15.239	2264	2270	2280	rVB2	138350	338803	24.27%	2.592%
39	15.398	2291	2297	2304	rBV	122071	212518	15.23%	1.626%
40	15.486	2306	2312	2316	rBV2	84677	164401	11.78%	1.258%
41	15.551	2317	2323	2324	rBV6	58512	108421	7.77%	0.829%
42	15.727	2346	2353	2360	rBV2	101479	253454	18.16%	1.939%
43	15.810	2362	2367	2372	rVV6	64278	133999	9.60%	1.025%
44	15.898	2376	2382	2392	rVB3	104432	255536	18.31%	1.955%
45	16.027	2399	2404	2409	rBV	56275	98363	7.05%	0.752%
46	16.257	2436	2443	2450	rBV4	81316	202136	14.48%	1.546%
47	16.374	2459	2463	2469	rBV	91951	160828	11.52%	1.230%
48	16.463	2473	2478	2484	rVB5	76197	157250	11.27%	1.203%
49	16.715	2515	2521	2528	rBV8	70902	206170	14.77%	1.577%

Sum of corrected areas: 13073116

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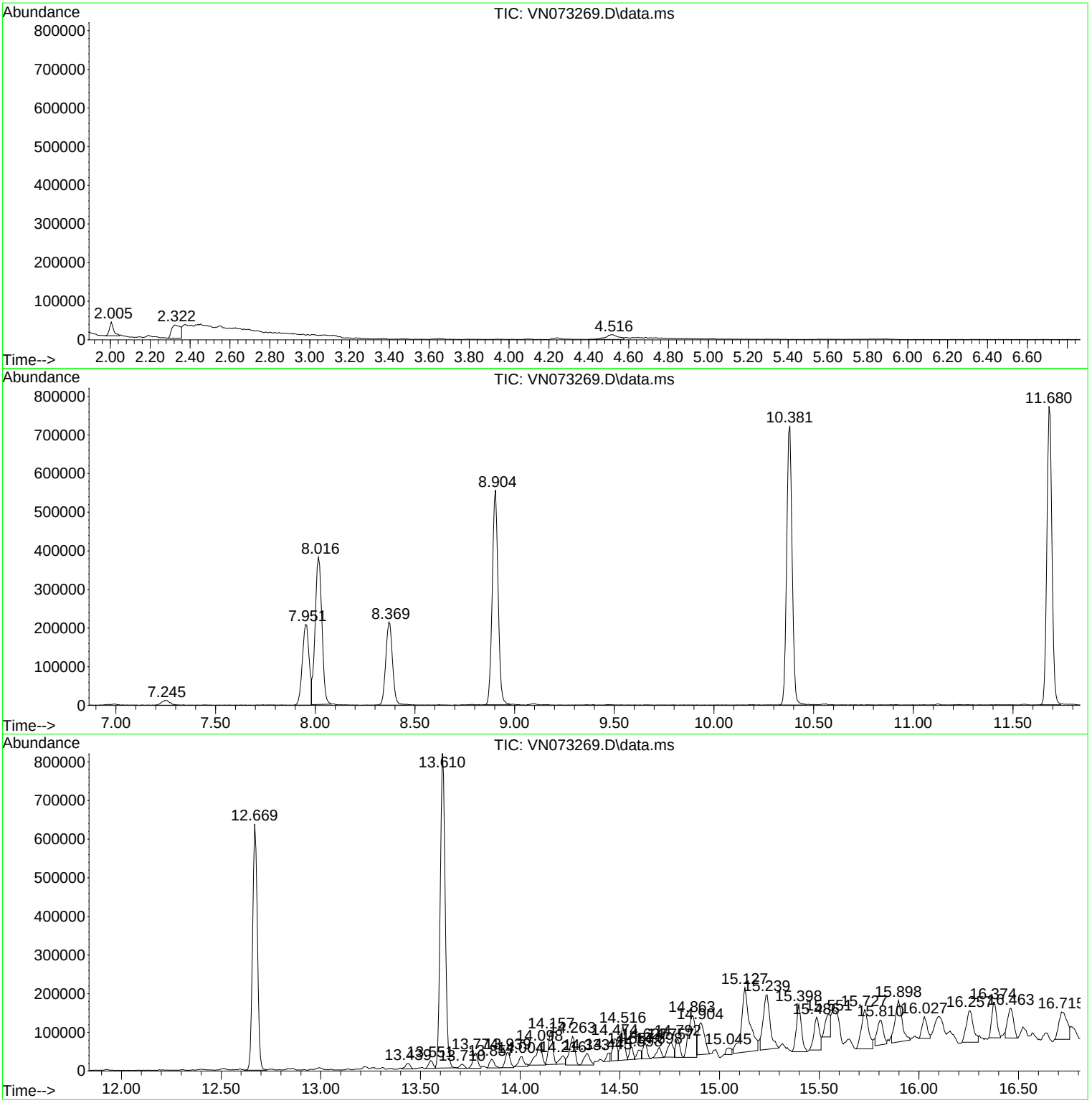
ClientSampleId :
152140-SPC-03-20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
Data File : VN073269.D
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MSVOA_N
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152140-SPC-03-20

