LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

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\82N081522W.M
Title : SW846 8260

Signal : TIC: VN073900.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.781	478	492	507	rBV	28310	115430	1.70%	0.215%
2	7.298	909	920	930	rBV	26630	75946	1.12%	0.141%
3	7.945	1019	1030	1035	rBV	362544	850122	12.49%	1.582%
4	8.010	1035	1041	1052	rVB	655922	1510170	22.19%	2.810%
5	8.363	1092	1101	1113	rBV	313856	716772	10.53%	1.334%
6	8.533	1123	1130	1143	rBV	314199	1073872	15.78%	1.998%
7	8.686	1148	1156	1176	rVB	735714	1891341	27.80%	3.519%
8	8.898	1183	1192	1210	rVB	871783	1840135	27.04%	3.424%
9	10.380	1435	1444	1451	rBV	1200915	2231215	32.79%	4.152%
10	11.686	1656	1666	1672	rBV	1347202	2452989	36.05%	4.565%
11	11.786	1672	1683	1689	rBV	517069	1401648	20.60%	2.608%
12	11.892	1694	1701	1724	rVB	2847721	5805203	85.32%	10.802%
13	12.221	1747	1757	1767	rBV	1379309	2350642	34.55%	4.374%
14	12.674	1827	1834	1844	rVB	1262595	2090596	30.72%	3.890%
15	12.957	1878	1882	1885	rVV	46352	80112	1.18%	0.149%
16	12.998	1885	1889	1895	rVB2	75191	135302	1.99%	0.252%
17	13.163	1910	1917	1924	rBV	48742	106055	1.56%	0.197%
18	13.310	1937	1942	1946	rBV	90292	136904	2.01%	0.255%
19	13.363	1946	1951	1956	rVB2	44676	71654	1.05%	0.133%
20	13.504	1970	1975	1979	rVB2	54753	82767	1.22%	0.154%
21	13.616	1987	1994	2004	rBV	1712681	3022145	44.41%	5.624%
22	13.816	2013	2028	2042	rBV2	1084634	3264598	47.98%	6.075%
23	13.939	2044	2049	2053	rVV4	74212	132843	1.95%	0.247%
24	13.998	2055	2059	2064	rVV3	57139	93327	1.37%	0.174%
25	14.098	2073	2076	2080	rVB	68601	99584	1.46%	0.185%
26	14.157	2081	2086	2092	rBV	258264	393105	5.78%	0.731%
27	14.268	2098	2105	2109	rBV3	266511	498550	7.33%	0.928%
28	14.310	2110	2112	2121	rVB3	102088	199771	2.94%	0.372%
29	14.392	2121	2126	2131	rVB4	96745	161553	2.37%	0.301%
30	14.445	2131	2135	2137	rBV3	83255	120160	1.77%	0.224%
31	14.480	2137	2141	2144	rBV2	103358	118157	1.74%	0.220%
32	14.521	2144	2148	2151	rVB	196612	265740	3.91%	0.494%
33	14.563	2151	2155	2160	rBV2	187775	350436	5.15%	0.652%
34	14.751	2181	2187	2191	rBV	384131	632213	9.29%	1.176%
35	14.792	2192	2194	2199	rVB3	78878	104902	1.54%	0.195%
36	14.868	2199	2207	2212	rBV3	766513	1707145	25.09%	3.177%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

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\82N081522W.M
Title : SW846 8260

37	14.927	2213	2217	2226	rVB7	155104	349977	5.14%	0.651%
38	15.015	2227	2232	2238	rBV2	395170	724968	10.65%	1.349%
39	15.127	2245	2251	2257	rBV4	350831	734849	10.80%	1.367%
40	15.245	2265	2271	2280	rBV3	231635	468476	6.88%	0.872%
41	15.433	2297	2303	2315	rVB	2219784	4093301	60.16%	7.617%
42	15.545	2318	2322	2334	rVB9	272022	751608	11.05%	1.399%
43	15.651	2335	2340	2345	rBV5	69714	160555	2.36%	0.299%
44	16.045	2402	2407	2413	rBV4	220038	550501	8.09%	1.024%
45	16.527	2483	2489	2498	rVB	1362290	2918766	42.90%	5.431%
46	16.739	2517	2525	2533	rVB	3039495	6804412	100.00%	12.662%

