LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30759

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\82N062821W.M
Title : SW846 8260

Signal : TIC: VN067542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.059	2225	2263	2287	rBV4	2749893	8160182	8.18%	1.456%
2	8.163	2287	2302	2325	rVV2	939320	2378839	2.39%	0.424%
3	8.287	2326	2348	2387	rVV	3640935	8624635	8.65%	1.539%
4	8.448	2387	2408	2428	rVV3	377750	1044588	1.05%	0.186%
5	8.555	2428	2448	2456	rVV4	662851	1629878	1.63%	0.291%
6	8.609	2458	2468	2490	rVV	1461674	4035831	4.05%	0.720%
7	8.700	2490	2502	2525	rVB2	445265	1032091	1.04%	0.184%
8	8.821	2526	2547	2581	rBV	4306570	8743220	8.77%	1.560%
9	8.965	2582	2601	2632	rBV3	667072	1727463	1.73%	0.308%
10	9.456	2750	2784	2796	rBV	2370208	5749217	5.77%	1.026%
11	9.507	2797	2803	2820	rVB2	570196	1018440	1.02%	0.182%
12	9.880	2907	2942	2963	rBV2	1088689	2280202	2.29%	0.407%
13	10.014	2981	2992	3005	rVB	1296786	2405584	2.41%	0.429%
14	10.078	3005	3016	3026	rBV	1038088	1910600	1.92%	0.341%
15	10.215	3047	3067	3094	rBV2	1125849	2653587	2.66%	0.473%
16	10.440	3137	3151	3160	rBV3	1575193	3106865	3.12%	0.554%
17	10.510	3161	3177	3204	rVV3	53128672	99697994	100.00%	17.785%
18	10.623	3205	3219	3235	rVB	2649872	4993754	5.01%	0.891%
19	10.878	3296	3314	3336	rBV8	665862	1757771	1.76%	0.314%
20	11.055	3360	3380	3392	rBV	627609	1151150	1.15%	0.205%
21	11.293	3462	3469	3479	rVB	880280	1275463	1.28%	0.228%
22	11.347	3480	3489	3502	rVB	999726	1754249	1.76%	0.313%
23	11.457	3519	3530	3538	rBV5	686658	1131033	1.13%	0.202%
24	11.529	3539	3557	3582	rVB5	3084079	7847368	7.87%	1.400%
25	11.629	3582	3594	3607	rBV	2525613	4173184	4.19%	0.744%
26	11.749	3628	3639	3651	rBV	740233	1273060	1.28%	0.227%
27	11.848	3663	3676	3695	rBV	3654444	7124921	7.15%	1.271%
28	11.958	3697	3717	3738	rVV3	26491409	51344263	51.50%	9.159%
29	12.034	3740	3745	3758	rVB3	1453402	2187128	2.19%	0.390%
30	12.178	3790	3799	3811	rVB4	846361	1529240	1.53%	0.273%
31	12.283	3812	3838	3855	rBV3	7269475	19215641	19.27%	3.428%
32	12.371	3862	3871	3881	rVB	2575977	4029043	4.04%	0.719%
33	12.455	3881	3902	3907	rBV8	1837792	4246260	4.26%	0.757%
34	12.583	3941	3950	3956	rBV3	1064553	1895393	1.90%	0.338%
35	12.739	4001	4008	4012	rBV4	801917	1061235	1.06%	0.189%
36	12.771	4013	4020	4030	rVB	3090904	4275502	4.29%	0.763%

LSC Area Percent Report

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Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30759

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Title : SW846 8260

37	12.921	4062	4076	4087	rVB	3017860	6204059	6.22%	1.107%
38	12.986	4087	4100	4108	rBV	11477245	19307341	19.37%	3.444%
39	13.053	4116	4125	4140	rVB2	32842927	53416434	53.58%	9.529%
40	13.112	4141	4147	4157	rVB4	1965039	2825157	2.83%	0.504%
41	13.160	4158	4165	4172	rBV3	945534	1279222	1.28%	0.228%
42	13.224	4174	4189	4204	rBV	4145329	9677656	9.71%	1.726%
43	13.289	4206	4213	4228	rVB4	3370274	5481036	5.50%	0.978%
44	13.372	4231	4244	4257	rBV	22820428	36399422	36.51%	6.493%
45	13.568	4304	4317	4326	rBV5	5158945	9774407	9.80%	1.744%
46	13.611	4328	4333	4341	rVB3	1992169	2425159	2.43%	0.433%
47	13.675	4351	4357	4362	rBV3	1878339	2530473	2.54%	0.451%
48	13.710	4363	4370	4379	rVV	5561218	8302056	8.33%	1.481%
49	13.747	4380	4384	4396	rVB3	2242347	2731511	2.74%	0.487%
50	13.873	4423	4431	4439	rBV2	6130081	8952045	8.98%	1.597%
51	13.914	4440	4446	4466	rVB4	6522950	13147750	13.19%	2.345%
52	13.997	4467	4477	4489	rBV2	16240325	24581124	24.66%	4.385%
53	14.134	4521	4528	4533	rBV2	2415238	3158812	3.17%	0.564%
54	14.219	4551	4560	4571	rVB	6088128	9296163	9.32%	1.658%
55	14.329	4590	4601	4612	rVB3	5118818	8297993	8.32%	1.480%
56	14.512	4660	4669	4676	rBV5	4223364	6556987	6.58%	1.170%
57	14.581	4689	4695	4704	rVB	4080338	5286744	5.30%	0.943%
58	14.624	4704	4711	4717	rBV2	2357125	3172832	3.18%	0.566%
59	14.729	4743	4750	4756	rBV4	1093983	1575458	1.58%	0.281%
60	14.815	4773	4782	4787	rBV3	3156402	5065116	5.08%	0.904%
61	14.930	4810	4825	4837	rBV5	6206855	15535551	15.58%	2.771%
62	15.091	4876	4885	4898	rBV	2200847	3725511	3.74%	0.665%
63	15.198	4918	4925	4935	rVB5	2021849	2818768	2.83%	0.503%
64	15.617	5074	5081	5091	rBV3	1319174	2138349	2.14%	0.381%
65	16.341	5338	5351	5368	rVB5	1427815	3445062	3.46%	0.615%
66	16.620	5444	5455	5501	rVB	1798329	4995747	5.01%	0.891%

