LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070934.D
Acq On : 3 Feb 2022 16:59
Operator : JC/MD
Sample : N1381-05
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

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\82N020222W.M
Title : SW846 8260

Signal : TIC: VN070934.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.016	2223	2247	2258	rBV	487137	1184474	6.05%	0.417%
2	8.078	2258	2270	2292	rVB	1052224	2468028	12.61%	0.869%
3	8.284	2329	2347	2363	rBV2	84669	197242	1.01%	0.069%
4	8.432	2384	2402	2428	rBV	598307	1385232	7.08%	0.488%
5	8.965	2580	2601	2650	rVB	1461664	3094455	15.81%	1.090%
6	9.454	2751	2783	2797	rBV	1033657	2444652	12.49%	0.861%
7	9.636	2837	2851	2863	rBV	111881	211894	1.08%	0.075%
8	9.727	2864	2885	2910	rVB3	182943	447782	2.29%	0.158%
9	9.872	2917	2939	2959	rBV4	243801	518183	2.65%	0.183%
10	10.017	2976	2993	3002	rBV2	208521	411129	2.10%	0.145%
11	10.073	3003	3014	3018	rVV6	158909	267913	1.37%	0.094%
12	10.108	3020	3027	3043	rVB	375041	653974	3.34%	0.230%
13	10.199	3044	3061	3071	rBV3	248554	595818	3.04%	0.210%
14	10.357	3096	3120	3132	rBV8	78402	248051	1.27%	0.087%
15	10.438	3132	3150	3182	rBV3	3884035	8804341	44.97%	3.101%
16	10.561	3184	3196	3202	rBV2	211584	368655	1.88%	0.130%
17	10.609	3203	3214	3237	rVB6	622595	1718392	8.78%	0.605%
18	10.738	3239	3262	3266	rBV4	178041	383507	1.96%	0.135%
19	10.778	3266	3277	3295	rVB	1095907	2080041	10.63%	0.733%
20	10.875	3297	3313	3324	rBV3	589510	1277273	6.52%	0.450%
21	10.961	3336	3345	3358	rVB2	495382	825354	4.22%	0.291%
22	11.049	3358	3378	3392	rBV2	1392282	2514968	12.85%	0.886%
23	11.151	3393	3416	3432	rBV	887074	2066823	10.56%	0.728%
24	11.221	3433	3442	3451	rBV3	594341	948462	4.84%	0.334%
25	11.291	3457	3468	3478	rBV	2115129	3305176	16.88%	1.164%
26	11.344	3478	3488	3501	rVB	3001819	5219208	26.66%	1.838%
27	11.398	3502	3508	3516	rVB	331012	406562	2.08%	0.143%
28	11.452	3517	3528	3538	rBV3	1717735	2948094	15.06%	1.038%
29	11.495	3539	3544	3554	rVB2	375005	517399	2.64%	0.182%
30	11.548	3555	3564	3580	rVB	1407679	2558966	13.07%	0.901%
31	11.621	3580	3591	3602	rBV3	653113	1138236	5.81%	0.401%
32	11.672	3604	3610	3623	rVB7	138638	203961	1.04%	0.072%
33	11.744	3624	3637	3659	rBV	2079296	3890819	19.88%	1.370%
34	11.835	3662	3671	3678	rBV	321725	496229	2.53%	0.175%
35	11.878	3679	3687	3693	rBV	673277	971678	4.96%	0.342%
36	11.924	3694	3704	3716	rVB5	1165259	2440754	12.47%	0.860%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
DB-11(15-20)-02-02-22

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Title : SW846 8260

37	11.988	3716	3728	3736	rBV	2750602	4898276	25.02%	1.725%
38	12.090	3756	3766	3779	rBV6	365802	802060	4.10%	0.283%
39	12.173	3782	3797	3809	rVB5	639846	1583799	8.09%	0.558%
40	12.254	3810	3827	3841	rBV5	3199976	7655989	39.11%	2.697%
41	12.366	3862	3869	3879	rVB	2979980	4311076	22.02%	1.518%
42	12.417	3879	3888	3891	rBV3	1123570	1522404	7.78%	0.536%
43	12.457	3893	3903	3906	rBV3	2422429	3523582	18.00%	1.241%
44	12.578	3940	3948	3957	rBV	1516977	2364504	12.08%	0.833%
45	12.734	3994	4006	4018	rVB3	2831428	4864441	24.85%	1.713%
46	12.817	4019	4037	4045	rBV8	1328939	3360688	17.17%	1.184%
47	12.913	4058	4073	4085	rVB2	4653492	12119536	61.91%	4.269%
48	12.972	4086	4095	4106	rVV6	1337805	2713272	13.86%	0.956%
49	13.055	4110	4126	4137	rVV7	4849739	13003774	66.43%	4.580%
50	13.106	4140	4145	4158	rVB4	2644067	4009544	20.48%	1.412%
51	13.198	4171	4179	4187	rBV4	1329789	1818015	9.29%	0.640%
52	13.286	4205	4212	4238	rVB6	2082323	4991061	25.50%	1.758%
53	13.383	4241	4248	4252	rBV4	736120	968457	4.95%	0.341%
54	13.498	4284	4291	4301	rVB2	3438017	5240310	26.77%	1.846%
55	13.565	4303	4316	4341	rVB4	5154122	13072262	66.78%	4.604%
56	13.672	4347	4356	4376	rVB	2438444	4886347	24.96%	1.721%
57	13.940	4442	4456	4465	rBV2	2441858	4654199	23.77%	1.639%
58	13.999	4466	4478	4488	rBV4	6701748	11427601	58.37%	4.025%
59	14.217	4550	4559	4573	rVB2	7300736	11560080	59.05%	4.072%
60	14.327	4590	4600	4613	rVB5	4363052	8251307	42.15%	2.906%
61	14.506	4657	4667	4674	rBV3	5139979	8699781	44.44%	3.064%
62	14.619	4700	4709	4717	rBV	2234010	3465648	17.70%	1.221%
63	14.673	4719	4729	4742	rVV3	2860169	5815655	29.71%	2.048%
64	14.820	4774	4784	4792	rBV3	1254756	2599344	13.28%	0.916%
65	14.917	4808	4820	4835	rBV4	9661505	19576405	100.00%	6.895%
66	14.981	4836	4844	4857	rVB3	2935459	4946135	25.27%	1.742%
67	15.236	4934	4939	4953	rVV4	1274008	2190221	11.19%	0.771%
68	15.306	4956	4965	4979	rVB6	3786114	7852491	40.11%	2.766%
69	15.560	5049	5060	5069	rBV3	2493187	5091803	26.01%	1.793%
70	16.016	5223	5230	5244	rVB	3188713	5640829	28.81%	1.987%
71	16.341	5337	5351	5369	rVB5	3089777	7243717	37.00%	2.551%
72	16.614	5440	5453	5497	rVB	6611255	17968364	91.79%	6.329%