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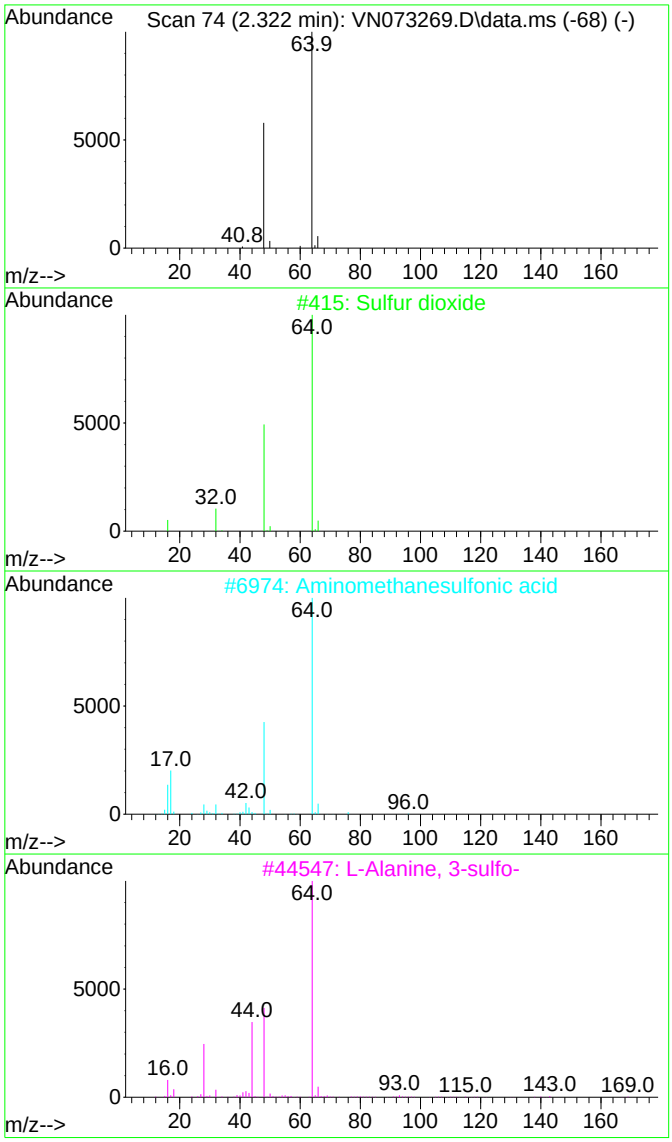
Quant Title : SW846 8260

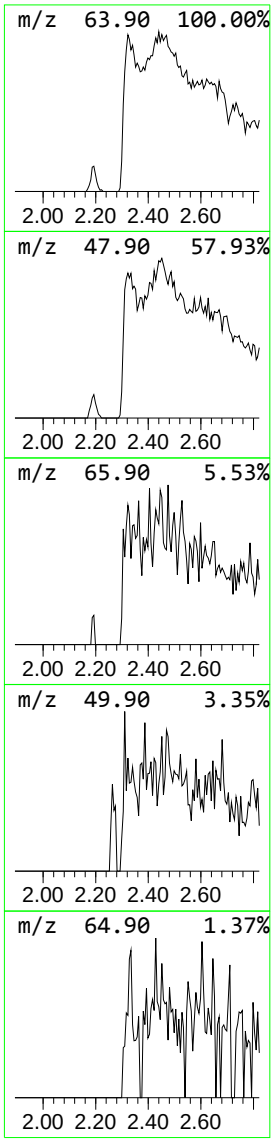
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	6.12 ug/l	108394	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

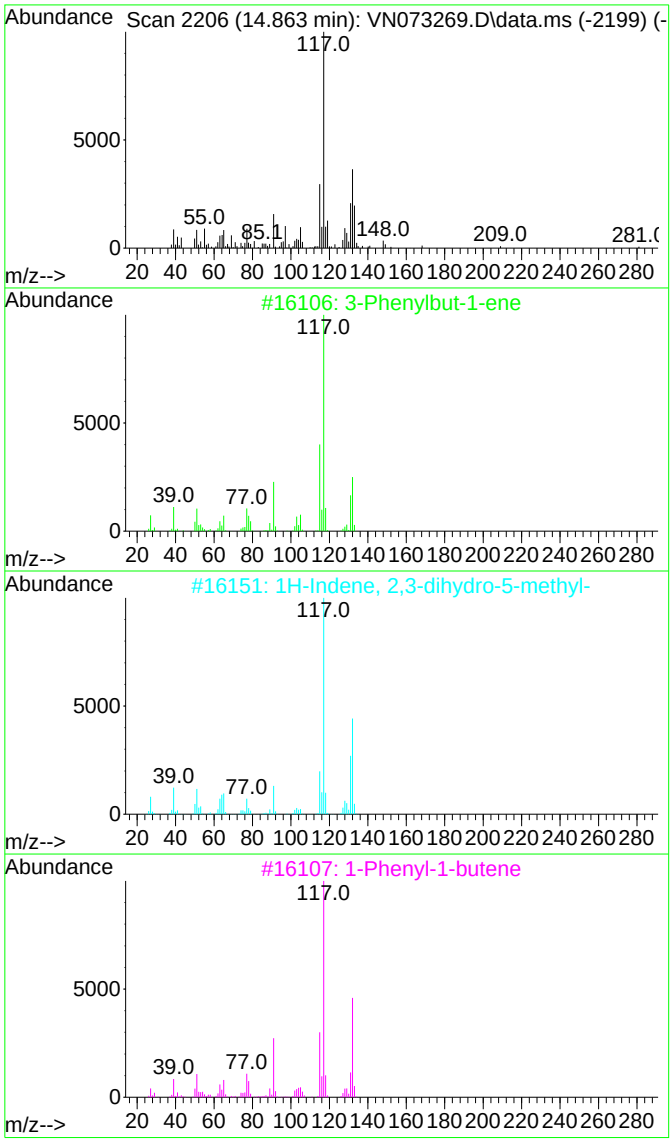
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

