LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN069920.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	86	102	114	rBV	418329	953407	5.12%	0.939%
2	2.445	162	170	195	rVB	799793	1360320	7.31%	1.340%
3	3.143	414	430	458	rVB	1018438	2321147	12.47%	2.287%
4	3.524	556	572	599	rVB6	138226	442193	2.38%	0.436%
5	3.993	728	747	771	rVB3	135987	363430	1.95%	0.358%
6	4.261	824	847	875	rBV6	47784	205976	1.11%	0.203%
7	5.082	1132	1153	1166	rBV4	92675	322386	1.73%	0.318%
8	5.374	1235	1262	1311	rBV2	959653	3483934	18.72%	3.432%
9	5.618	1326	1353	1389	rVB2	990268	3471464	18.65%	3.420%
10	6.498	1646	1681	1708	rBV3	407141	1421190	7.64%	1.400%
11	7.147	1900	1923	1942	rBV2	191732	547525	2.94%	0.539%
12	7.844	2168	2183	2204	rVB2	90009	238805	1.28%	0.235%
13	8.024	2225	2250	2261	rBV3	934943	2272564	12.21%	2.239%
14	8.086	2261	2273	2295	rVV	1738236	4116825	22.12%	4.056%
15	8.174	2297	2306	2329	rVB5	84455	220312	1.18%	0.217%
16	8.458	2385	2412	2431	rBV3	7328750	18610132	100.00%	18.334%
17	8.536	2433	2441	2455	rVB	354171	729770	3.92%	0.719%
18	8.968	2580	2602	2627	rBV	2696101	5675388	30.50%	5.591%
19	9.791	2896	2909	2930	rBV3	79620	205055	1.10%	0.202%
20	10.014	2984	2992	3007	rVB2	124001	243063	1.31%	0.239%
21	10.202	3046	3062	3093	rBV2	276046	750695	4.03%	0.740%
22	10.440	3134	3151	3169	rBV	4256401	8051560	43.26%	7.932%
23	10.947	3326	3340	3359	rVB2	201309	394268	2.12%	0.388%
24	11.089	3367	3393	3398	rBV4	260456	552410	2.97%	0.544%
25	11.130	3399	3408	3432	rVB	786678	1434009	7.71%	1.413%
26	11.588	3568	3579	3589	rBV	140276	245121	1.32%	0.241%
27	11.744	3619	3637	3663	rBV	4562200	8431407	45.31%	8.306%
28	11.843	3666	3674	3696	rVB4	109177	274444	1.47%	0.270%
29	12.278	3813	3836	3855	rBV5	72837	232241	1.25%	0.229%
30	12.731	3990	4005	4028	rBV	3659217	6536126	35.12%	6.439%
31	12.919	4059	4075	4093	rBV	193447	382133	2.05%	0.376%
32	13.219	4172	4187	4202	rBV	257975	532587	2.86%	0.525%
33	13.675	4342	4357	4376	rBV	4214500	7332692	39.40%	7.224%
34	13.838	4407	4418	4422	rBV	296905	436869	2.35%	0.430%
35	13.876	4423	4432	4465	rVB	1361392	2692022	14.47%	2.652%
36	14.002	4467	4479	4491	rBV2	330836	575800	3.09%	0.567%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

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\82N120221W.M
Title : SW846 8260

37	14.217	4547	4559	4571	rBV	761839	1209097	6.50%	1.191%
38	14.327	4588	4600	4612	rVB3	1186754	1990833	10.70%	1.961%
39	14.463	4643	4651	4659	rBV4	132689	198169	1.06%	0.195%
40	14.538	4671	4679	4688	rBV	523773	679983	3.65%	0.670%
41	14.622	4703	4710	4717	rBV2	161963	200910	1.08%	0.198%
42	14.812	4771	4781	4791	rBV3	353689	627527	3.37%	0.618%
43	14.930	4808	4825	4838	rBV2	1198511	2563038	13.77%	2.525%
44	15.083	4873	4882	4897	rBV2	352041	574148	3.09%	0.566%
45	15.196	4912	4924	4933	rBV5	514354	1020484	5.48%	1.005%
46	15.308	4954	4966	4984	rVB4	666693	1592393	8.56%	1.569%
47	15.504	5031	5039	5051	rVB	580135	985958	5.30%	0.971%
48	15.560	5053	5060	5070	rVB2	183234	275193	1.48%	0.271%
49	15.804	5139	5151	5167	rBV2	378304	748056	4.02%	0.737%
50	16.107	5255	5264	5276	rBV3	200646	359624	1.93%	0.354%
51	16.343	5337	5352	5379	rBV3	486740	1126120	6.05%	1.109%
52	16.617	5443	5454	5485	rVB4	501908	1294034	6.95%	1.275%