Sum of corrected areas: 560568819

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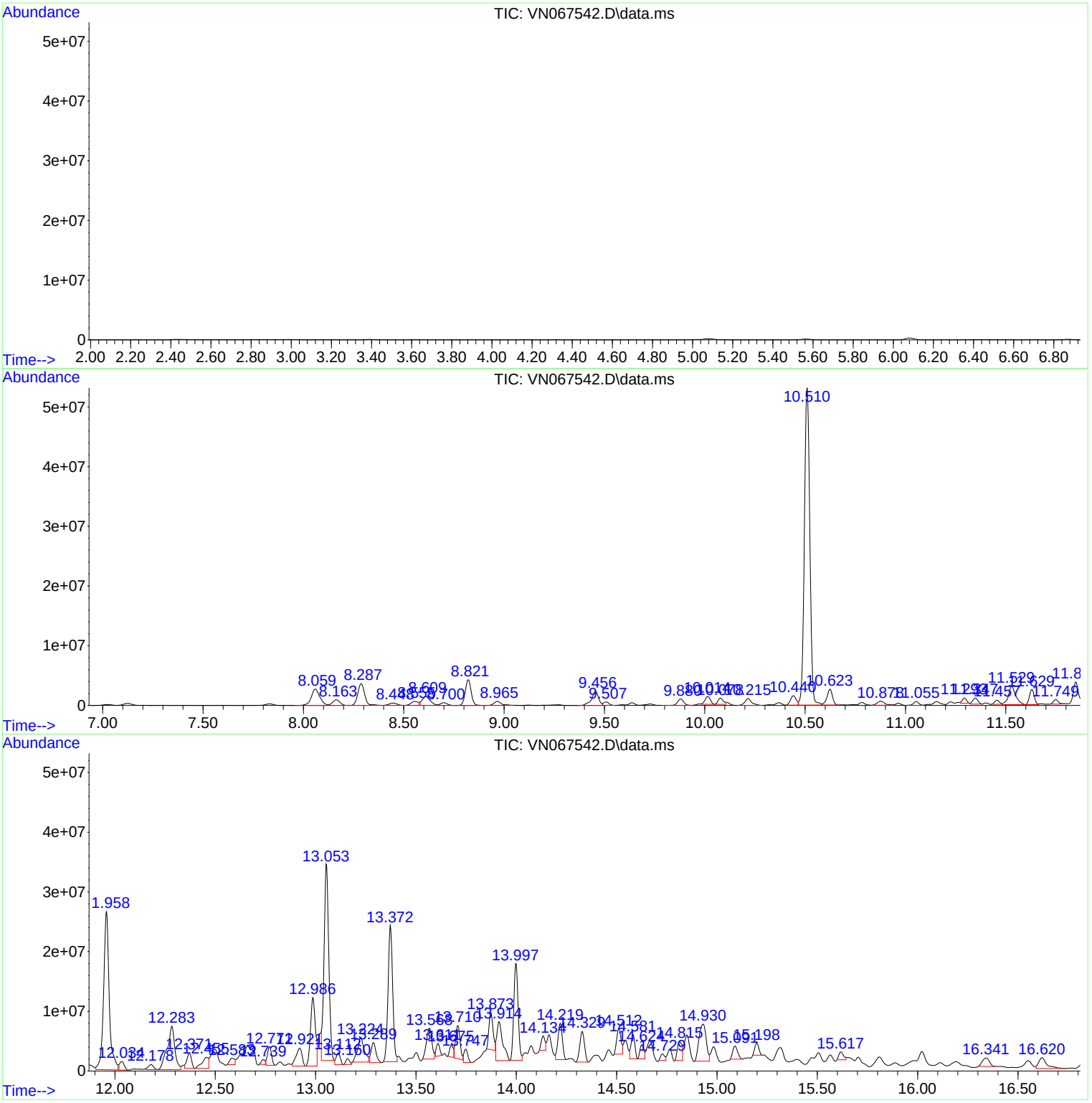
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : VN067542.D
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Instrument : MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

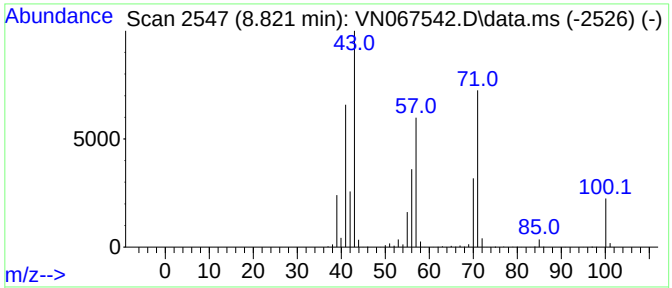
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

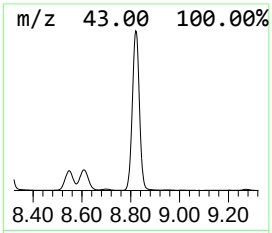
****

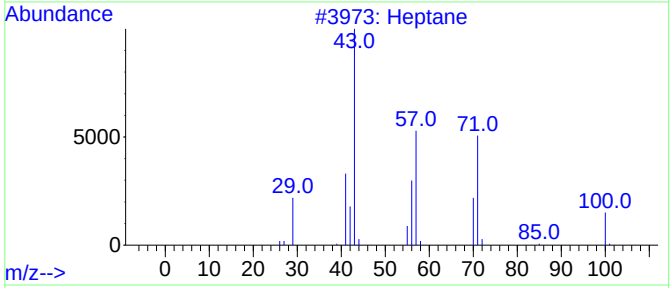
Peak Number 1 Heptane Concentration Rank 5

