LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

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\82N112320W.M
Title : SW846 8260

Signal : TIC: VN064897.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.978	66	74	87	rVB2	6623	10350	1.00%	0.109%
2	3.785	620	636	659	rBV	17060	50936	4.94%	0.535%
3	7.547	1788	1806	1816	rBV2	112615	288197	27.96%	3.028%
4	7.621	1818	1829	1846	rVV	202639	487345	47.27%	5.120%
5	7.698	1846	1853	1866	rVB4	4742	10724	1.04%	0.113%
6	7.830	1880	1894	1909	rBV2	20958	49061	4.76%	0.515%
7	7.984	1925	1942	1965	rBV	117578	275137	26.69%	2.891%
8	8.396	2057	2070	2083	rBV3	26354	53172	5.16%	0.559%
9	8.547	2101	2117	2135	rBV	325899	674322	65.41%	7.085%
10	9.045	2260	2272	2283	rVB7	13130	29609	2.87%	0.311%
11	9.691	2465	2473	2481	rBV5	5799	10594	1.03%	0.111%
12	9.836	2501	2518	2539	rVB4	6169	16087	1.56%	0.169%
13	9.952	2544	2554	2565	rBV3	6593	13292	1.29%	0.140%
14	10.058	2573	2587	2597	rBV	517950	946069	91.77%	9.940%
15	10.122	2597	2607	2625	rVB	441450	799321	77.54%	8.398%
16	10.251	2636	2647	2656	rVB4	8745	15519	1.51%	0.163%
17	10.830	2818	2827	2835	rBV4	14007	31797	3.08%	0.334%
18	11.379	2985	2998	3017	rVB	500900	884616	85.81%	9.294%
19	11.482	3022	3030	3039	rVB2	13505	20919	2.03%	0.220%
20	11.592	3052	3064	3085	rBV4	56117	142179	13.79%	1.494%
21	12.376	3291	3308	3323	rBV	449360	900706	87.37%	9.463%
22	12.566	3360	3367	3373	rBV	25742	39327	3.81%	0.413%
23	12.627	3378	3386	3393	rBV	94494	163999	15.91%	1.723%
24	12.704	3404	3410	3422	rVB2	81129	129488	12.56%	1.360%
25	12.804	3435	3441	3450	rVB3	11140	15025	1.46%	0.158%
26	12.862	3450	3459	3468	rBV	42505	71442	6.93%	0.751%
27	13.013	3495	3506	3519	rBV	176247	295835	28.70%	3.108%
28	13.080	3521	3527	3533	rVB3	8583	13186	1.28%	0.139%
29	13.315	3590	3600	3623	rVB2	557711	1030895	100.00%	10.831%
30	13.424	3627	3634	3646	rVB	24251	41306	4.01%	0.434%
31	13.514	3647	3662	3668	rBV	69400	126721	12.29%	1.331%
32	13.559	3669	3676	3678	rBV	69623	82598	8.01%	0.868%
33	13.775	3737	3743	3747	rBV2	25125	33192	3.22%	0.349%
34	13.862	3762	3770	3779	rVB2	51064	78757	7.64%	0.827%

LSC Area Percent Report

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Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

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\82N112320W.M
Title : SW846 8260

35	13.968	3794	3803	3815	rVV5	40294	75496	7.32%	0.793%
36	14.100	3836	3844	3853	rBV3	29602	54046	5.24%	0.568%
37	14.183	3865	3870	3875	rBV	17620	20961	2.03%	0.220%
38	14.219	3876	3881	3888	rVV2	34867	47599	4.62%	0.500%
39	14.270	3891	3897	3916	rVB4	33702	93777	9.10%	0.985%
40	14.405	3933	3939	3946	rBV3	18024	22730	2.20%	0.239%
41	14.450	3946	3953	3962	rBV3	26442	50569	4.91%	0.531%
42	14.559	3977	3987	4000	rBV6	64815	143233	13.89%	1.505%
43	14.620	4001	4006	4013	rVB	12615	17997	1.75%	0.189%
44	14.929	4094	4102	4115	rVB7	30115	62164	6.03%	0.653%
45	15.103	4144	4156	4167	rBV2	88030	168941	16.39%	1.775%
46	15.209	4184	4189	4197	rVB7	17816	24724	2.40%	0.260%
47	15.382	4236	4243	4258	rVB5	25253	50739	4.92%	0.533%
48	15.733	4345	4352	4364	rVB5	14439	26924	2.61%	0.283%
49	15.852	4380	4389	4402	rVB	67620	133652	12.96%	1.404%
50	16.119	4460	4472	4493	rVB2	225609	478334	46.40%	5.026%
51	16.308	4519	4531	4553	rVB2	94689	214099	20.77%	2.249%