Sum of corrected areas: 101504837

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
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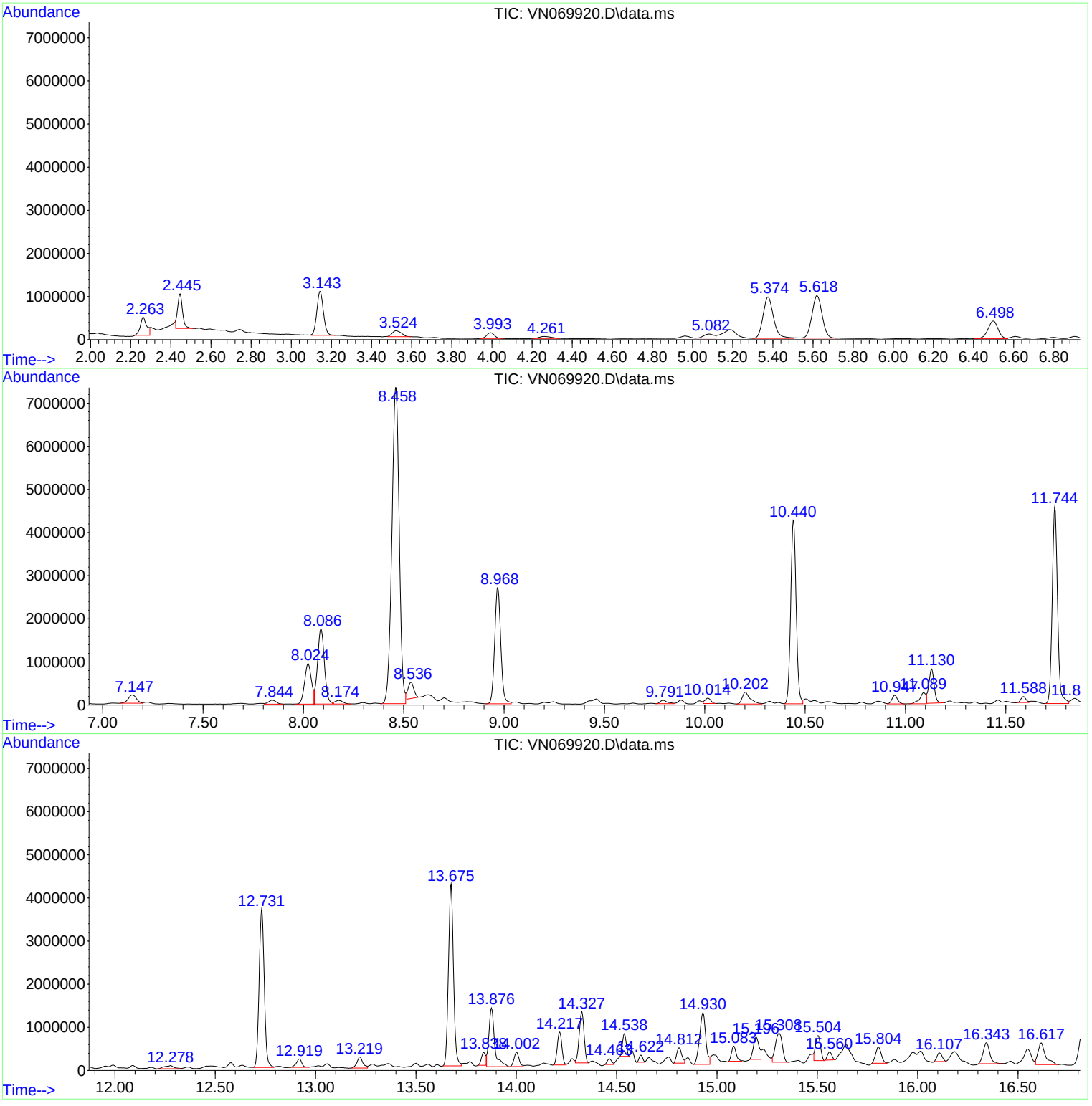
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

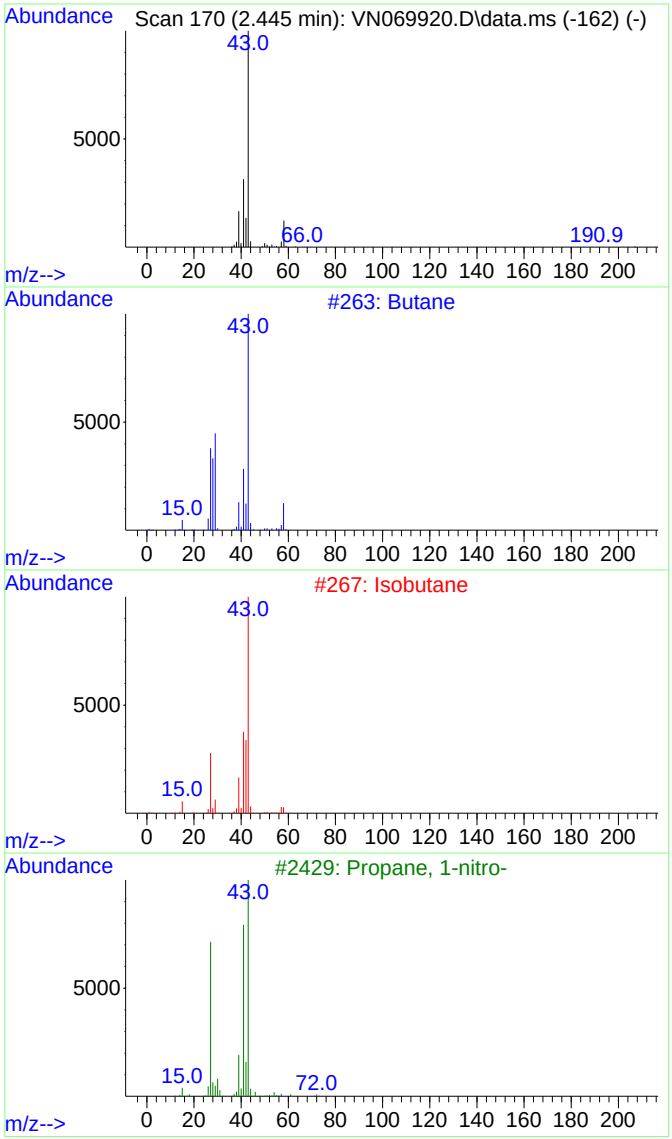
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