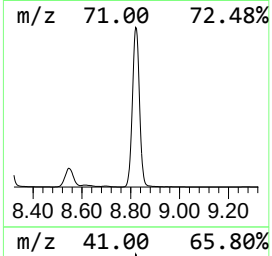
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.821	253.07 ug/l	8743220	1,4-Difluorobenzene	8.968

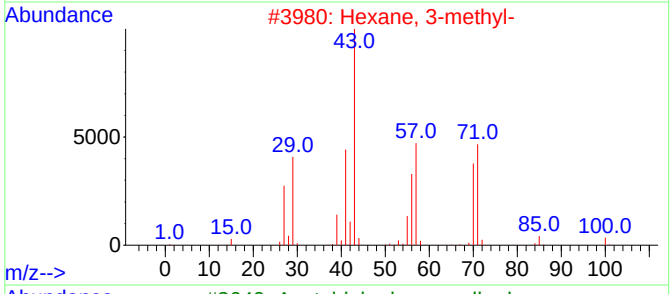
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
4	3-Hexanone	100	C6H12O	000589-38-8	43
5	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	37

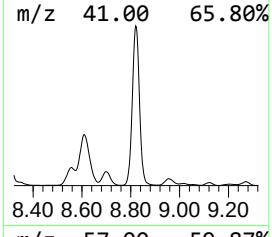


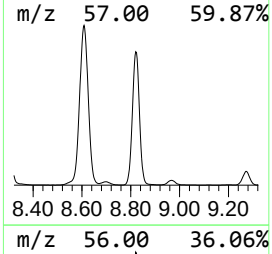


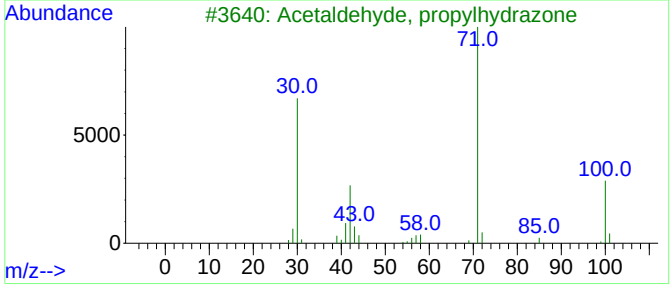


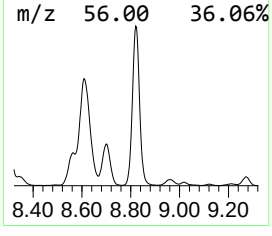












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

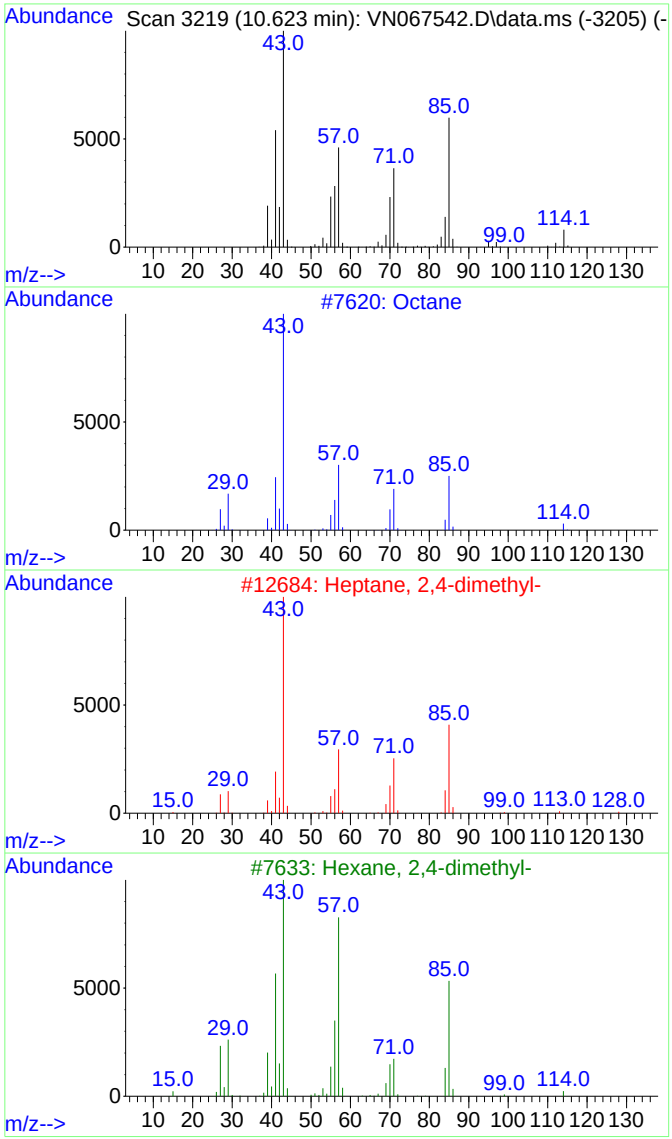
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

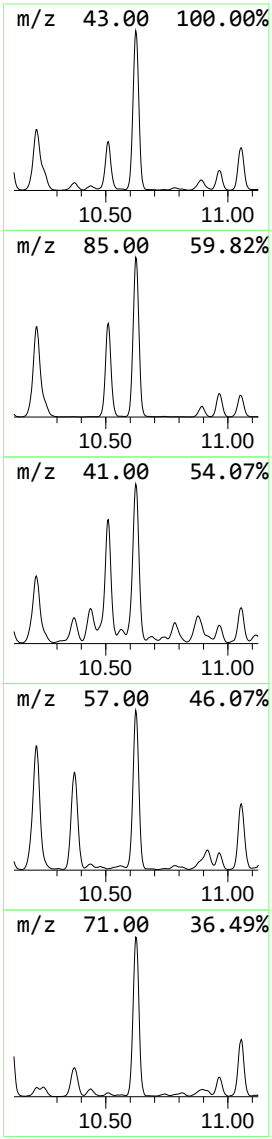
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Octane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.623	196.13 ug/l	4993750	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	91
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
4	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	59
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53





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Instrument : MSVOA_N
ClientSampleId : 30759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