Sum of corrected areas: 9517708

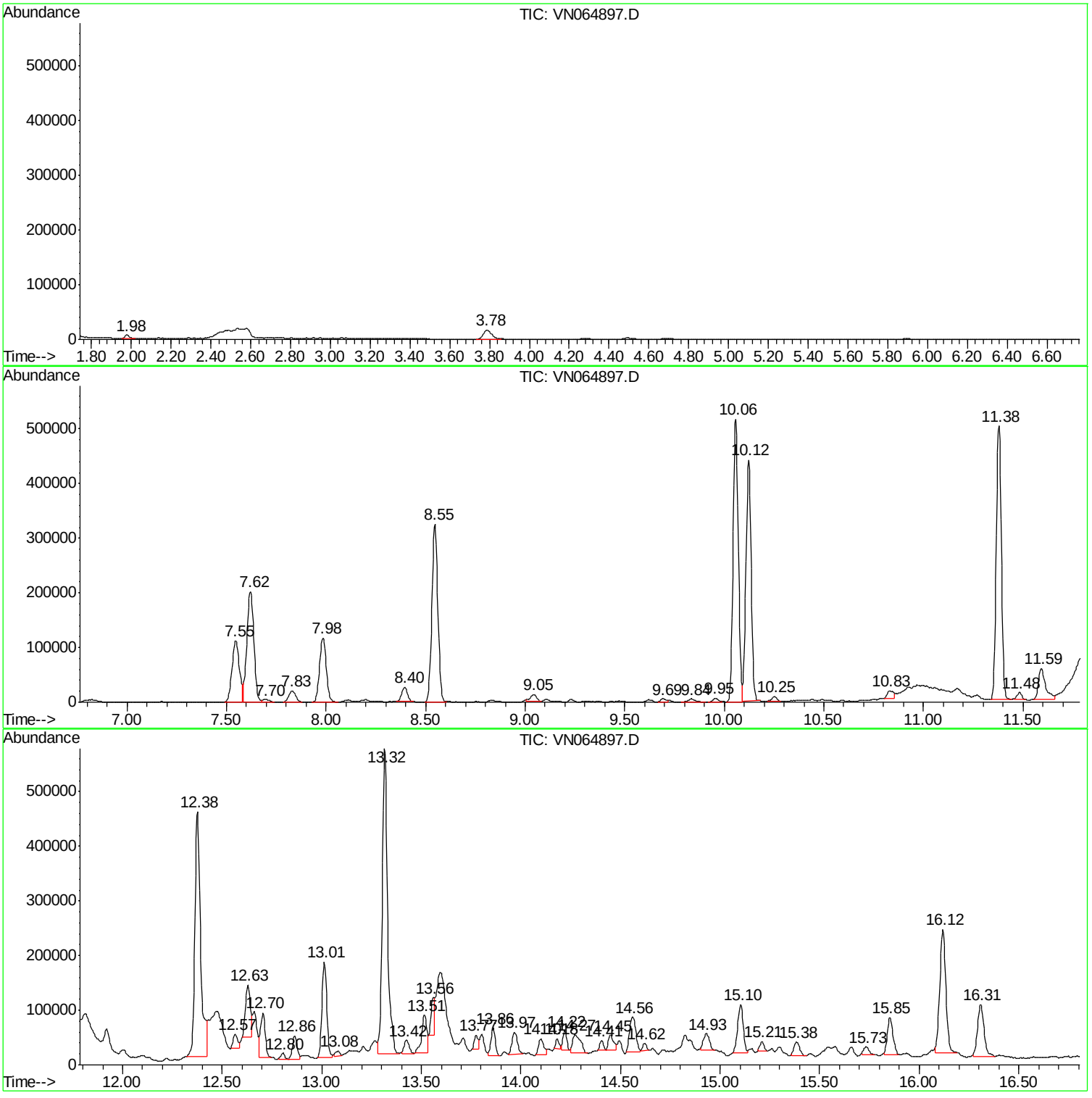
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