Sum of corrected areas: 283906702

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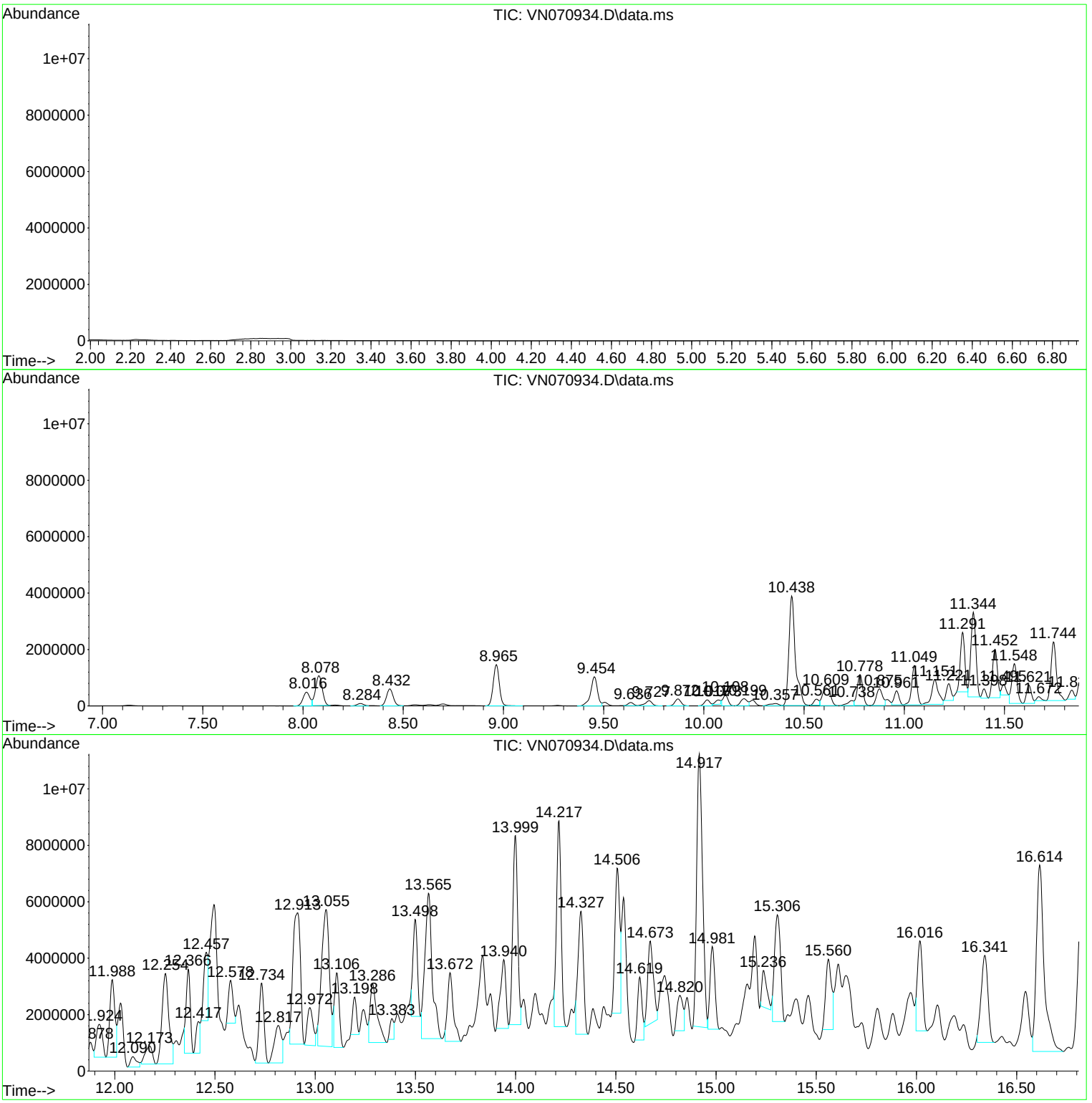
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070934.D
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Operator : JC/MD
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DB-11(15-20)-02-02-22

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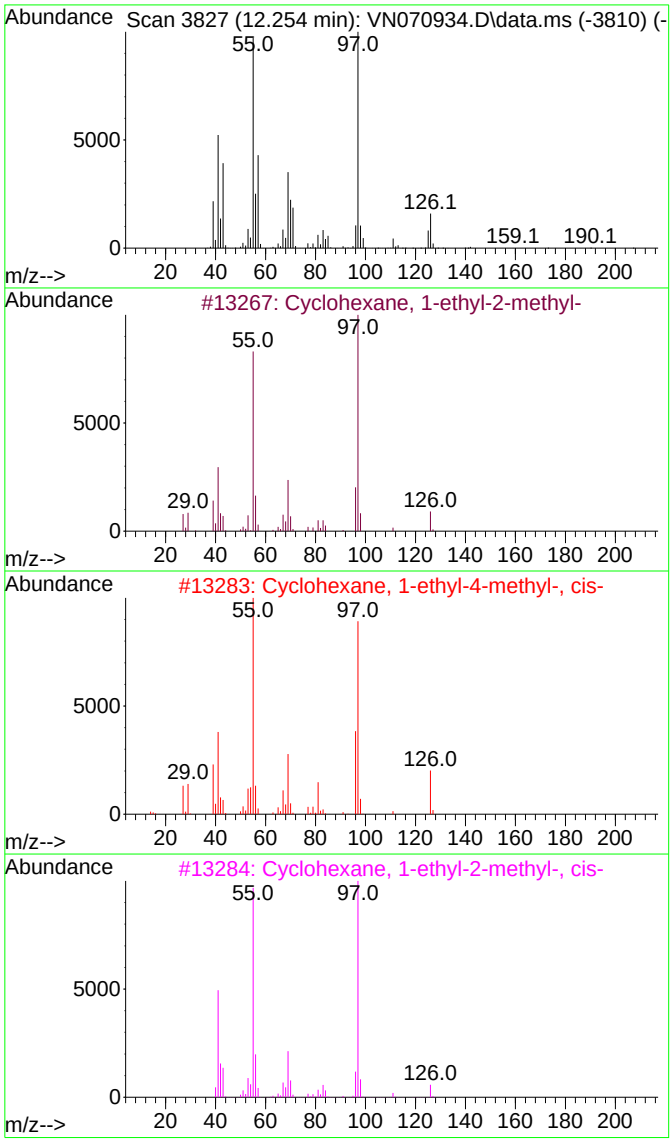
Quant Title : SW846 8260