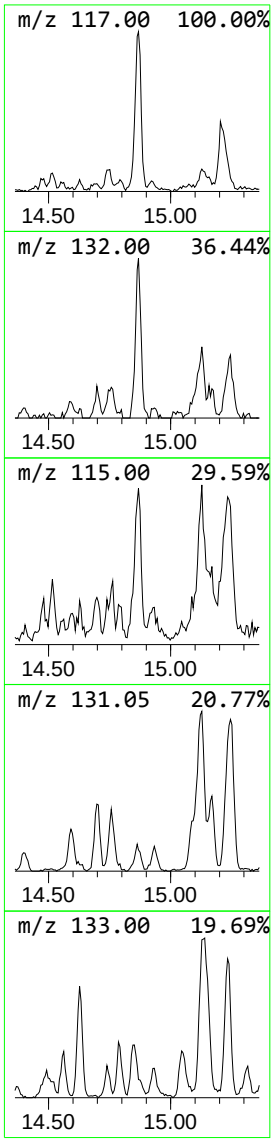
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Phenylbut-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	9.64 ug/l	269147	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	70
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
Data File : VN073269.D
Acq On : 30 Jun 2022 16:37
Operator : JC\MD
Sample : N3554-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

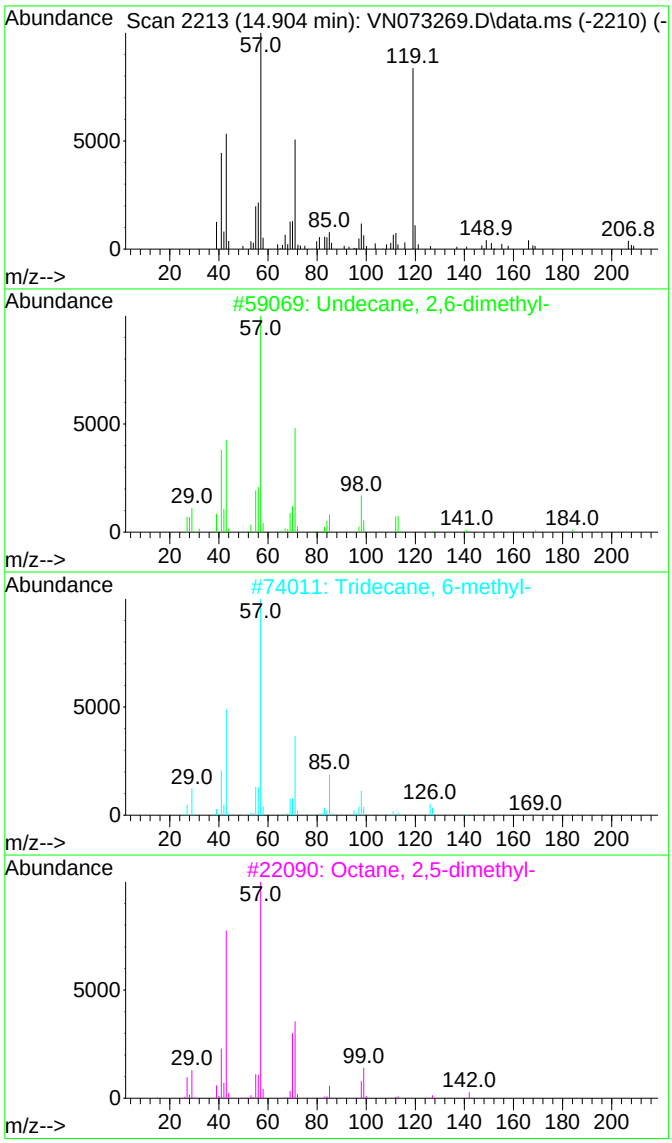
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

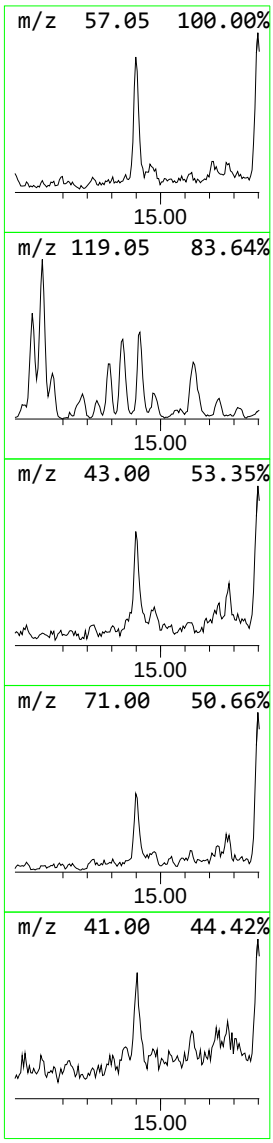
****

Peak Number 3 unknown14.904 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	6.48 ug/l	180863	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	35
2	Tridecane, 6-methyl-	198	C14H30	013287-21-3	27
3	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	27
4	Decane, 2-methyl-	156	C11H24	006975-98-0	27
5	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	22