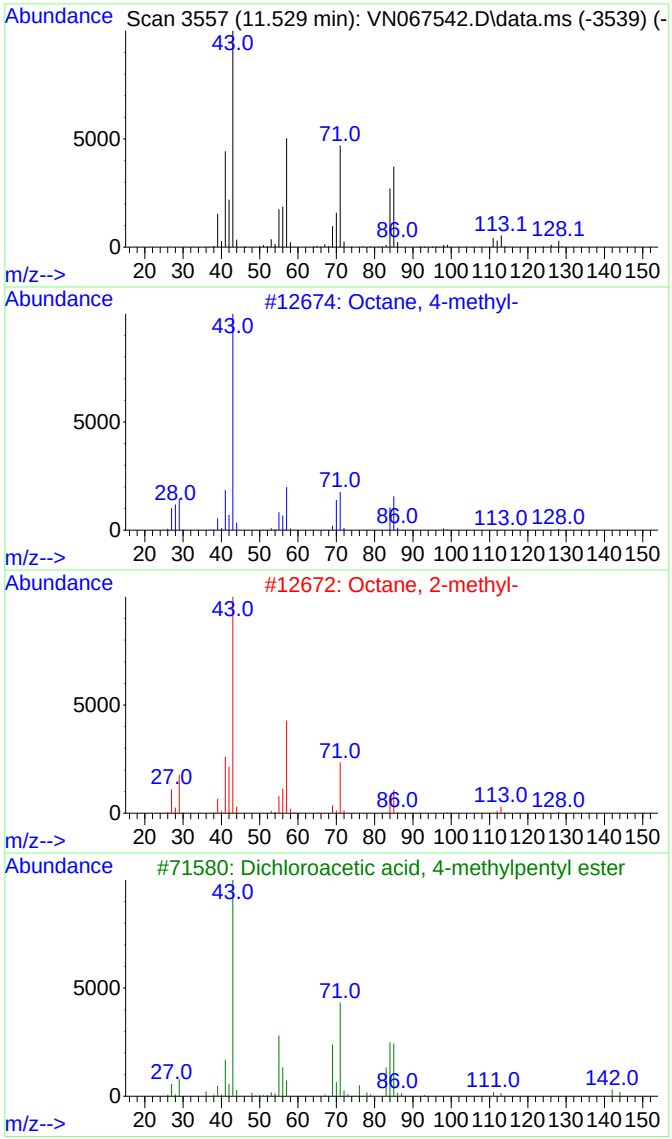
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

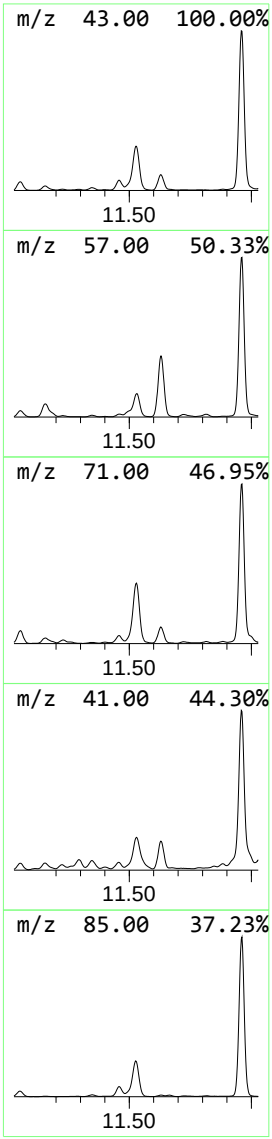
****

Peak Number 3 Octane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	308.21 ug/l	7847370	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	80
2	Octane, 2-methyl-	128	C9H20	003221-61-2	64
3	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	53
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	47
5	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47





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Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

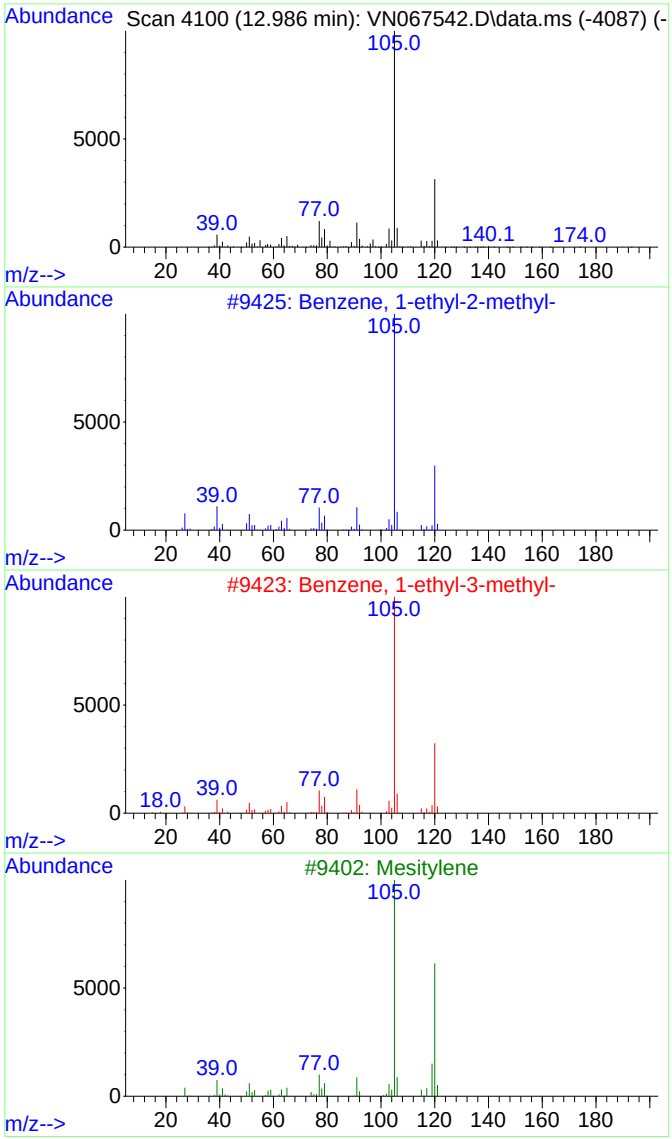
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