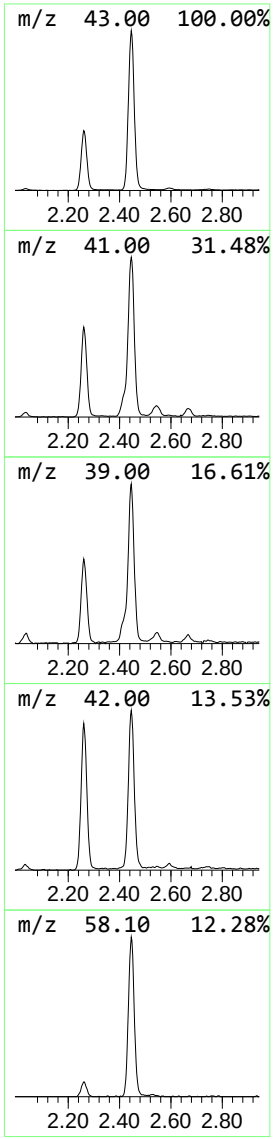
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.445	16.52 ug/l	1360320	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
2	Isobutane	58	C4H10	000075-28-5	9
3	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5
5	Acetone	58	C3H6O	000067-64-1	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

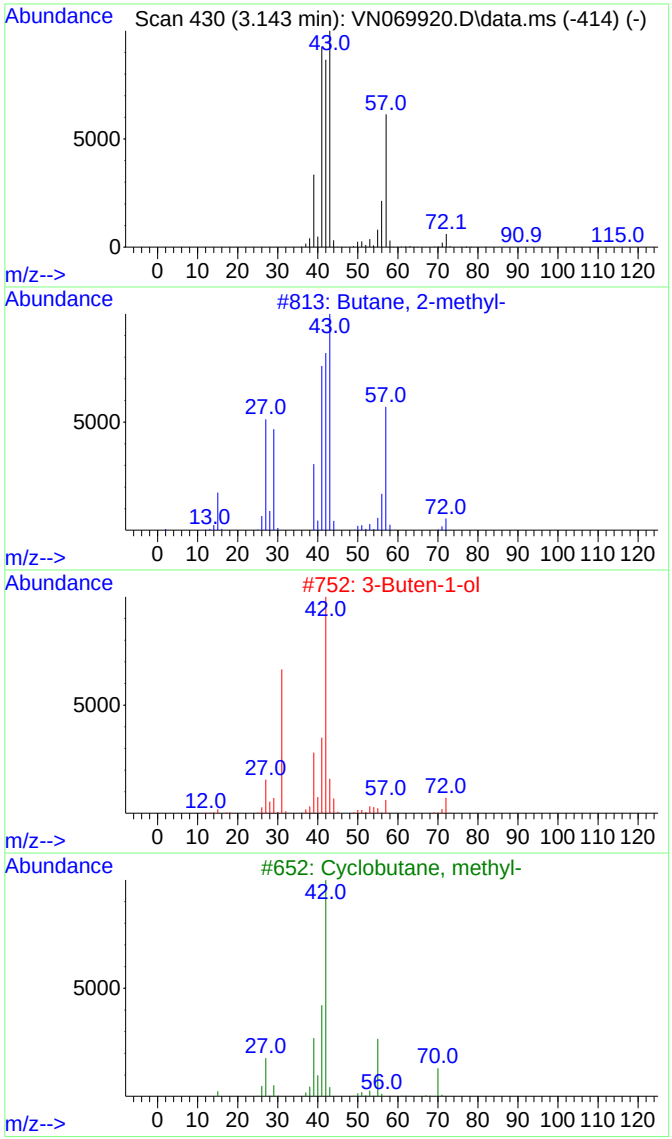
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

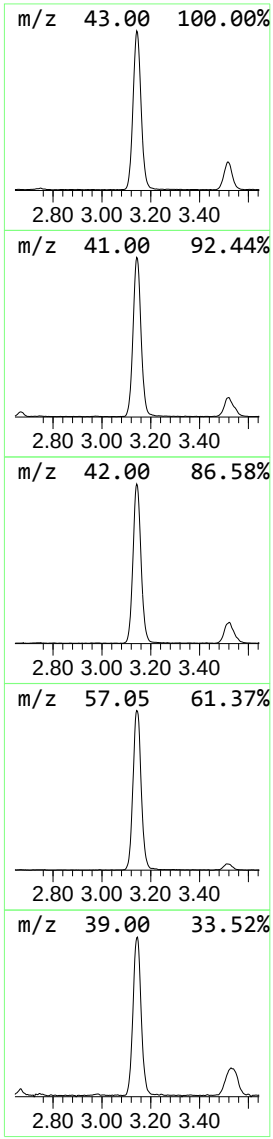
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	28.19 ug/l	2321150	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	38
4	Pentane	72	C5H12	000109-66-0	36
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