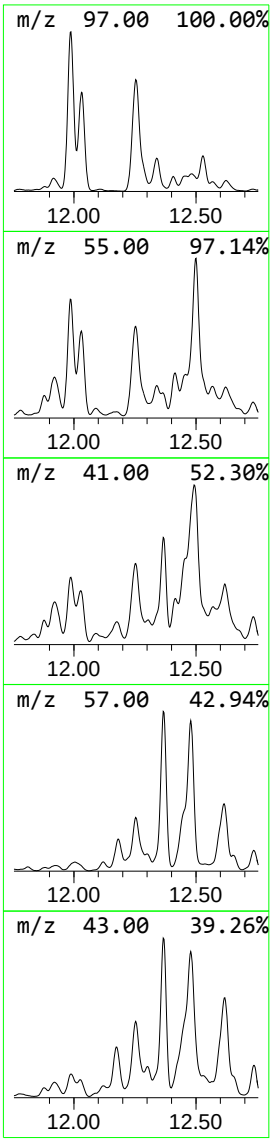
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.254	98.39 ug/l	7655990	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	74
2	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	64
3	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	64
4	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
5	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
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Operator : JC/MD
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

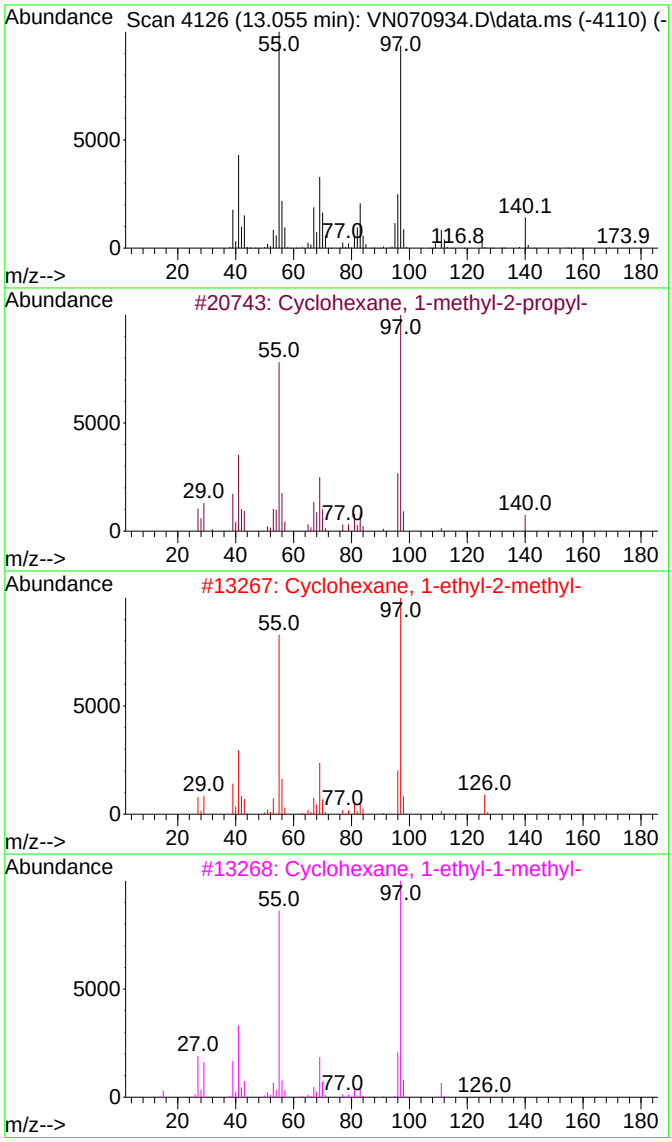
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

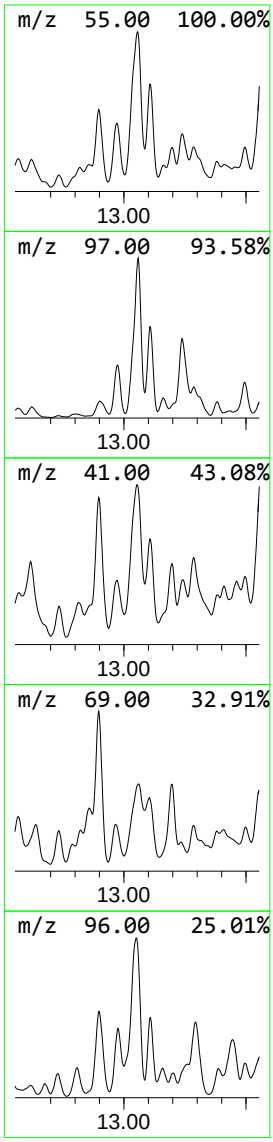
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1-methyl-2-pro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.055	133.06 ug/l	13003800	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	74
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	59
3	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	58
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	52
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070934.D
Acq On : 3 Feb 2022 16:59
Operator : JC/MD
Sample : N1381-05
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