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

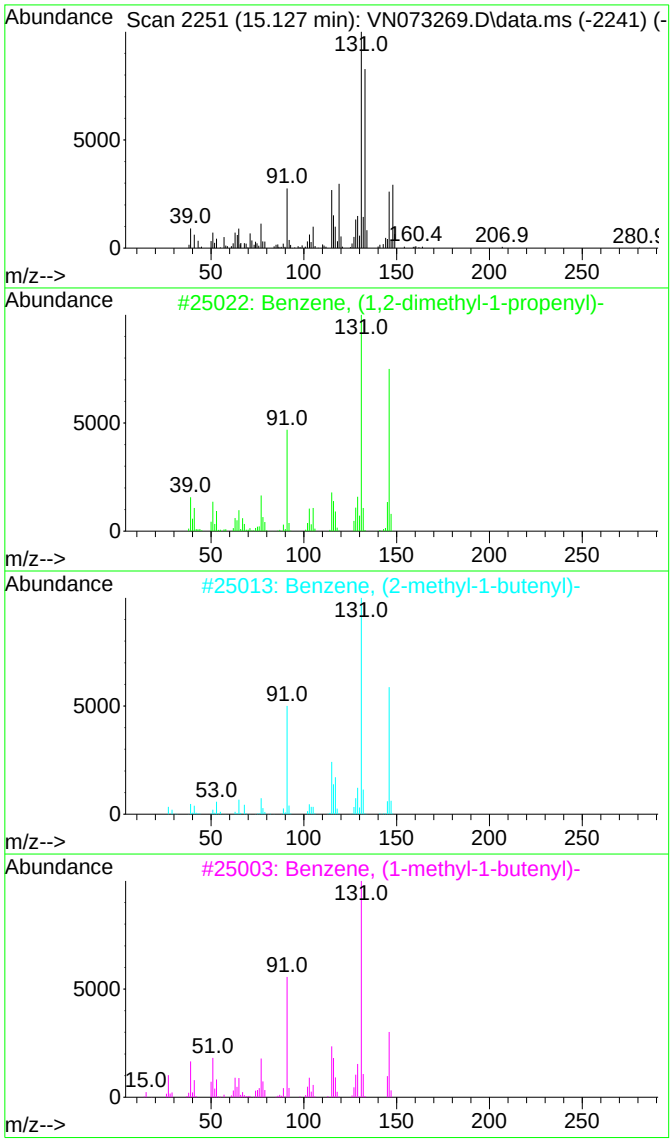
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

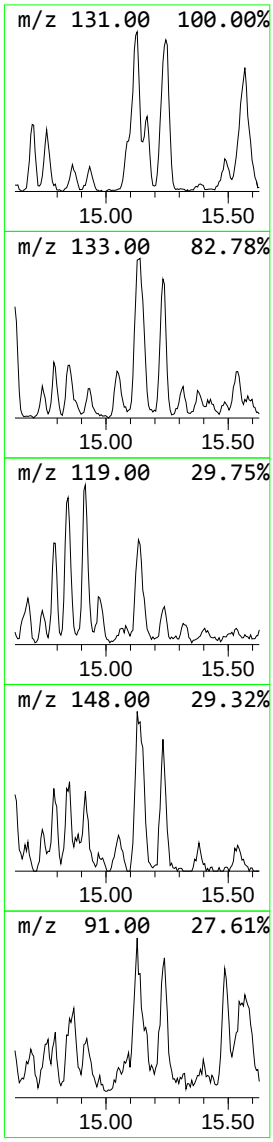
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, (1,2-dimethyl-1-pr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	17.41 ug/l	486142	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	90
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	86
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	70
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
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Instrument :
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ClientSampleId :
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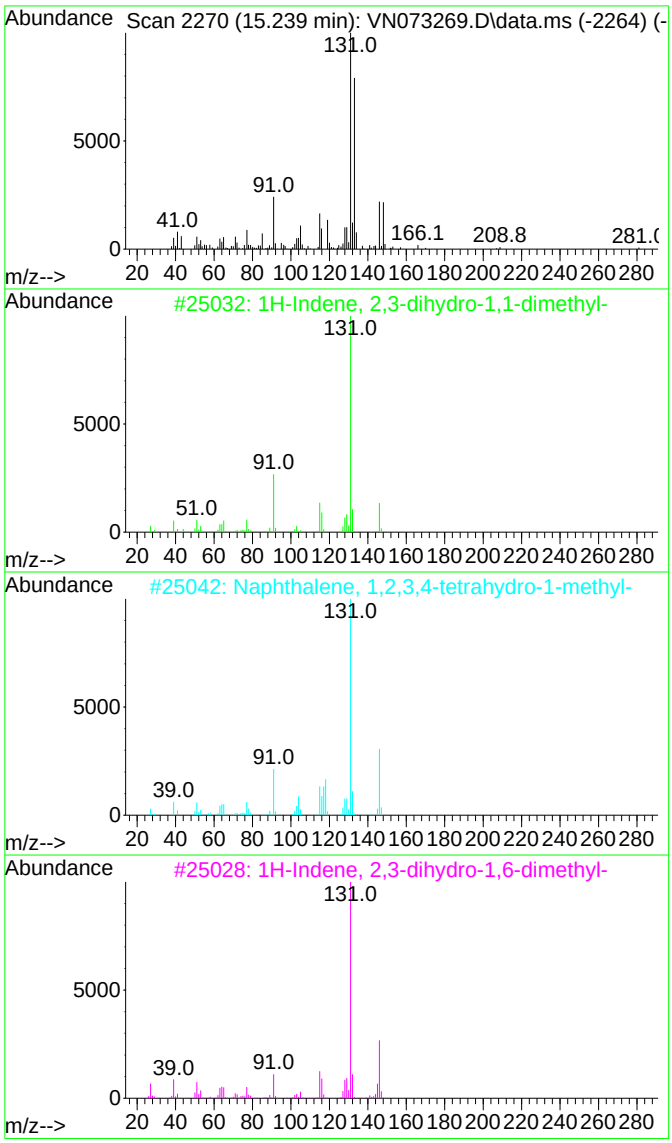
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