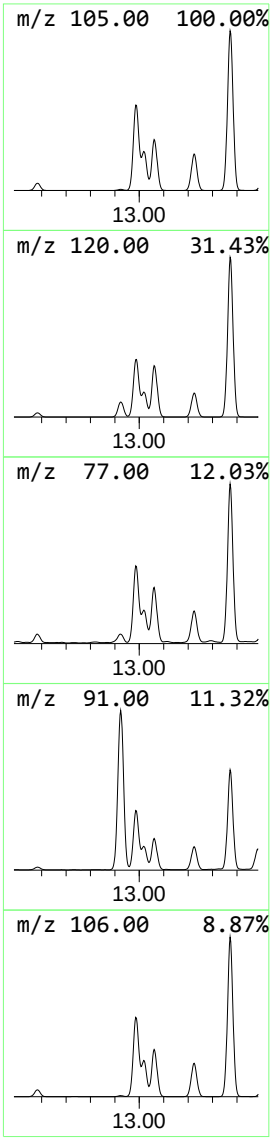
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	381.50 ug/l	19307300	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





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Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30759

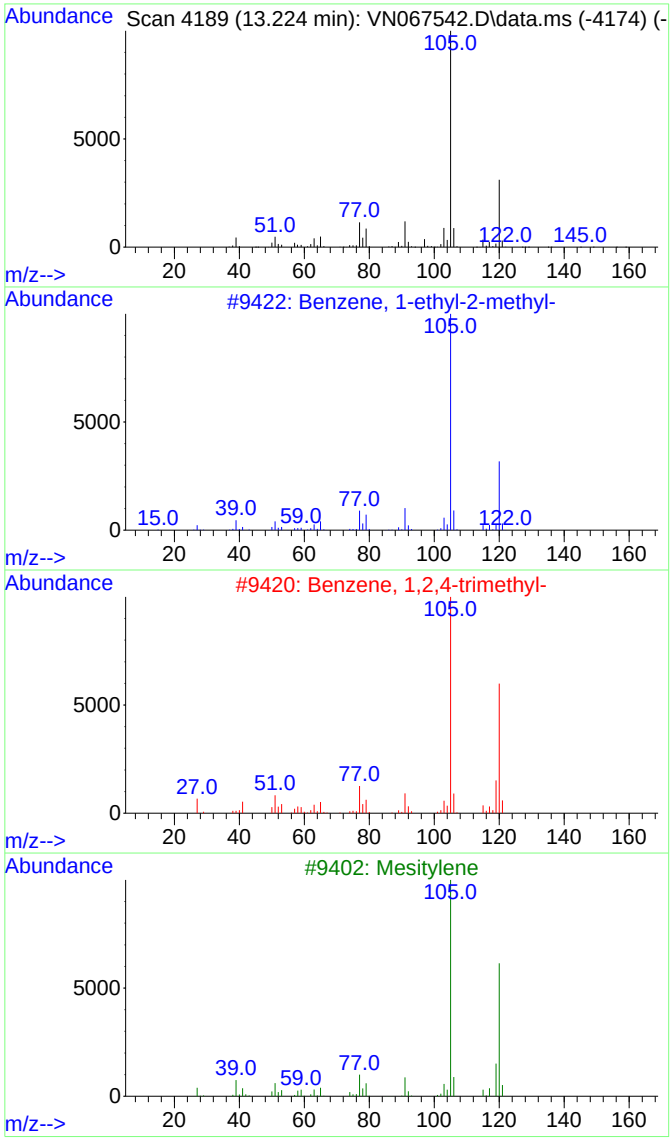
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

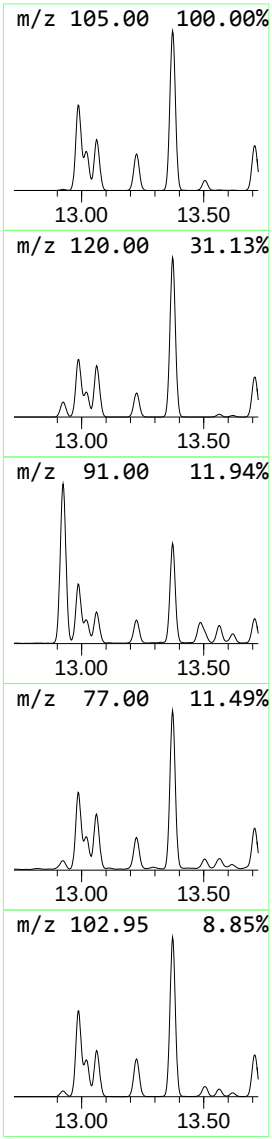
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.224	191.22 ug/l	9677660	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Operator : JC/MD
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Quant Title : SW846 8260