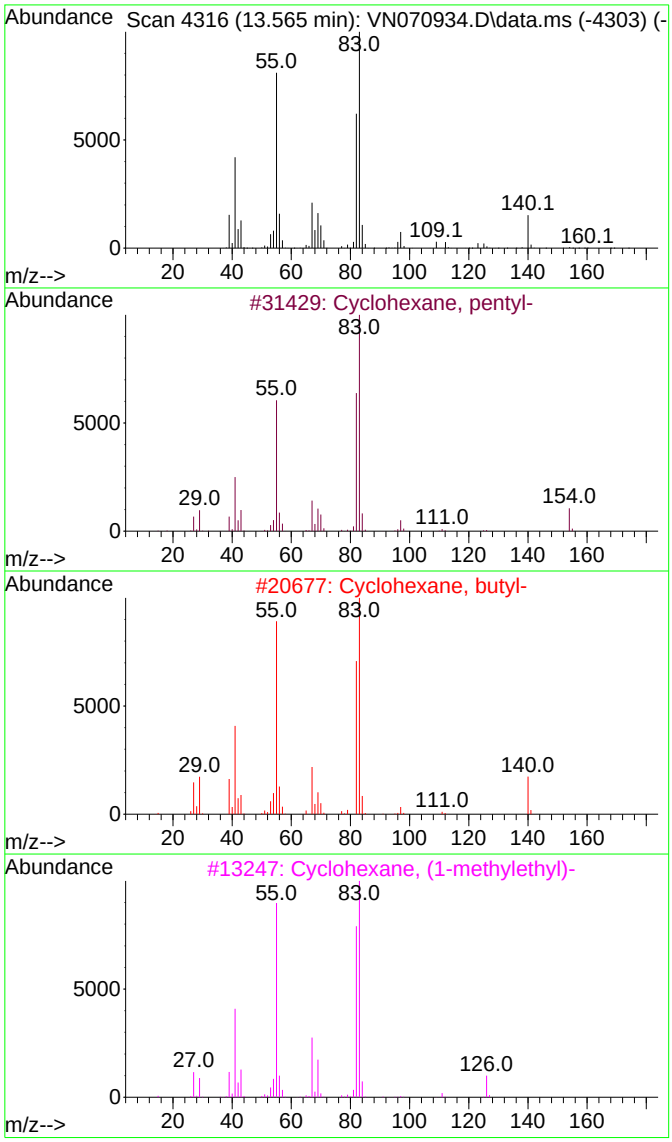
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

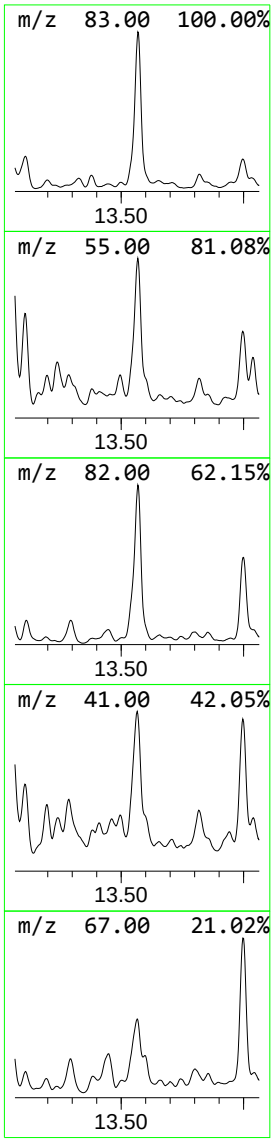
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, pentyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.565	133.76 ug/l	13072300	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	91
2	Cyclohexane, butyl-	140	C10H20	001678-93-9	91
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	80
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	78
5	Cyclohexane, octyl-	196	C14H28	001795-15-9	78





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Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

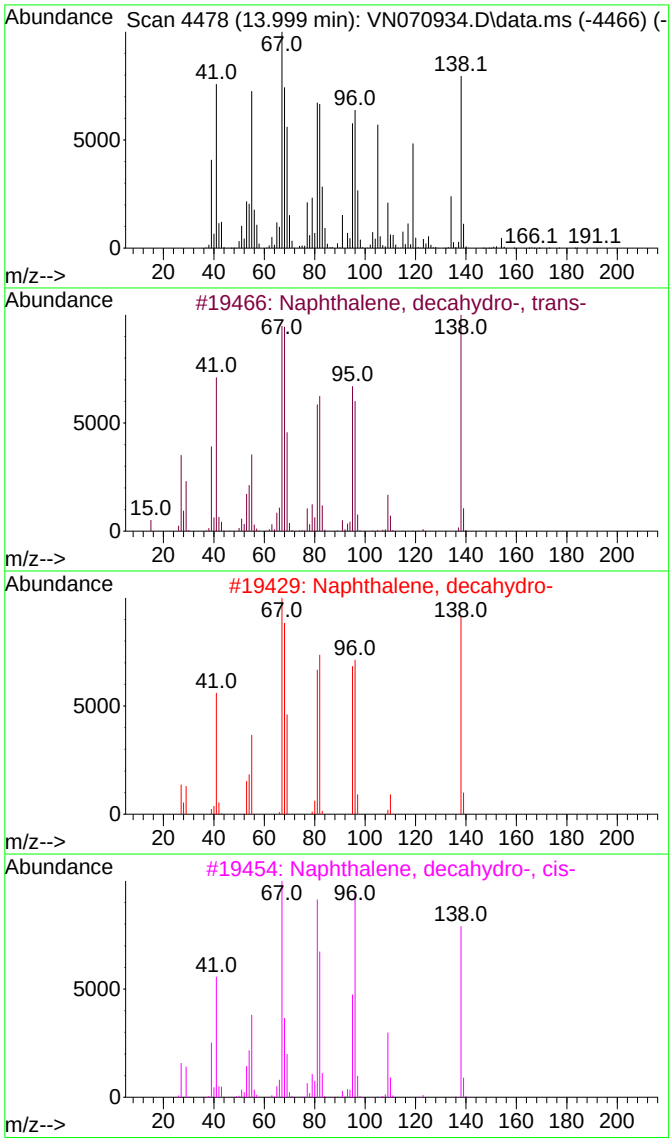
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