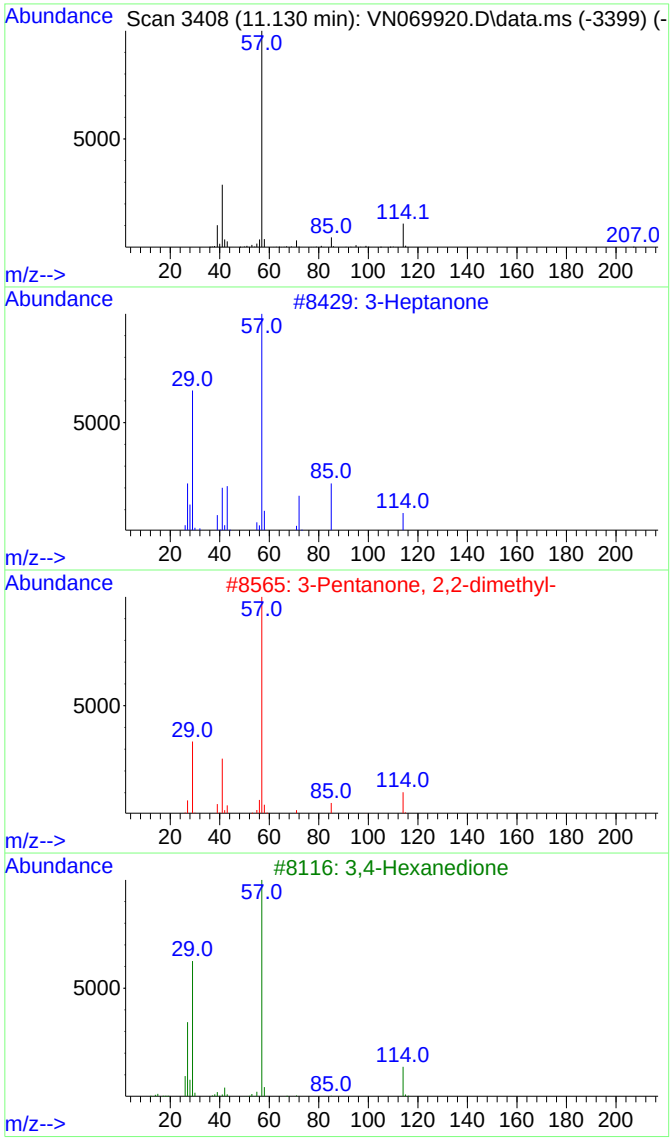
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

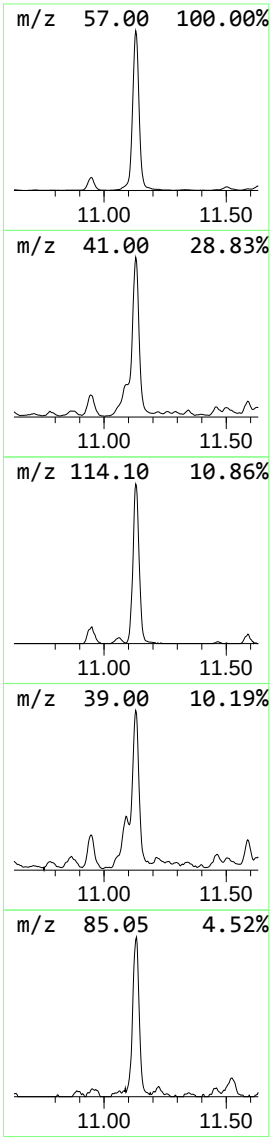
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Heptanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.130	8.50 ug/l	1434010	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone	114	C7H14O	000106-35-4	53
2	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	53
3	3,4-Hexanedione	114	C6H10O2	004437-51-8	52
4	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	50
5	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

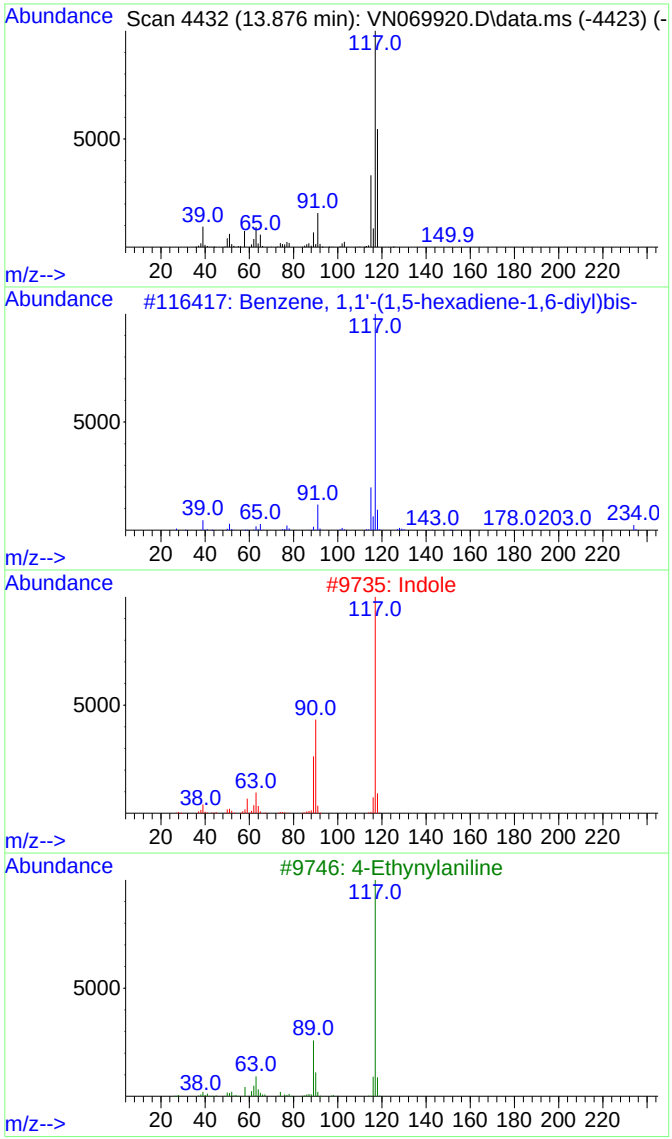
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