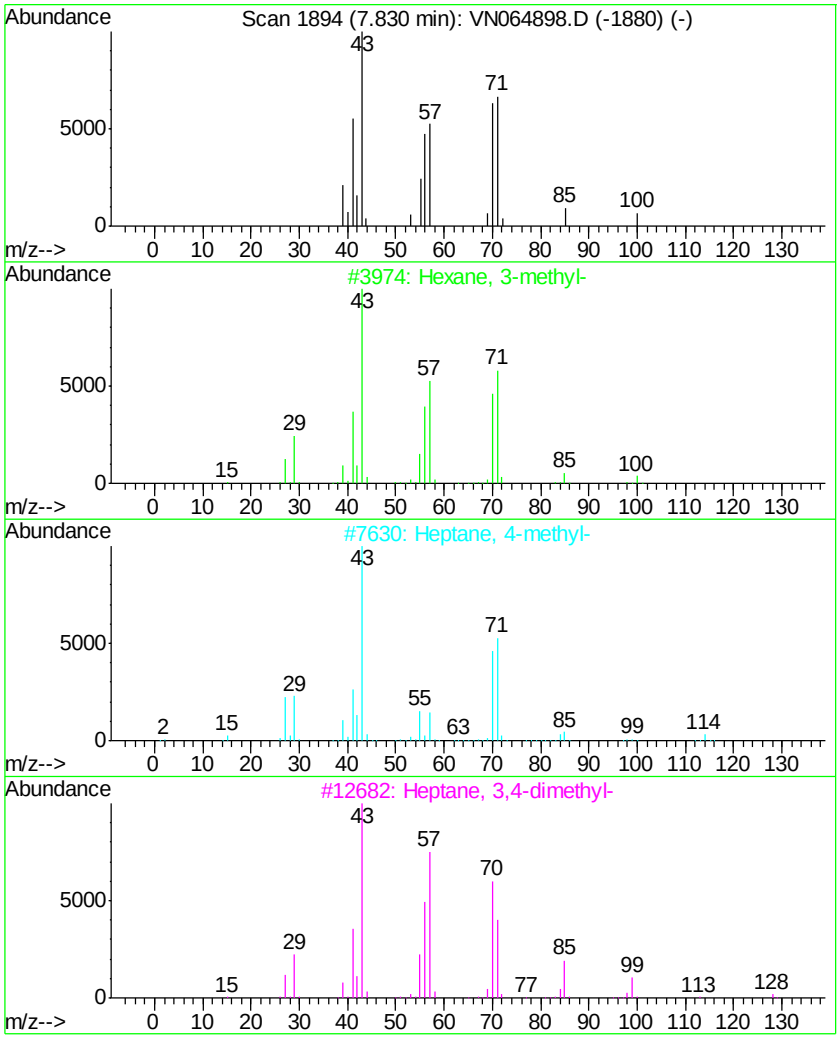
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

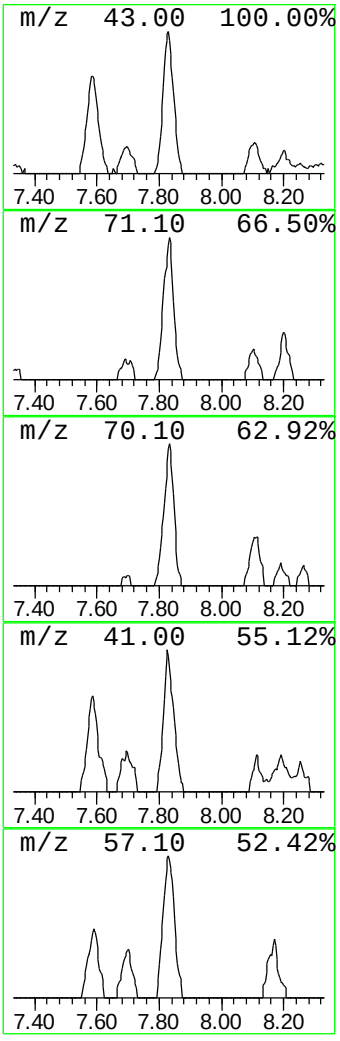
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.83	5.03 ug/l	49061	Pentafluorobenzene	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
3	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	56
4	Heptane	100	C7H16	000142-82-5	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

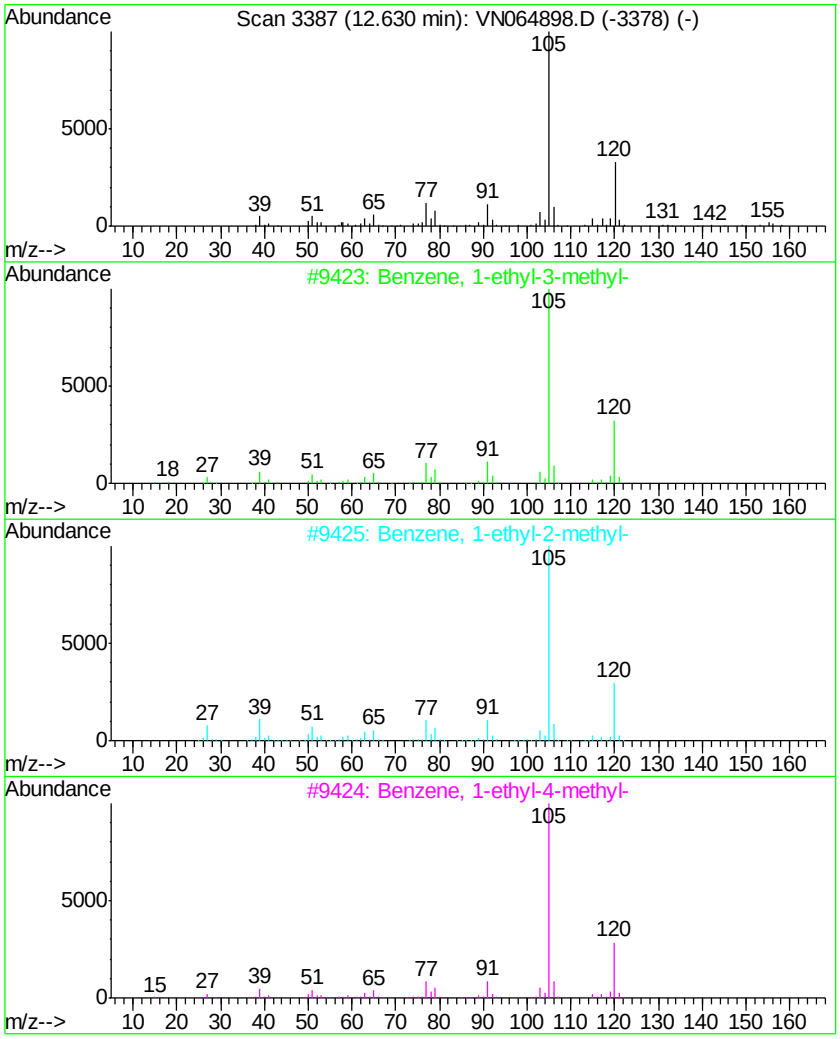
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