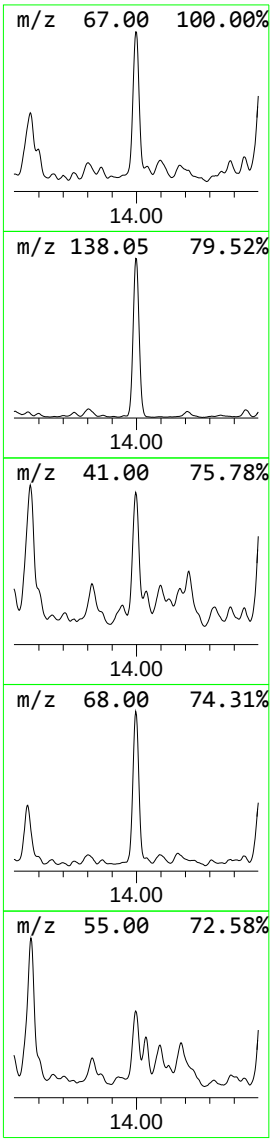
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, decahydro-, tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	116.93 ug/l	11427600	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	96
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	94
3	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	92
4	1,1'-Bicyclopentyl	138	C10H18	001636-39-1	76
5	Spiro[4.5]decane	138	C10H18	000176-63-6	64





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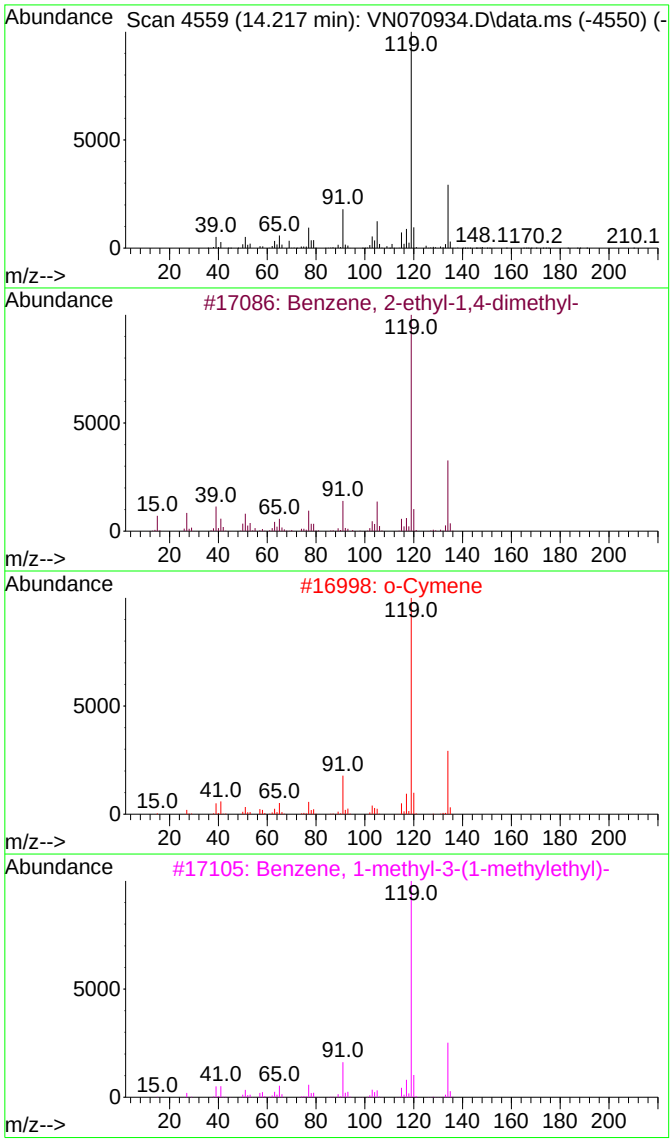
Quant Title : SW846 8260

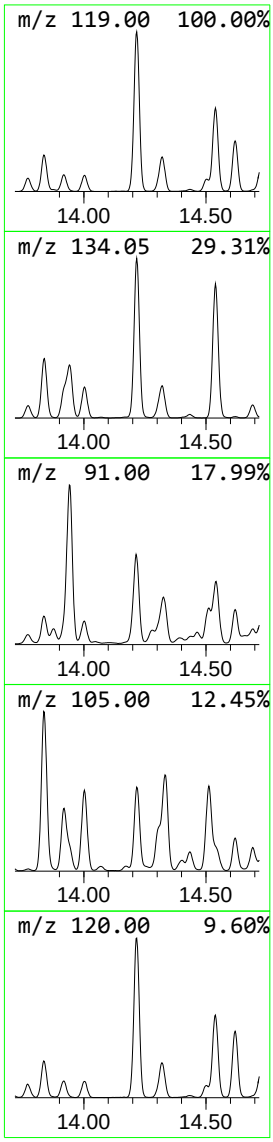
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	118.29 ug/l	11560100	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





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Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

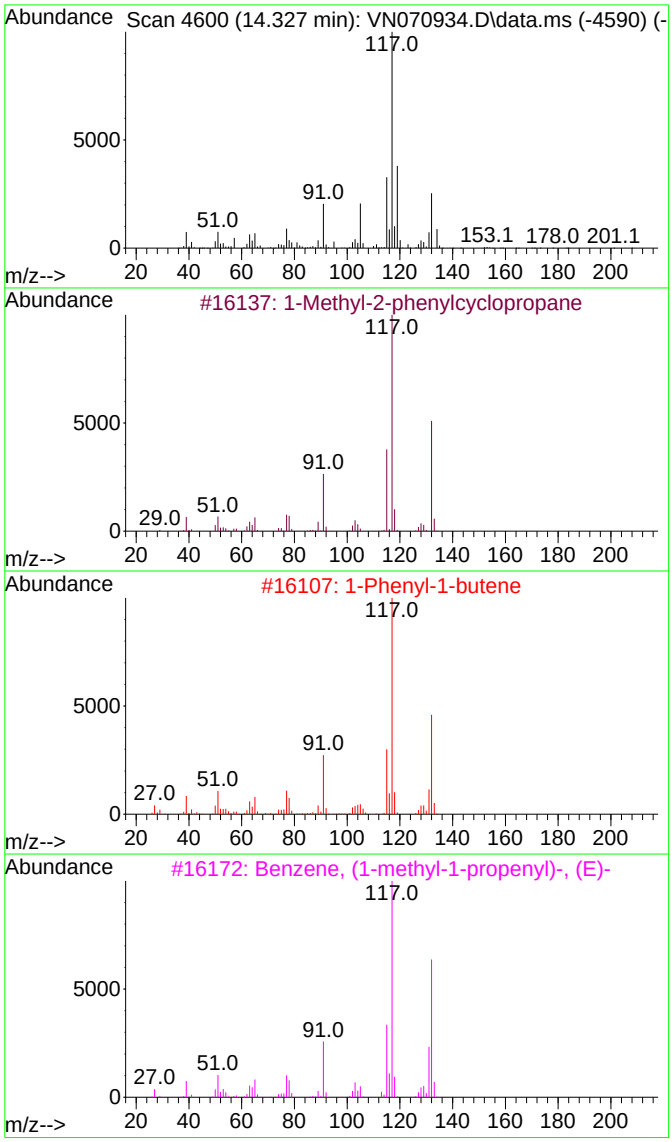
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