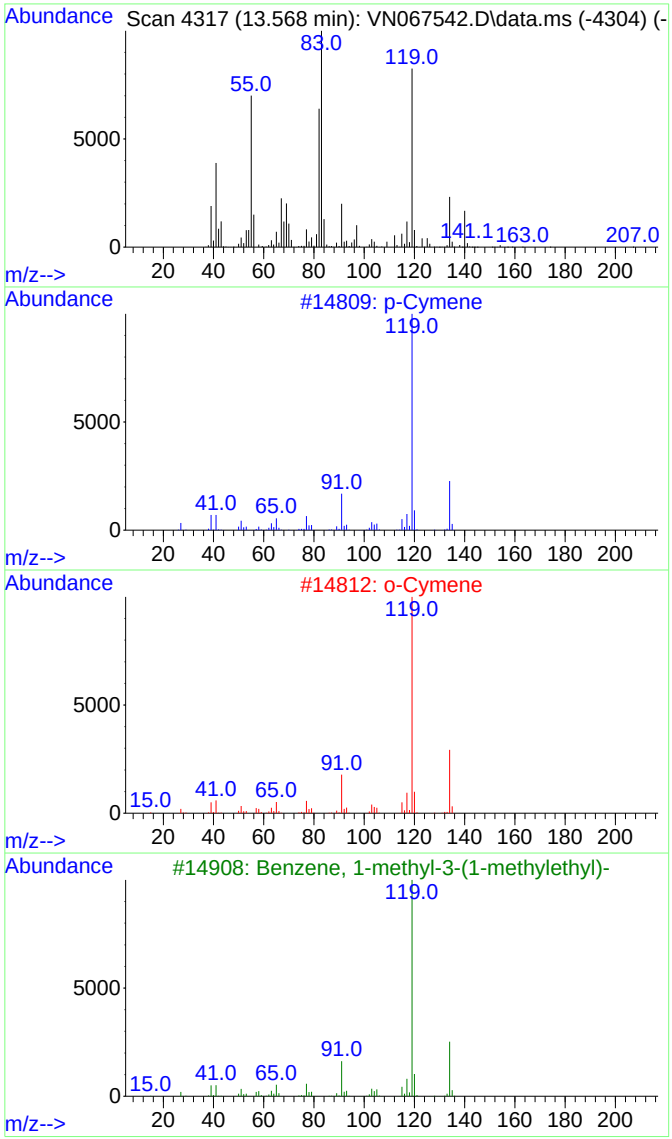
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

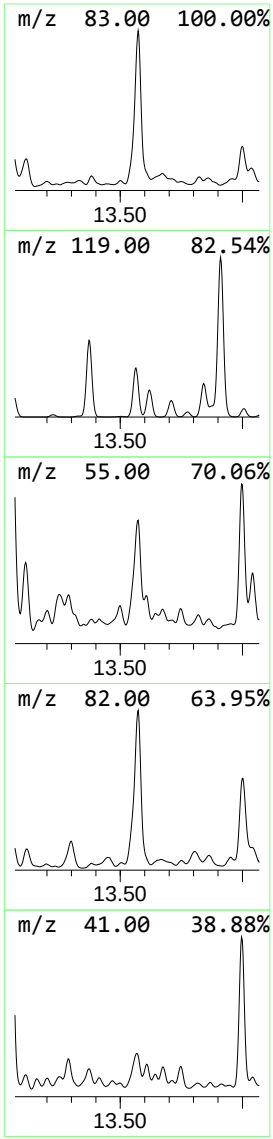
****

Peak Number 6 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	193.13 ug/l	9774410	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	78
2	o-Cymene	134	C10H14	000527-84-4	74
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	74
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	55
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

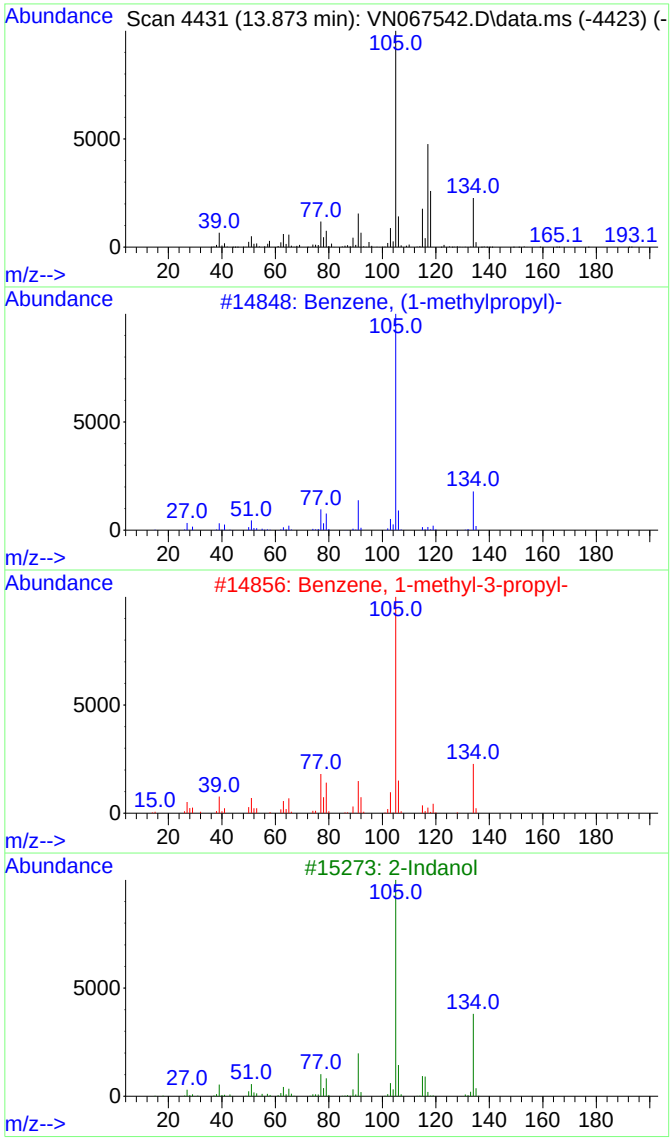
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

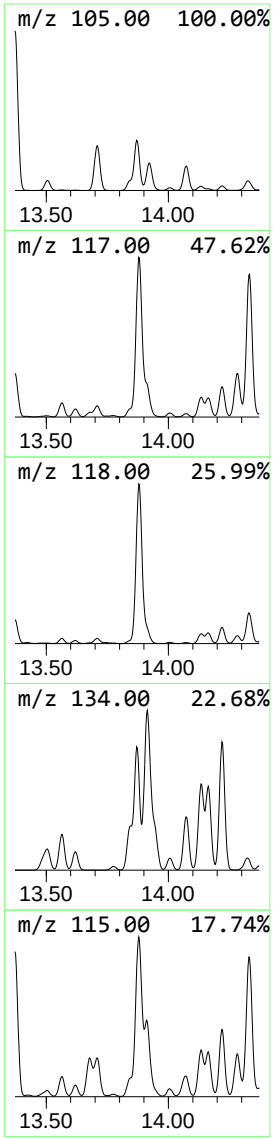
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (1-methylpropyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	176.88 ug/l	8952050	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	50
2	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	45
3	2-Indanol	134	C9H10O	004254-29-9	43
4	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	38
5	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	38