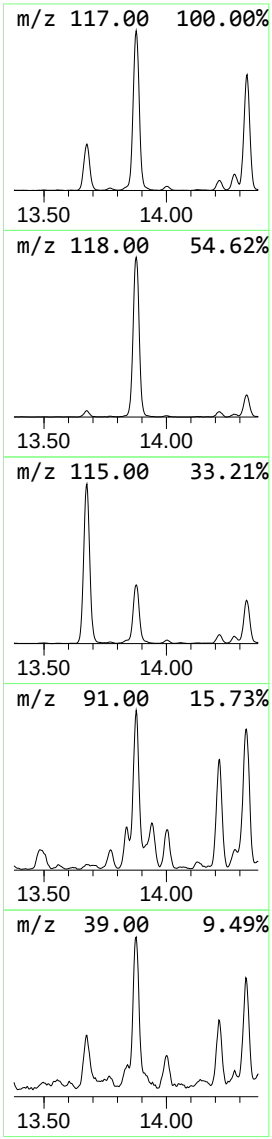
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	18.36 ug/l	2692020	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
2	Indole	117	C8H7N	000120-72-9	49
3	4-Ethynylaniline	117	C8H7N	014235-81-5	47
4	Deltacyclene	118	C9H10	007785-10-6	45
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

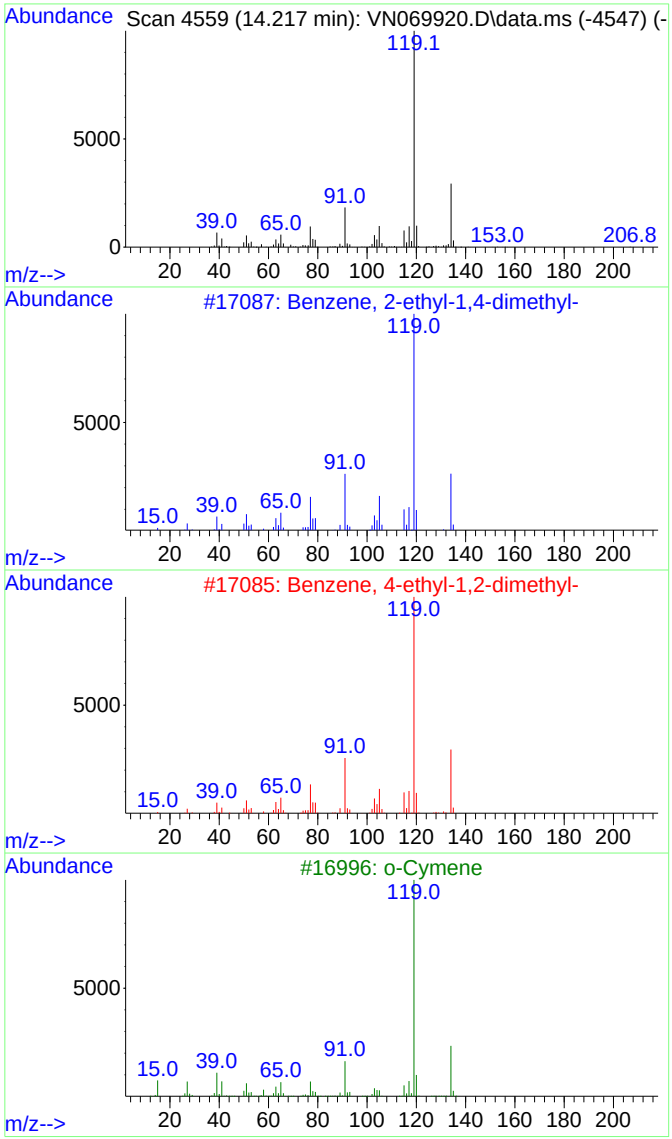
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

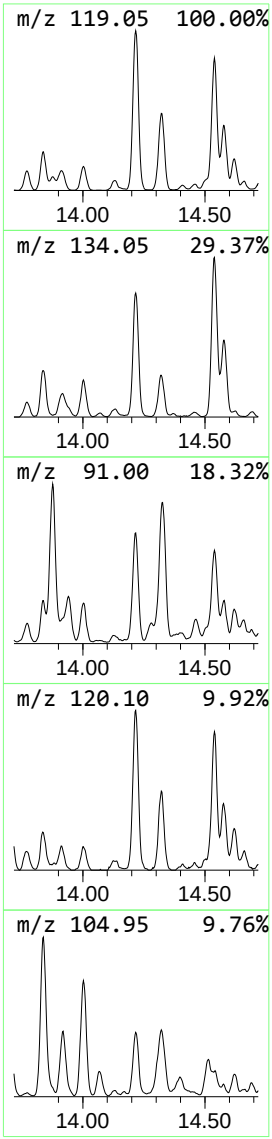
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	8.24 ug/l	1209100	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	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