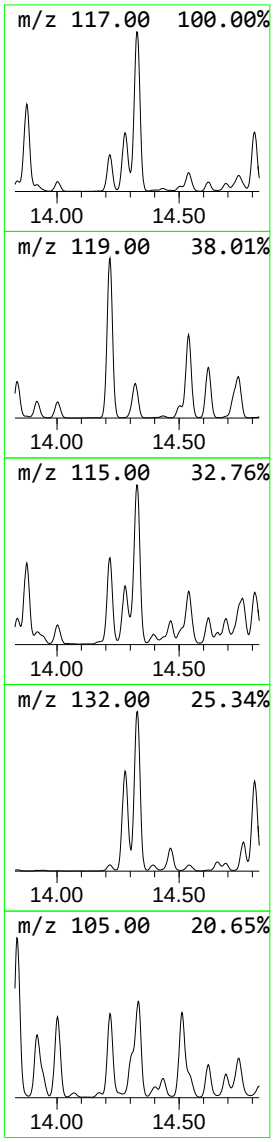
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Methyl-2-phenylcyclopropane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	84.43 ug/l	8251310	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	68





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Data File : VN070934.D
Acq On : 3 Feb 2022 16:59
Operator : JC/MD
Sample : N1381-05
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

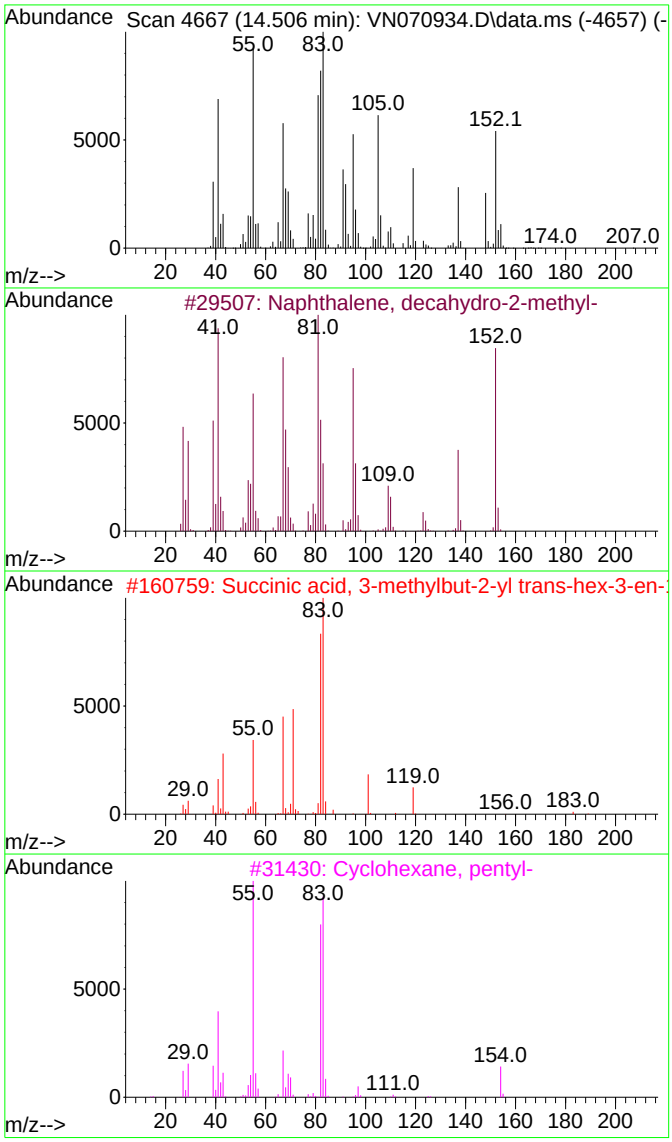
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

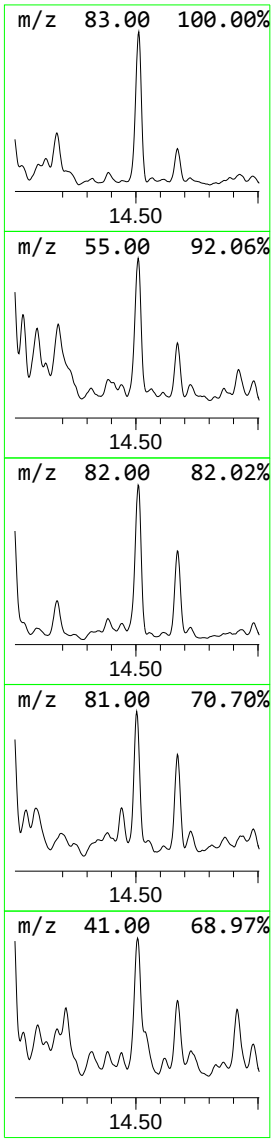
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, decahydro-2-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.506	89.02 ug/l	8699780	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	83
2	Succinic acid, 3-methylbut-2-yl ...	270	C15H26O4	1000391-11-1	49
3	Cyclohexane, pentyl-	154	C11H22	004292-92-6	46
4	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	46
5	Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	43