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Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

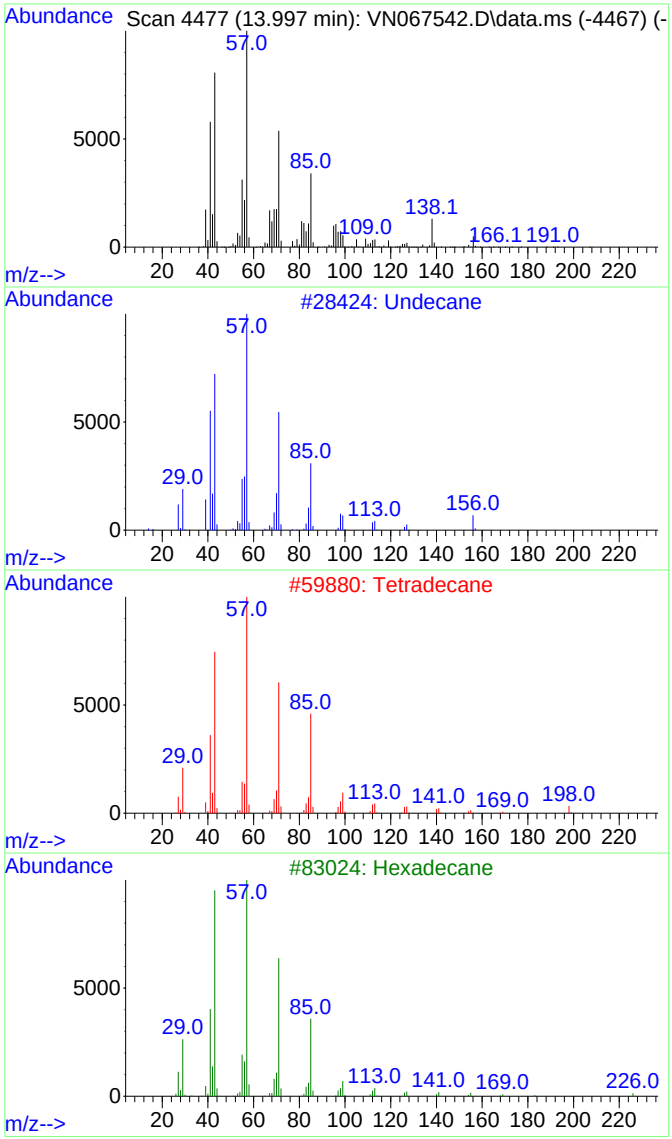
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

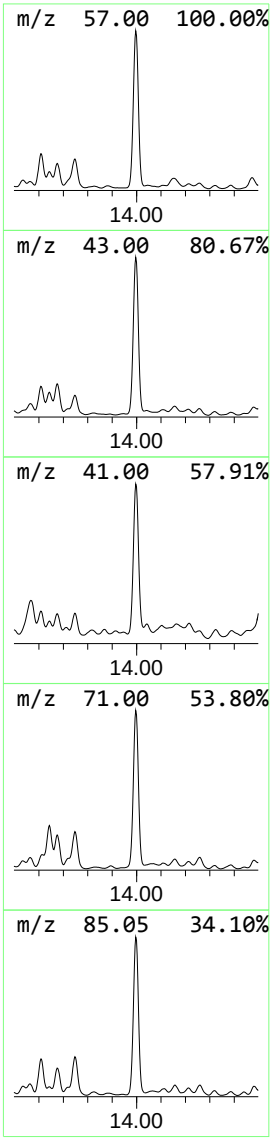
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	485.70 ug/l	24581100	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Tetradecane	198	C14H30	000629-59-4	50
3	Hexadecane	226	C16H34	000544-76-3	50
4	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	50
5	Octacosane	394	C28H58	000630-02-4	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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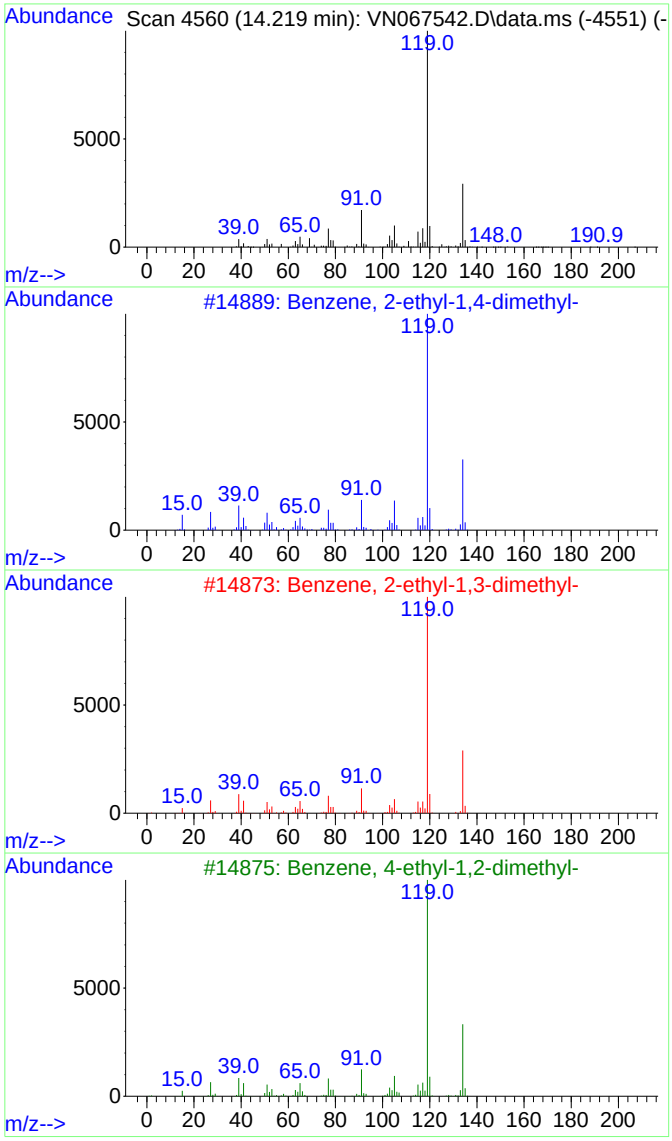
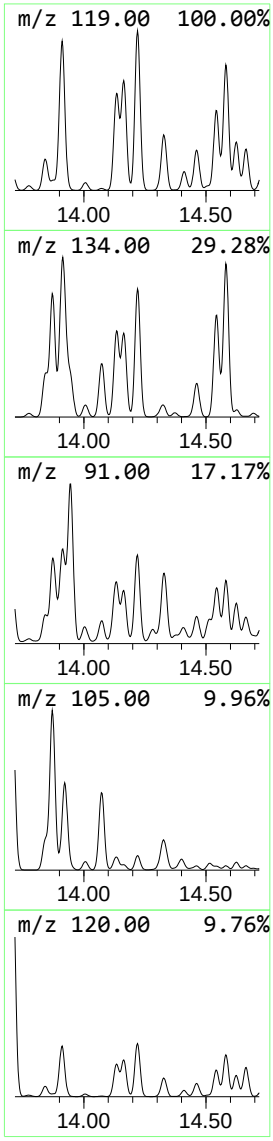
Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	183.68 ug/l	9296160	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