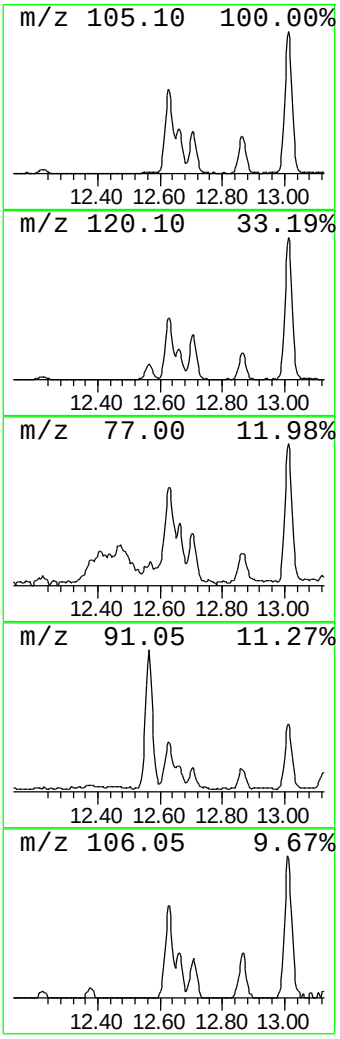
****

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.95 ug/l	163999	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87
5	Mesitylene	120	C9H12	000108-67-8	87





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

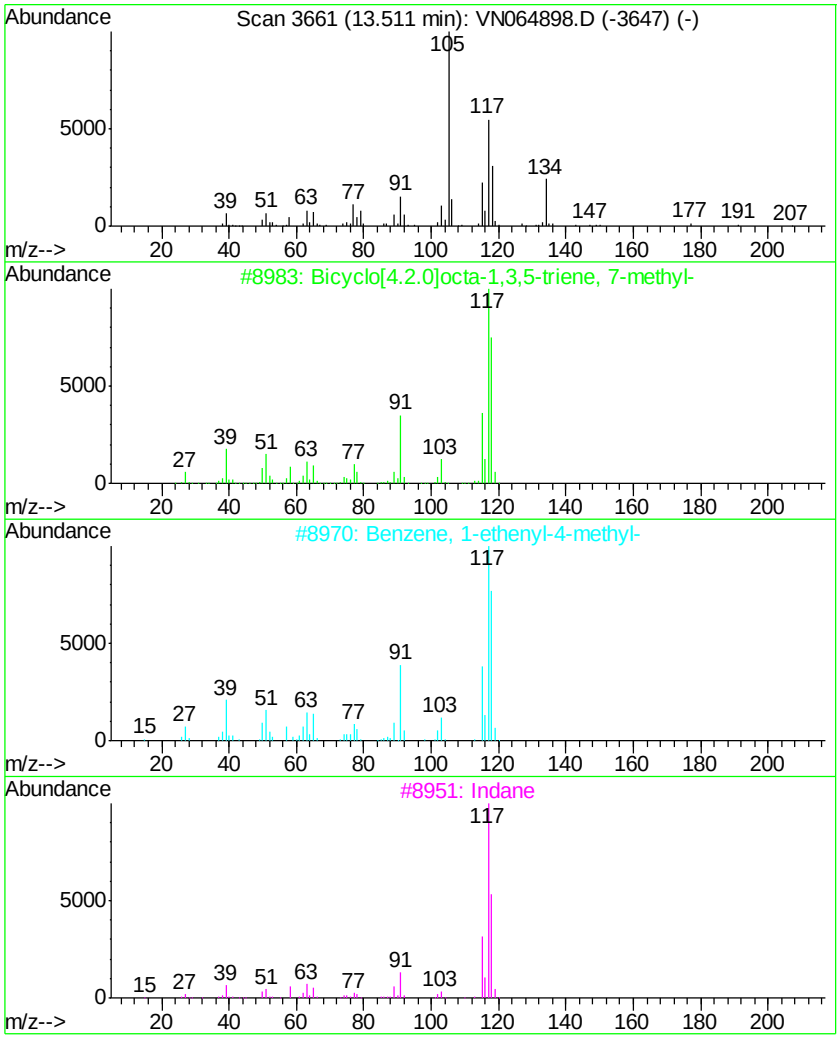
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