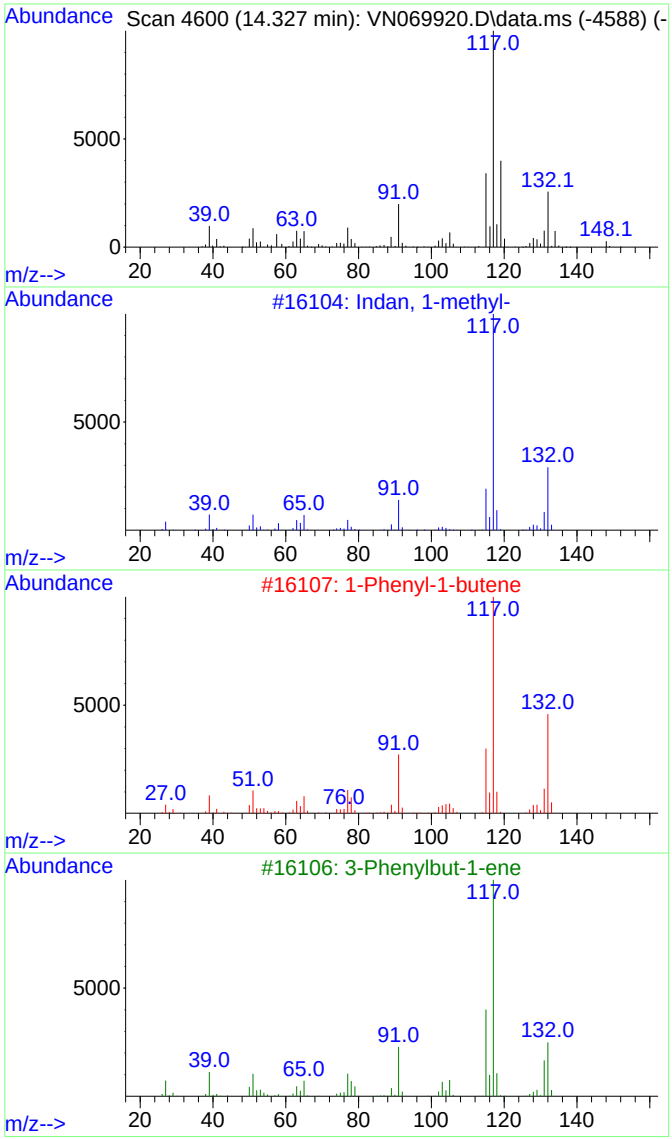
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

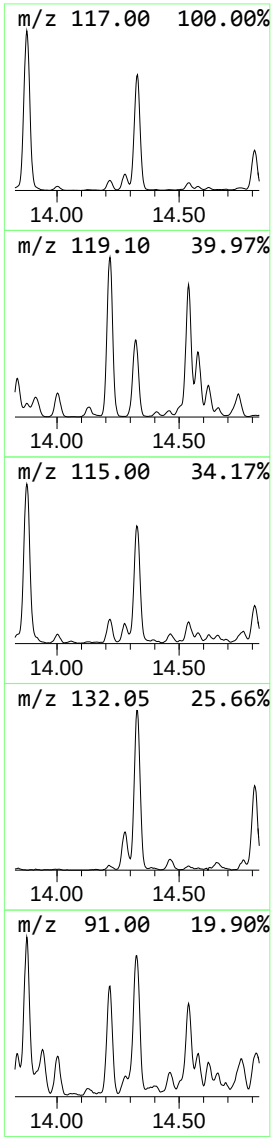
****

Peak Number 7 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	13.57 ug/l	1990830	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	76
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	76
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	68
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68





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Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

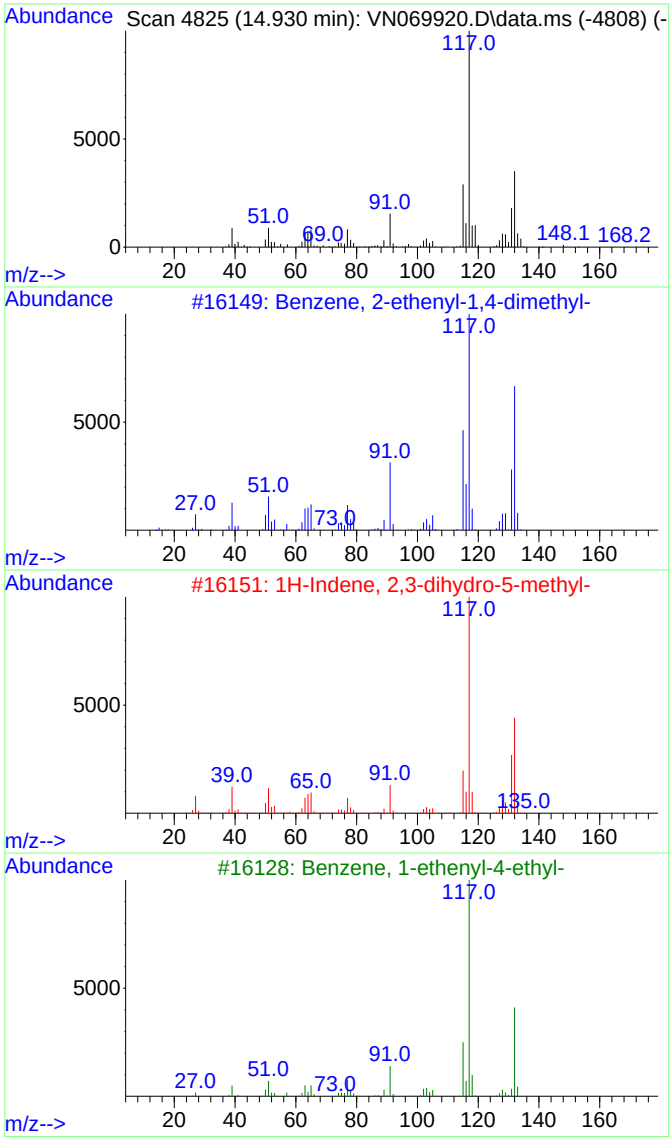
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