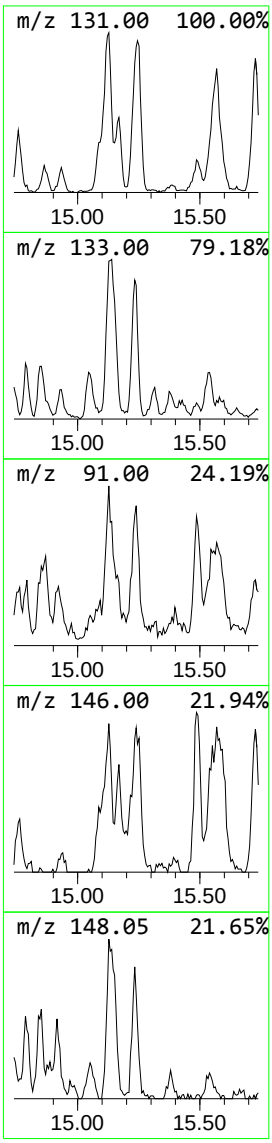
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Indene, 2,3-dihydro-1,1-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	12.14 ug/l	338803	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	55
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	49
3	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	49
4	Cyclopropane, 1-chloro-1-methyl-...	166	C10H11Cl	1000161-07-9	46
5	2-Butene, 3-chloro-1-phenyl-, (Z)-	166	C10H11Cl	016608-68-7	46





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

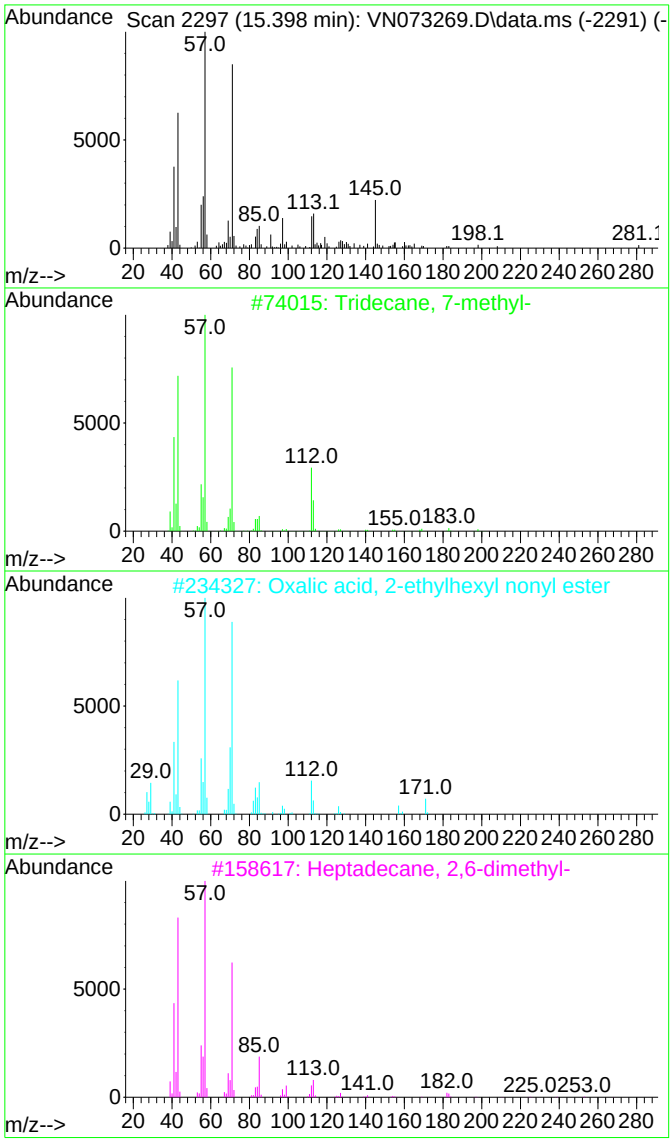
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

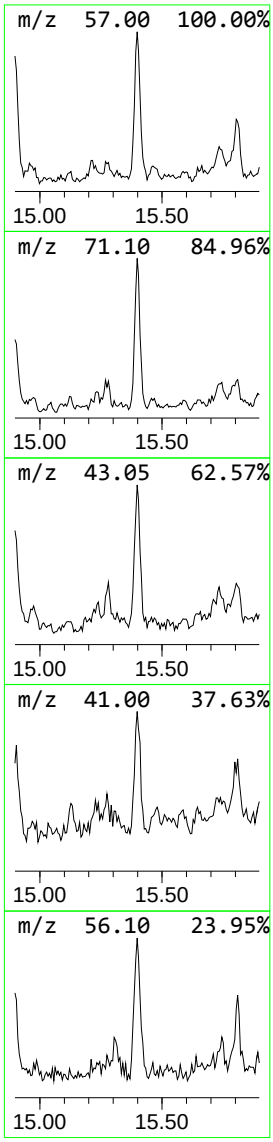
****

Peak Number 6 Tridecane, 7-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	7.61 ug/l	212518	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	70
2	Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	64
3	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	59
4	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	53
5	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	53