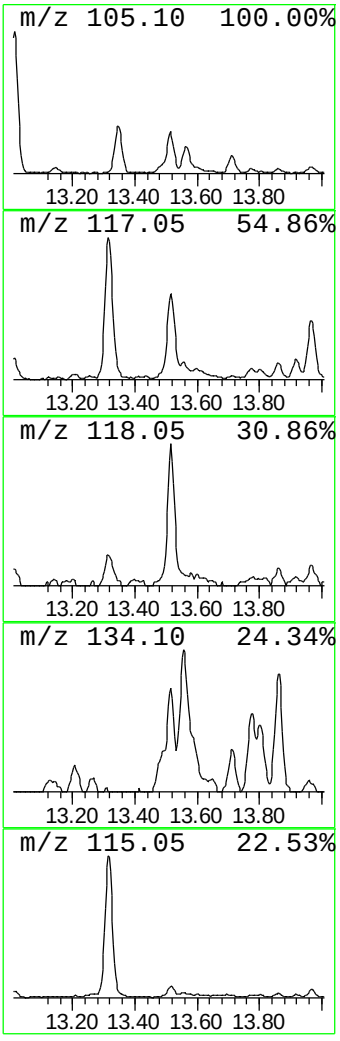
****

Peak Number 3 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	6.15 ug/l	126721	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	50
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	50
3	Indane	118	C9H10	000496-11-7	46
4	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	45
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

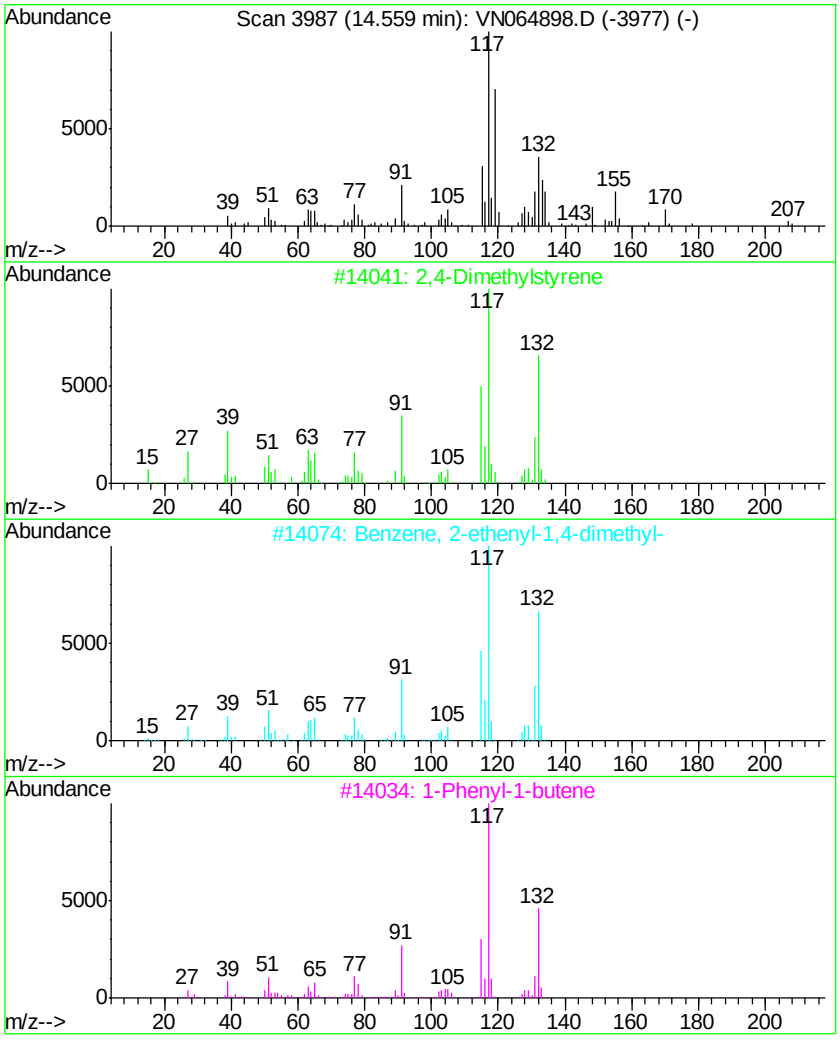
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