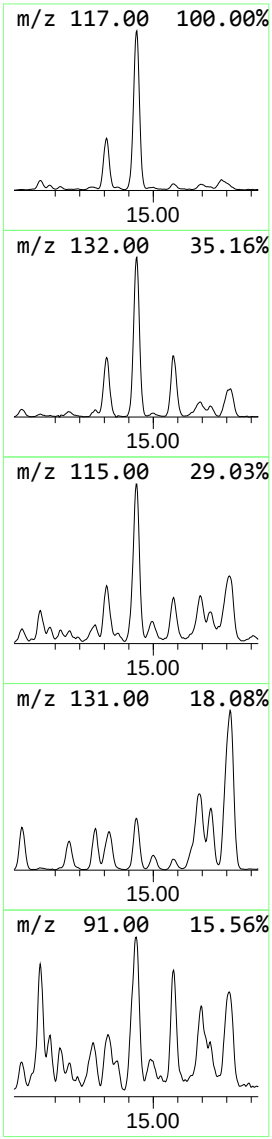
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	17.48 ug/l	2563040	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

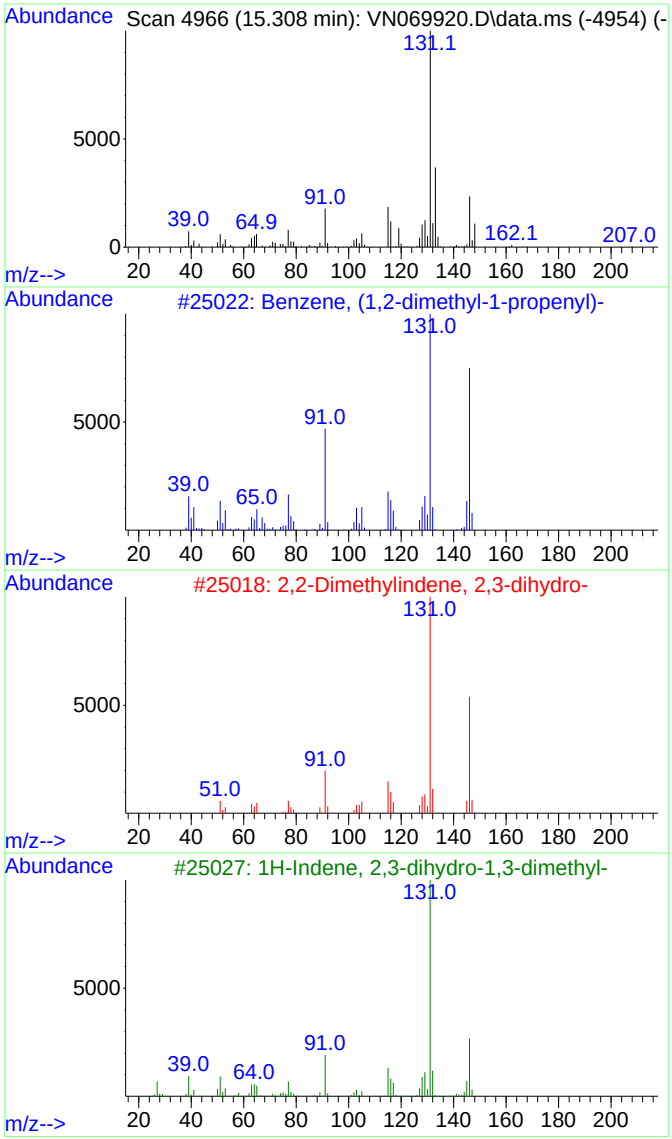
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