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Data File : VN070934.D
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Operator : JC/MD
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Instrument :
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ClientSampleId :
DB-11(15-20)-02-02-22

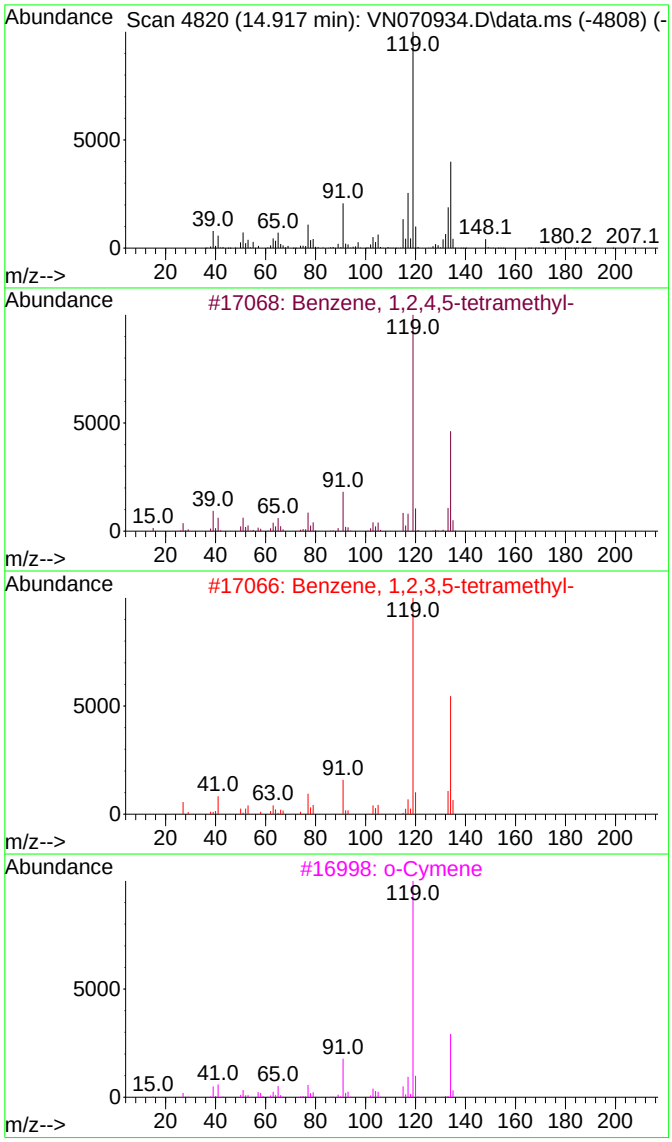
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

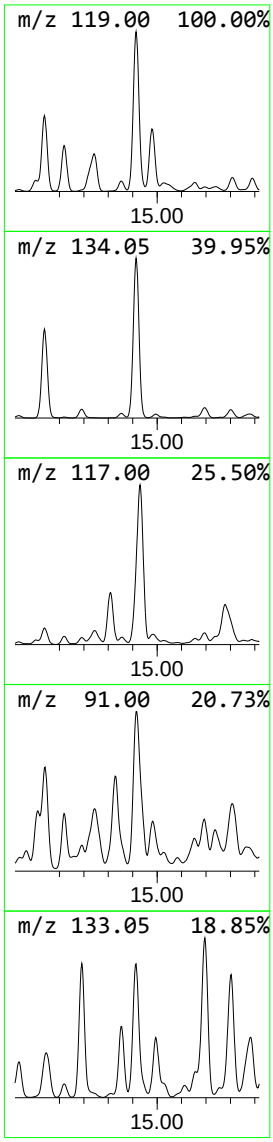
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.917	200.32 ug/l	19576400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
3	o-Cymene	134	C10H14	000527-84-4	81
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81





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Data File : VN070934.D
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Operator : JC/MD
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

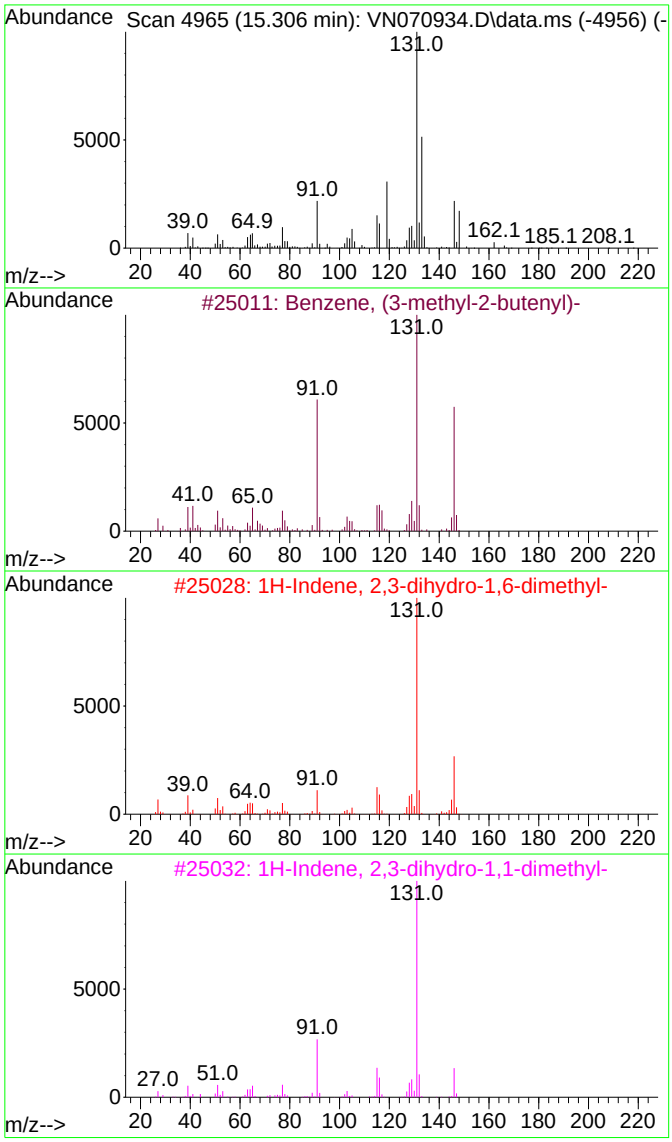
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