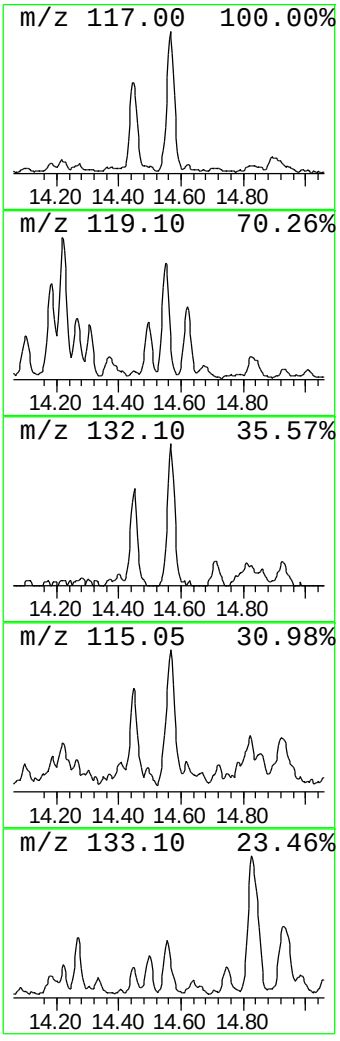
****

Peak Number 4 2,4-Dimethylstyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	6.95 ug/l	143233	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylstyrene	132	C10H12	002234-20-0	74
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	74
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	55
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	55
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

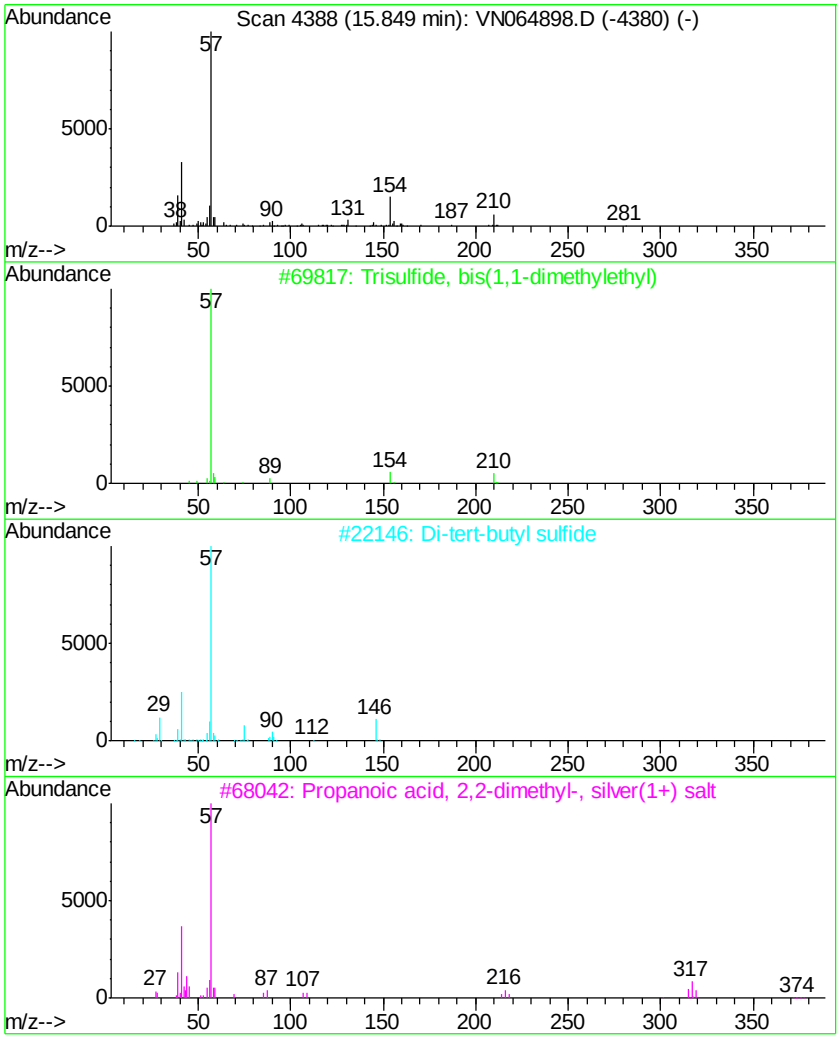
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

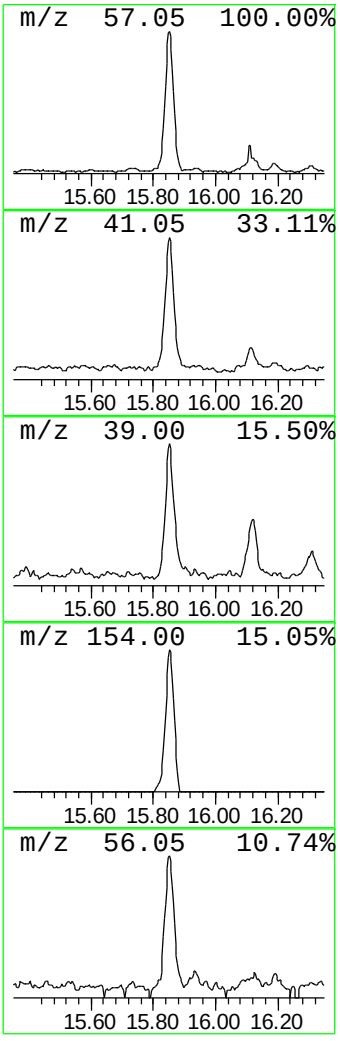
****

Peak Number 5 Trisulfide, bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	6.48 ug/l	133652	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	72
2	Di-tert-butyl sulfide	146	C8H18S	000107-47-1	47
3	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	37
4	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	25
5	Propanoyl chloride	92	C3H5ClO	000079-03-8	23