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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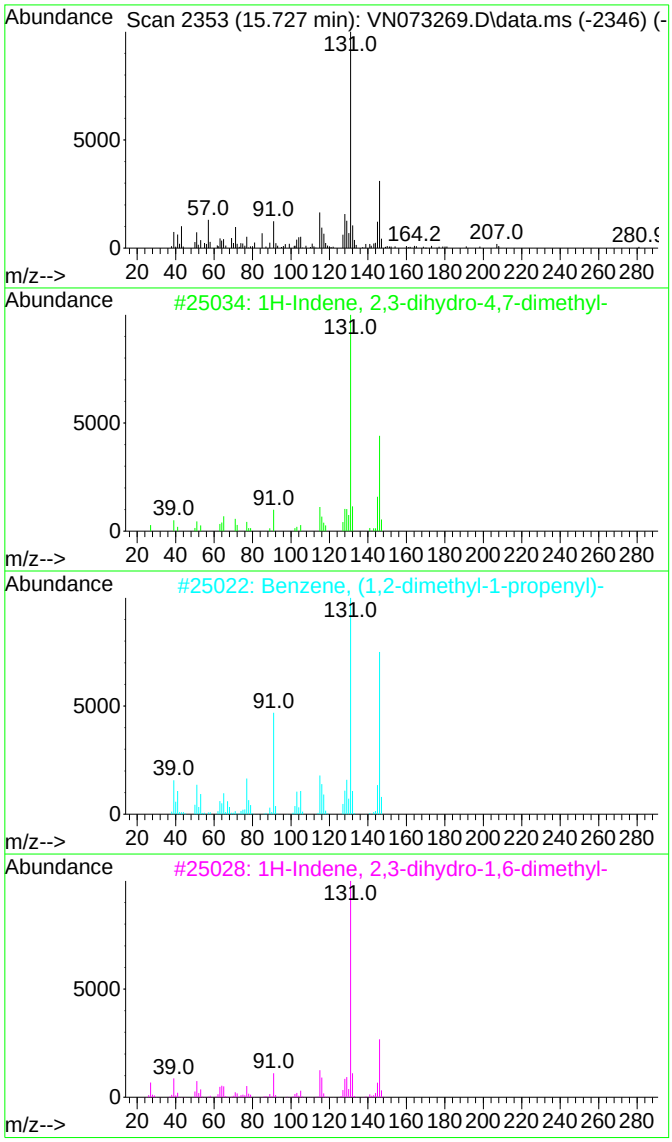
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

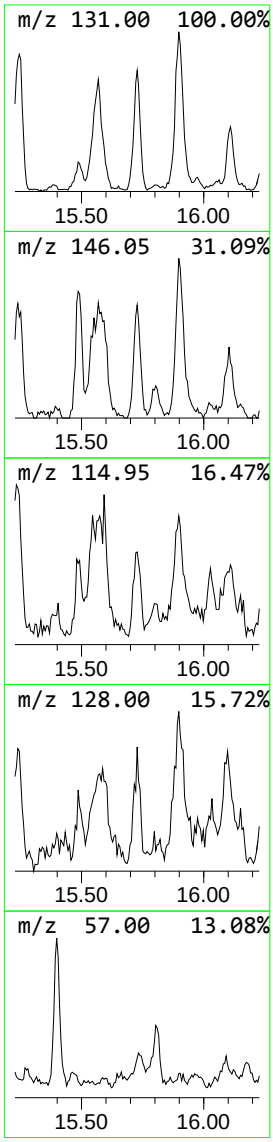
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.727	9.08 ug/l	253454	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	97
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	95
3	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
4	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	93
5	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	93





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Data File : VN073269.D
Acq On : 30 Jun 2022 16:37
Operator : JC\MD
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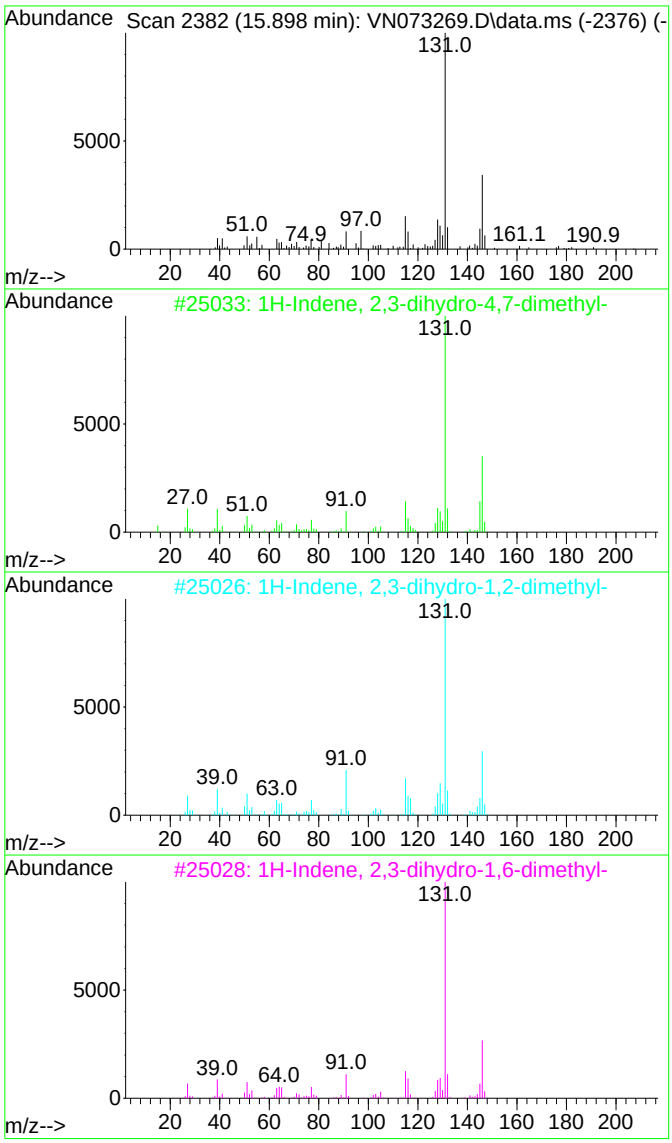
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