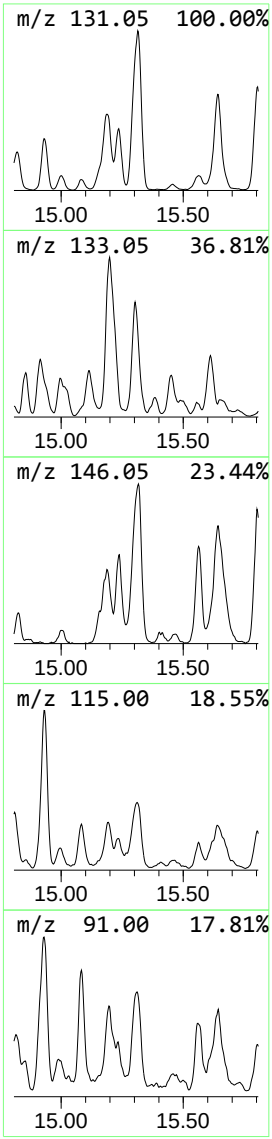
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1,2-dimethyl-1-pr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.308	10.86 ug/l	1592390	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	90
2	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	81
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	81
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

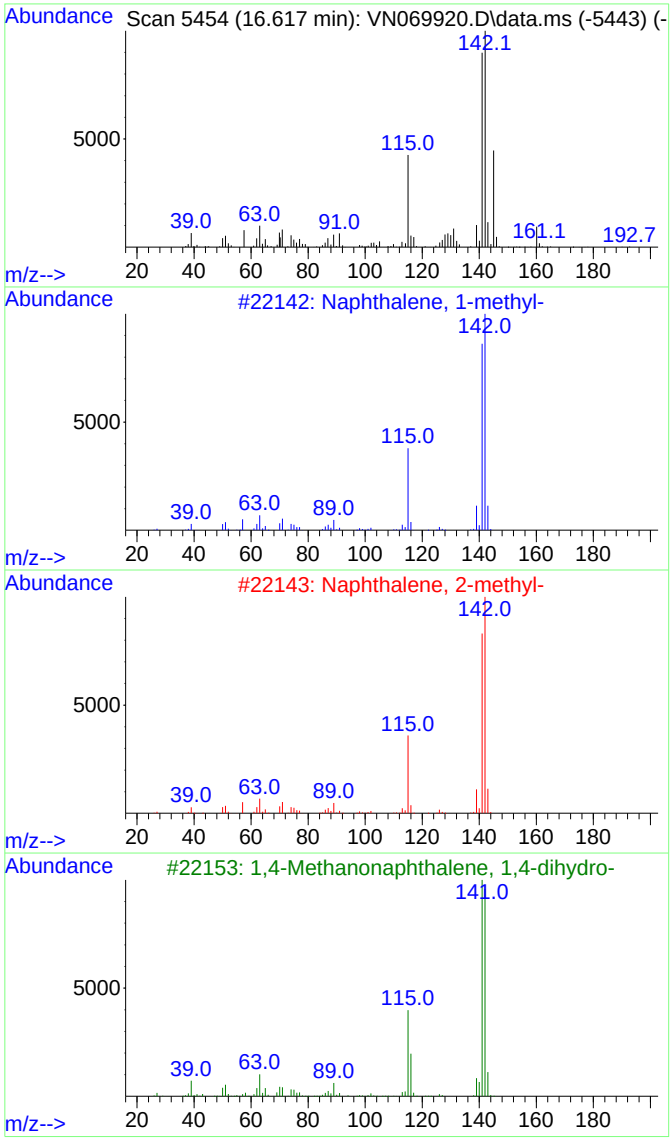
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

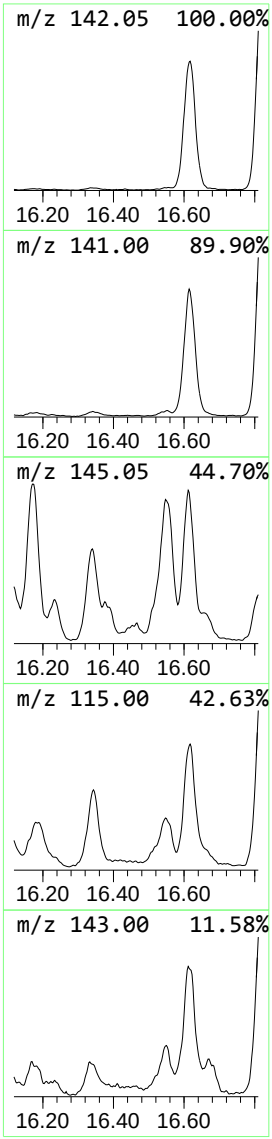
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.617	8.82 ug/l	1294030	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	89
4	Benzocycloheptatriene	142	C11H10	000264-09-5	76
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069920.D
Acq On : 9 Dec 2021 18:53
Operator : JC/MD
Sample : M4969-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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
Butane	2.445	16.5	ug/l	1360320	1	8.086	4116830	50.0
Butane, 2-methyl-	3.143	28.2	ug/l	2321150	1	8.086	4116830	50.0
3-Heptanone	11.130	8.5	ug/l	1434010	3	11.744	8431410	50.0
Benzene, 1,1'-(...	13.876	18.4	ug/l	2692020	4	13.675	7332690	50.0
Benzene, 2-ethy...	14.217	8.2	ug/l	1209100	4	13.675	7332690	50.0
Indan, 1-methyl-	14.327	13.6	ug/l	1990830	4	13.675	7332690	50.0
Benzene, 2-ethe...	14.930	17.5	ug/l	2563040	4	13.675	7332690	50.0
Benzene, (1,2-d...	15.308	10.9	ug/l	1592390	4	13.675	7332690	50.0
Naphthalene, 1-...	16.617	8.8	ug/l	1294030	4	13.675	7332690	50.0