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

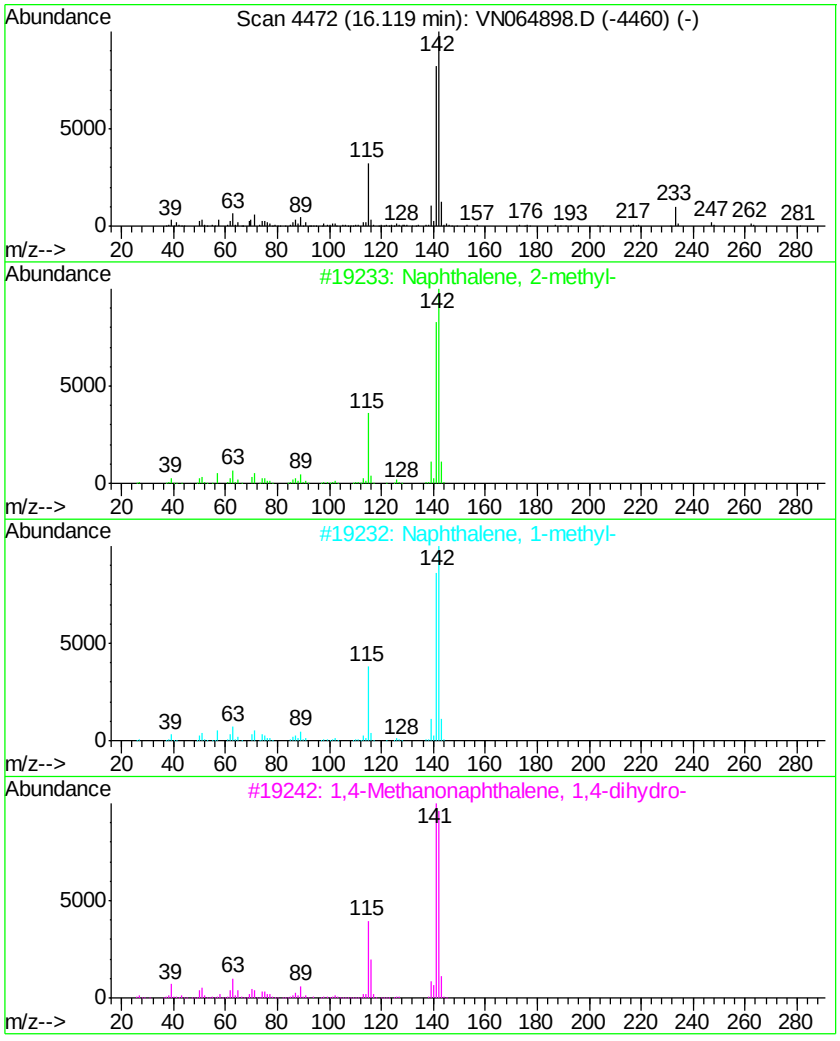
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

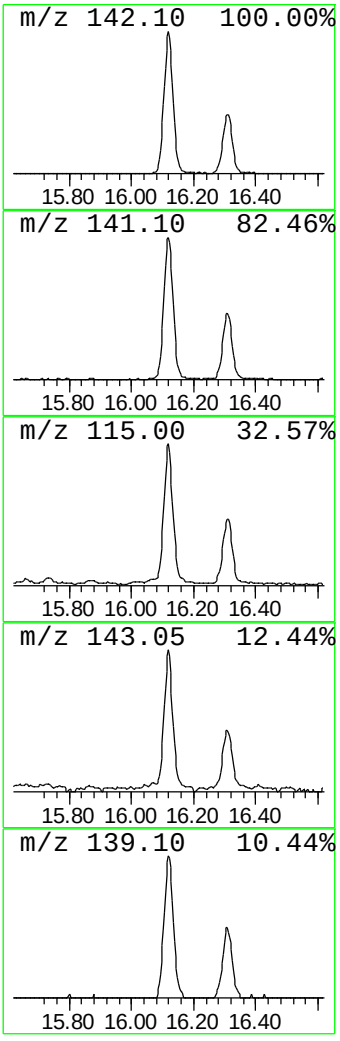
****

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	23.20 ug/l	478334	1,4-Dichlorobenzene-d4	13.32

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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	Naphthalene, 1-(2-hydroxypropyl)	186	C13H14O	027653-13-0	78