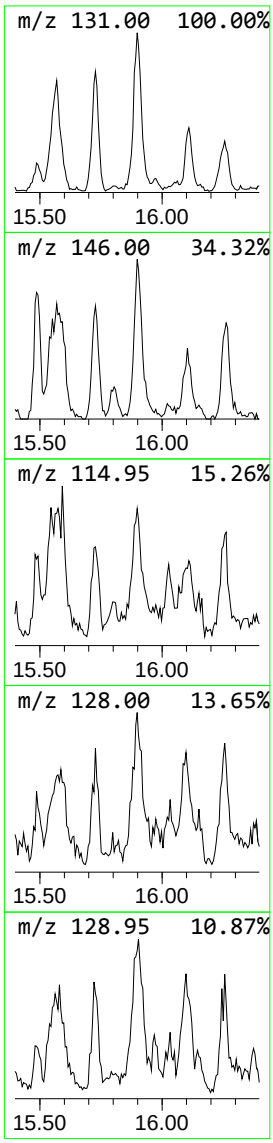
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	9.15 ug/l	255536	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	95
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	94
3	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	91
4	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	91
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	90





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Data File : VN073269.D
Acq On : 30 Jun 2022 16:37
Operator : JC\MD
Sample : N3554-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

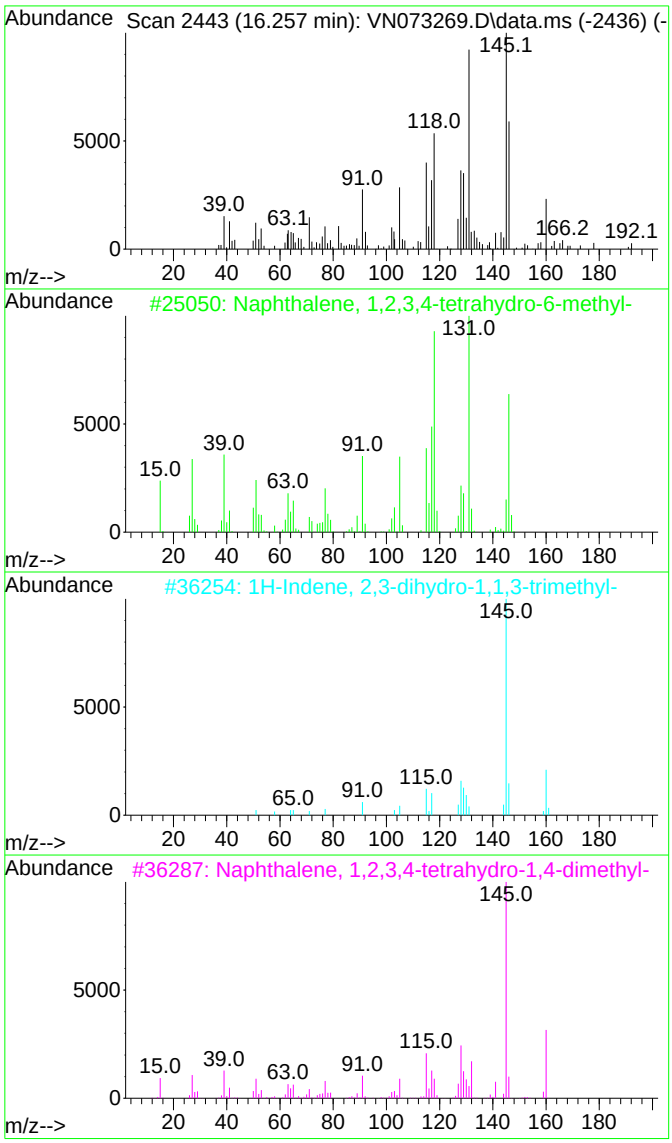
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

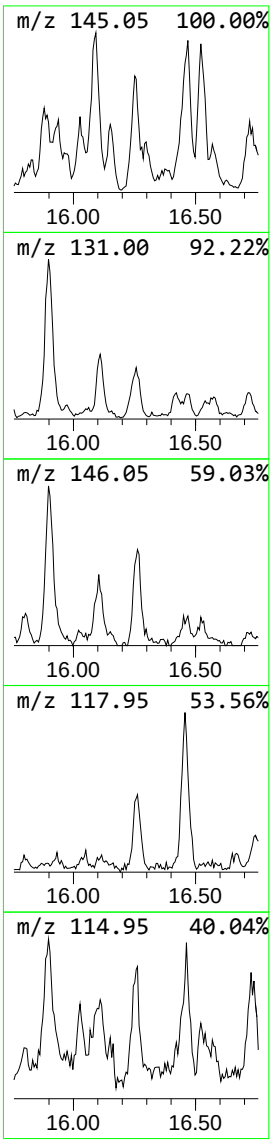
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	7.24 ug/l	202136	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	60
2	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	60
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	60
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	49
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
Data File : VN073269.D
Acq On : 30 Jun 2022 16:37
Operator : JC\MD
Sample : N3554-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