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Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30759

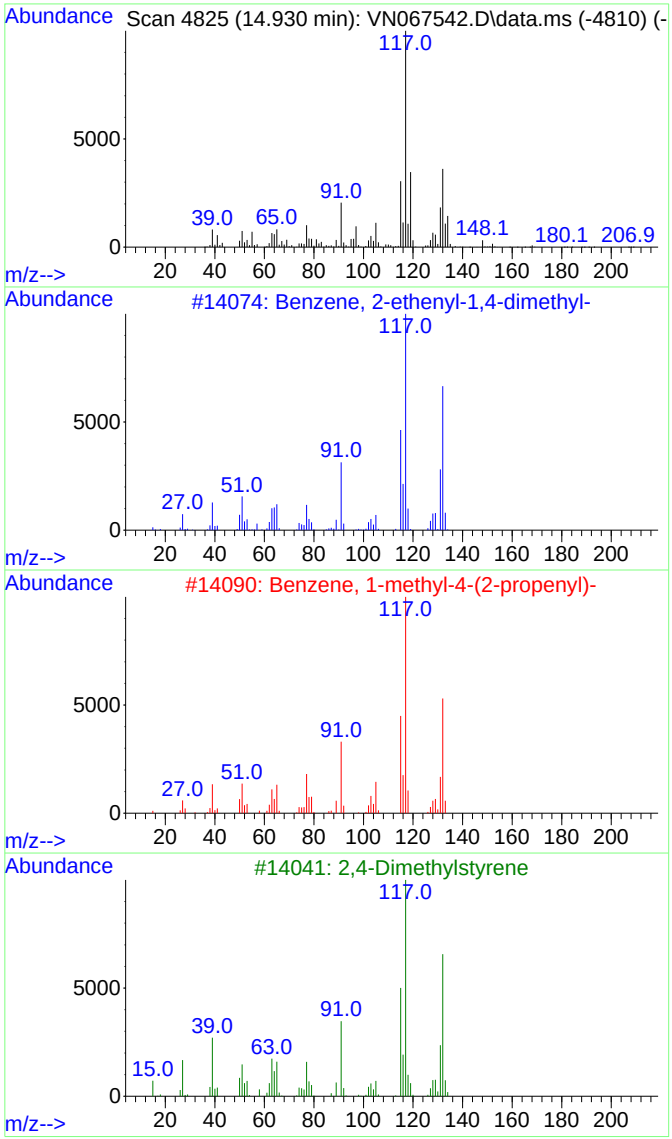
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

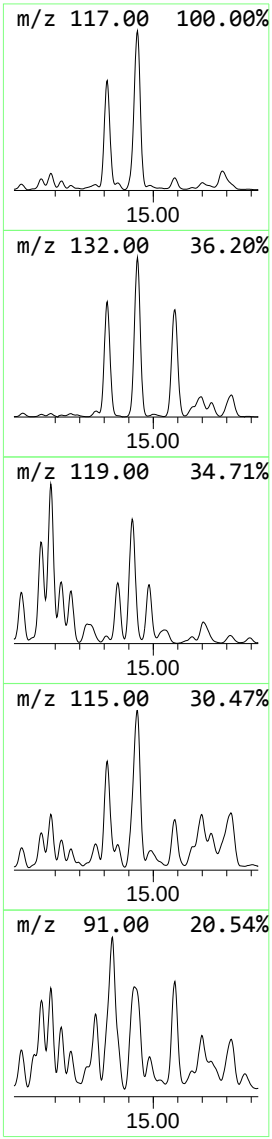
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	306.97 ug/l	15535600	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
3	2,4-Dimethylstyrene	132	C10H12	002234-20-0	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	76
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067542.D
Acq On : 28 Jun 2021 19:53
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Heptane	8.821	253.1	ug/l	8743220	2	8.968	1727460	50.0
Octane	10.623	196.1	ug/l	4993750	3	11.749	1273060	50.0
Octane, 4-methyl-	11.529	308.2	ug/l	7847370	3	11.749	1273060	50.0
Benzene, 1-ethy...	12.986	381.5	ug/l	19307300	4	13.678	2530470	50.0
Benzene, 1-ethy...	13.224	191.2	ug/l	9677660	4	13.678	2530470	50.0
o-Cymene	13.568	193.1	ug/l	9774410	4	13.678	2530470	50.0
Benzene, (1-met...	13.873	176.9	ug/l	8952050	4	13.678	2530470	50.0
Undecane	13.997	485.7	ug/l	24581100	4	13.678	2530470	50.0
Benzene, 2-ethy...	14.219	183.7	ug/l	9296160	4	13.678	2530470	50.0
Benzene, 2-ethe...	14.930	307.0	ug/l	15535600	4	13.678	2530470	50.0