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

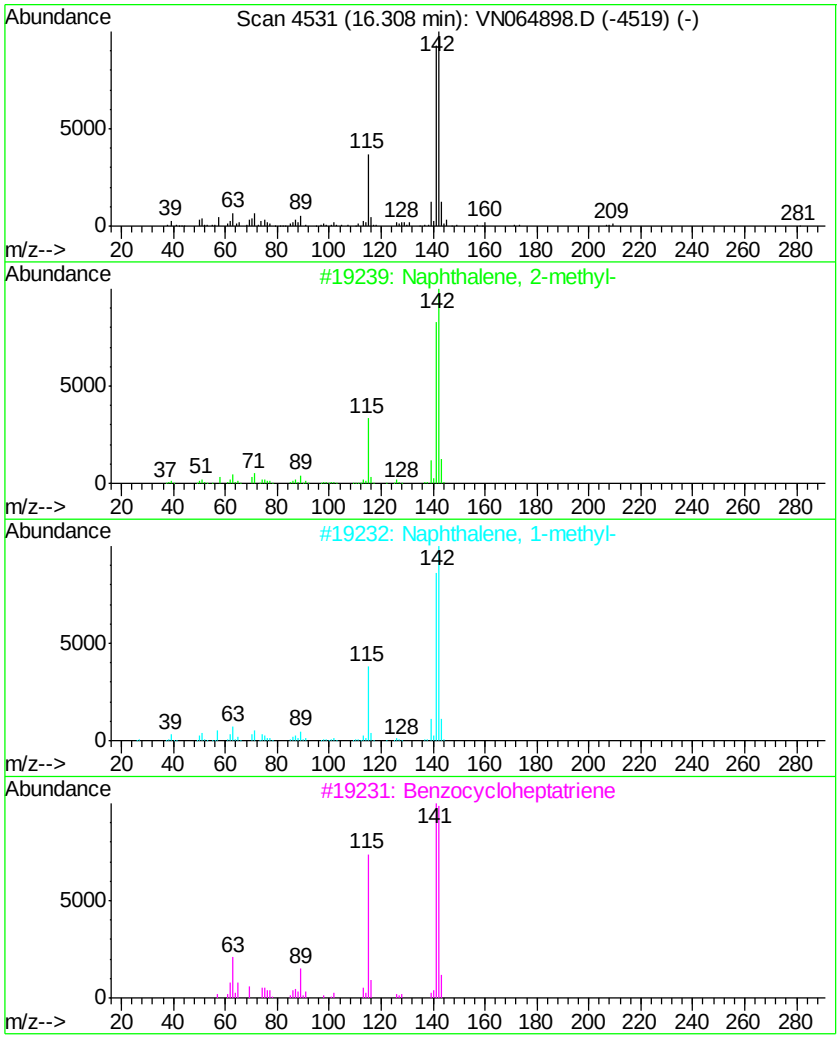
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

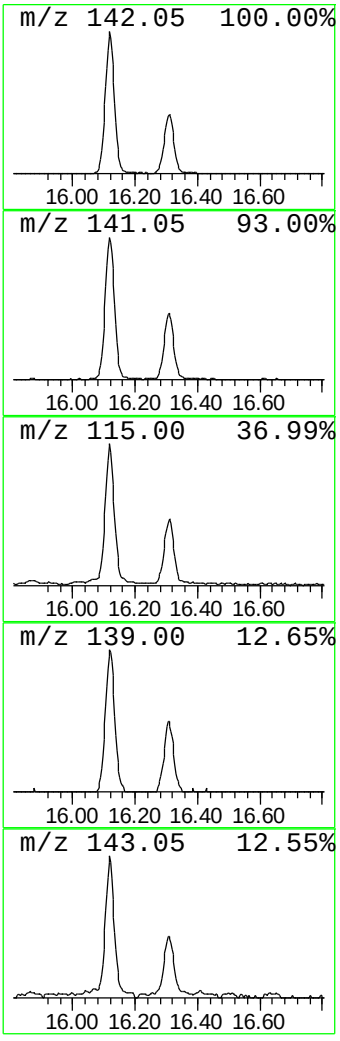
****

Peak Number 7 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	10.38 ug/l	214099	1,4-Dichlorobenzene-d4	13.32

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	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064898.D
Acq On : 3 Dec 2020 14:35
Operator : JC/MD
Sample : L4918-05
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.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
Hexane, 3-methyl-	7.83	5.0	ug/l	49061	1	7.62	487345	50.0
Benzene, 1-ethyl-...	12.63	8.0	ug/l	163999	4	13.32	1030900	50.0
Bicyclo[4.2.0]oct...	13.51	6.2	ug/l	126721	4	13.32	1030900	50.0
2,4-Dimethylstyrene	14.56	7.0	ug/l	143233	4	13.32	1030900	50.0
Trisulfide, bis(1...	15.85	6.5	ug/l	133652	4	13.32	1030900	50.0
Naphthalene, 1-me...	16.12	23.2	ug/l	478334	4	13.32	1030900	50.0
Benzocycloheptatr...	16.31	10.4	ug/l	214099	4	13.32	1030900	50.0