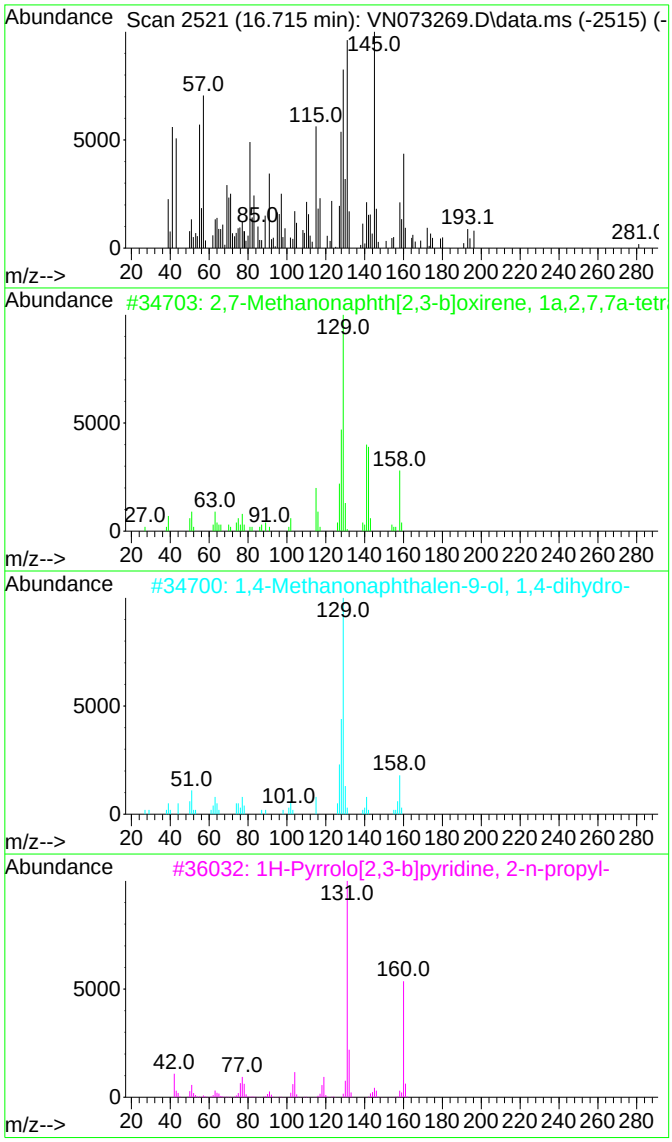
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

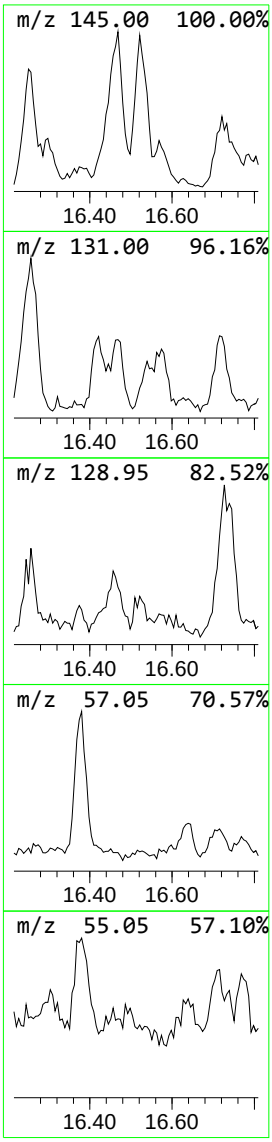
****

Peak Number 10 unknown16.715 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.715	7.39 ug/l	206170	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,7-Methanonaphth[2,3-b]oxirene,...	158	C11H10O	013137-34-3	41
2	1,4-Methanonaphthalen-9-ol, 1,4-...	158	C11H10O	004796-33-2	30
3	1H-Pyrrolo[2,3-b]pyridine, 2-n-p...	160	C10H12N2	1010212-02-1	20
4	Ethanone, 1-(2,3-dihydro-1H-inde...	160	C11H12O	004228-10-8	20
5	1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
Data File : VN073269.D
Acq On : 30 Jun 2022 16:37
Operator : JC\MD
Sample : N3554-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-03-20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
Sulfur dioxide	2.322	6.1	ug/l	108394	1	8.016	885267	50.0
3-Phenylbut-1-ene	14.863	9.6	ug/l	269147	4	13.610	1395780	50.0
unknown14.904	14.904	6.5	ug/l	180863	4	13.610	1395780	50.0
Benzene, (1,2-d...	15.127	17.4	ug/l	486142	4	13.610	1395780	50.0
1H-Indene, 2,3-...	15.239	12.1	ug/l	338803	4	13.610	1395780	50.0
Tridecane, 7-me...	15.398	7.6	ug/l	212518	4	13.610	1395780	50.0
1H-Indene, 2,3-...	15.727	9.1	ug/l	253454	4	13.610	1395780	50.0
1H-Indene, 2,3-...	15.898	9.2	ug/l	255536	4	13.610	1395780	50.0
Naphthalene, 1,...	16.257	7.2	ug/l	202136	4	13.610	1395780	50.0
unknown16.715	16.715	7.4	ug/l	206170	4	13.610	1395780	50.0