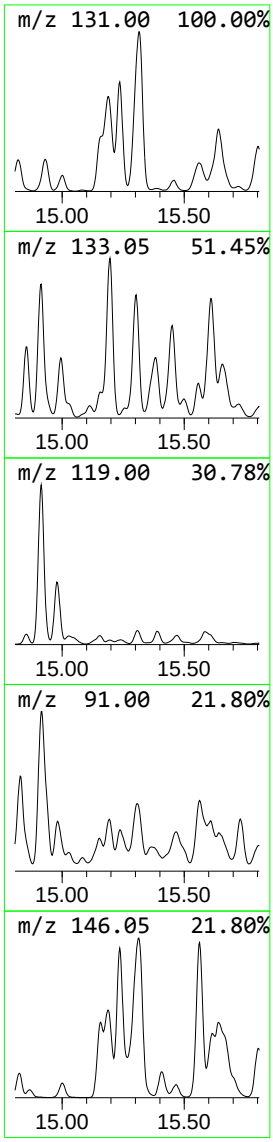
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (3-methyl-2-butenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.306	80.35 ug/l	7852490	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	91
2	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	64
3	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	64
4	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	64
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	64





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

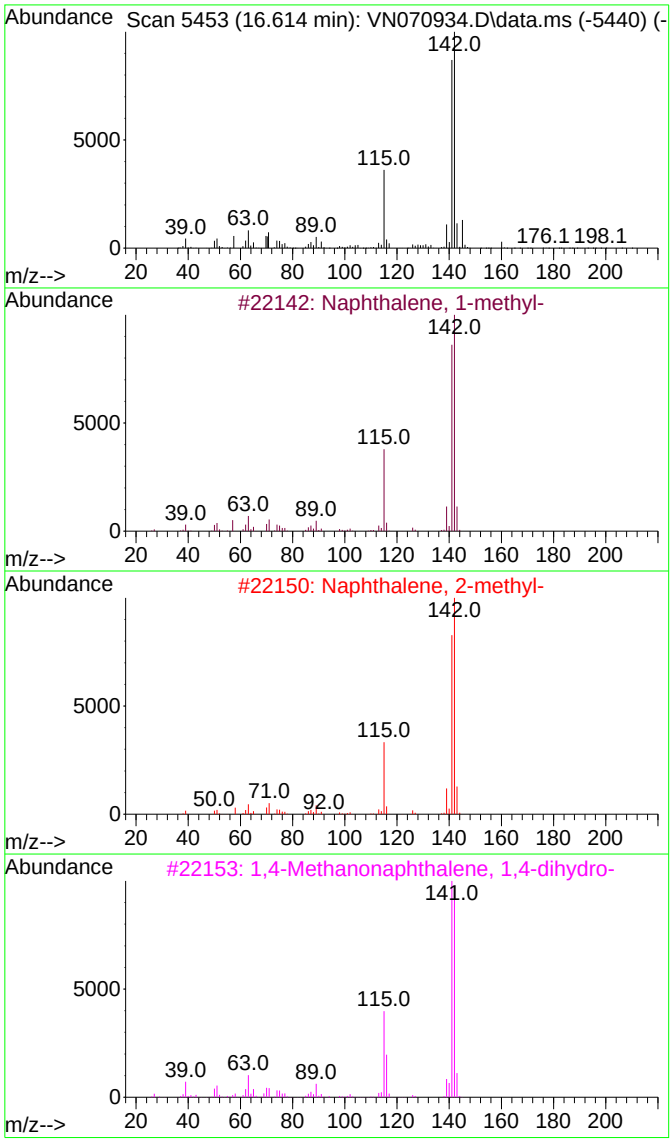
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

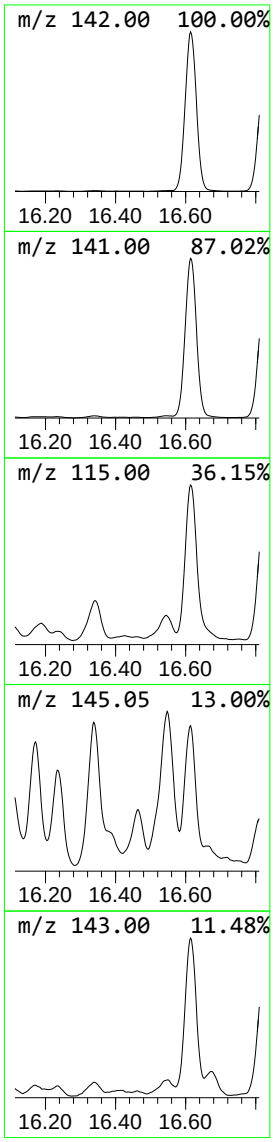
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.614	183.86 ug/l	17968400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4	Benzocycloheptatriene	142	C11H10	000264-09-5	87
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070934.D
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MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

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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
Cyclohexane, 1-...	12.254	98.4	ug/l	7655990	3	11.744	3890820	50.0
Cyclohexane, 1-...	13.055	133.1	ug/l	13003800	4	13.675	4886350	50.0
Cyclohexane, pe...	13.565	133.8	ug/l	13072300	4	13.675	4886350	50.0
Naphthalene, de...	13.999	116.9	ug/l	11427600	4	13.675	4886350	50.0
Benzene, 2-ethy...	14.217	118.3	ug/l	11560100	4	13.675	4886350	50.0
1-Methyl-2-phen...	14.327	84.4	ug/l	8251310	4	13.675	4886350	50.0
Naphthalene, de...	14.506	89.0	ug/l	8699780	4	13.675	4886350	50.0
Benzene, 1,2,4,...	14.917	200.3	ug/l	19576400	4	13.675	4886350	50.0
Benzene, (3-met...	15.306	80.3	ug/l	7852490	4	13.675	4886350	50.0
1,4-Methanonaph...	16.614	183.9	ug/l	17968400	4	13.675	4886350	50.0