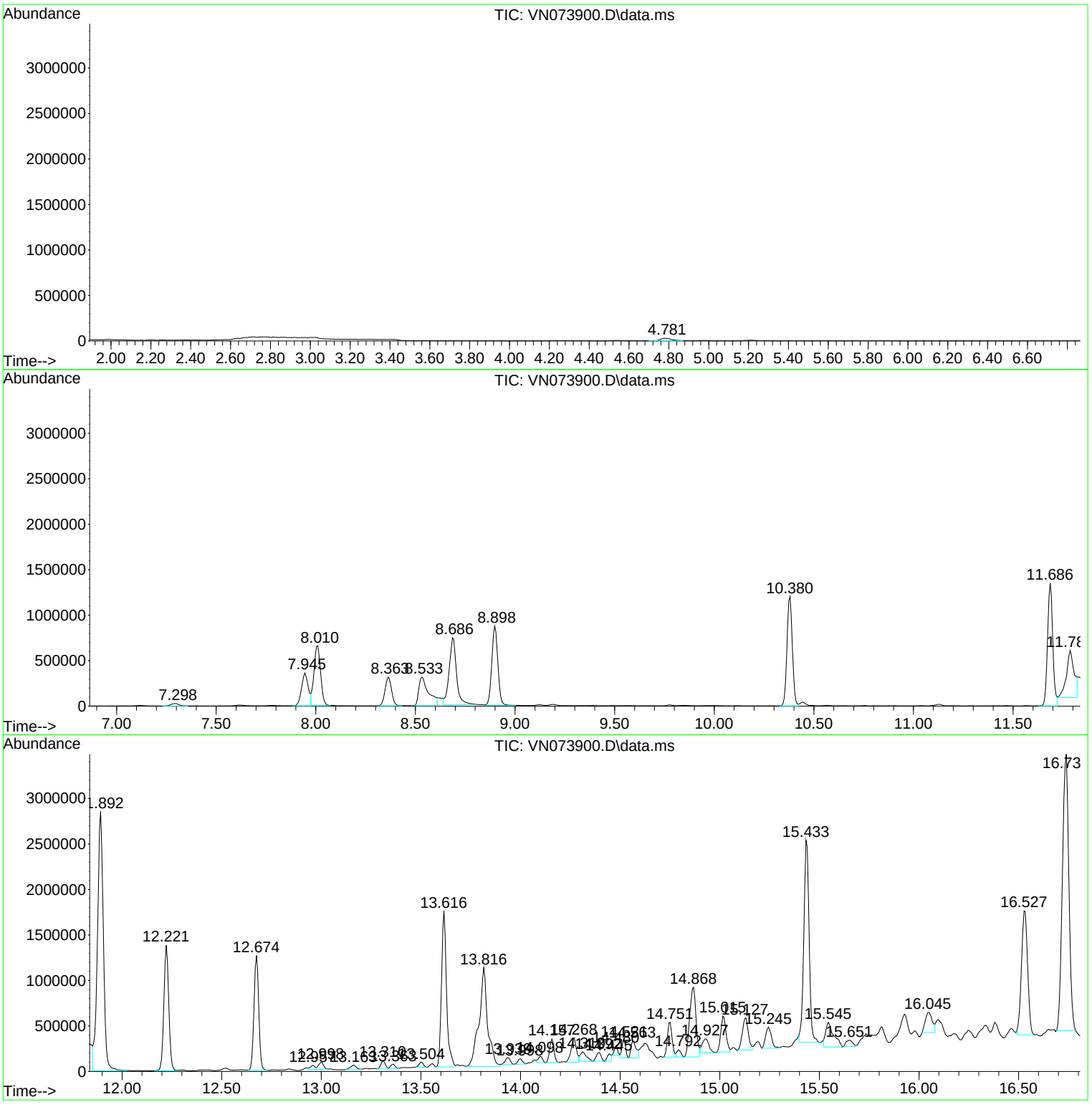
Sum of corrected areas: 53740517

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

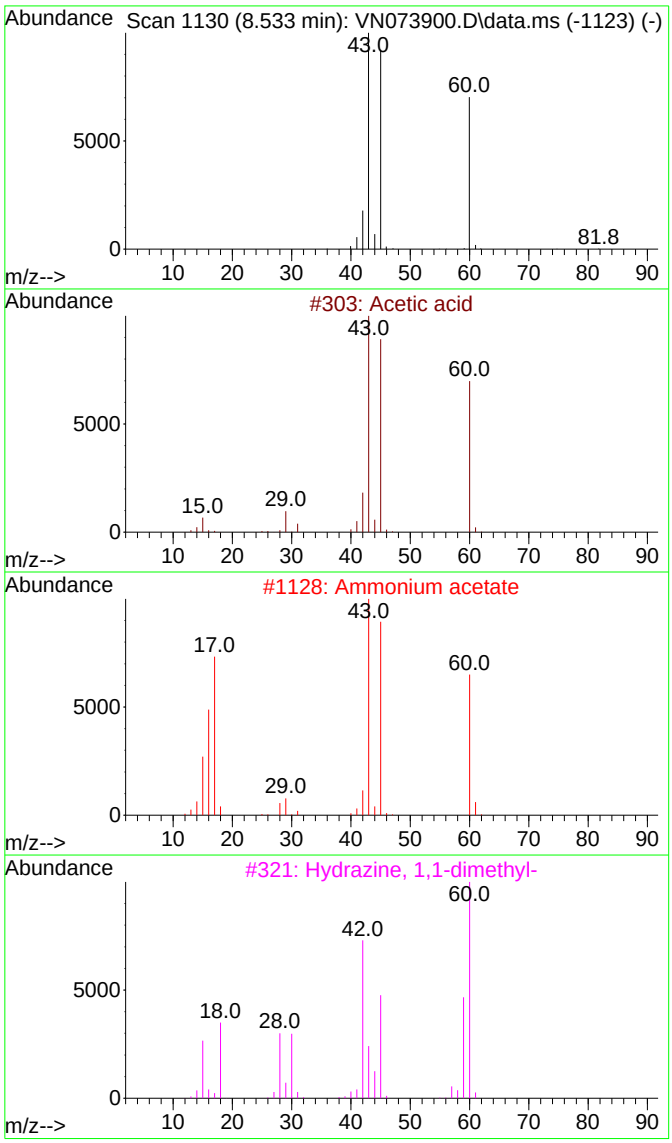
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

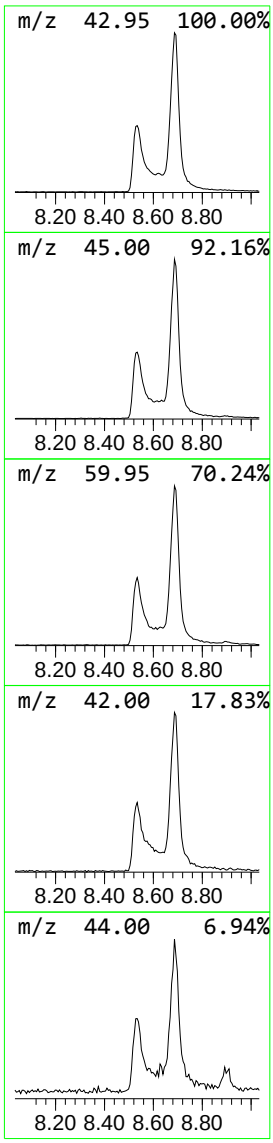
****

Peak Number 1 Acetic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.533	29.18 ug/l	1073870	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	91
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	5
5	Thiirane	60	C2H4S	000420-12-2	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

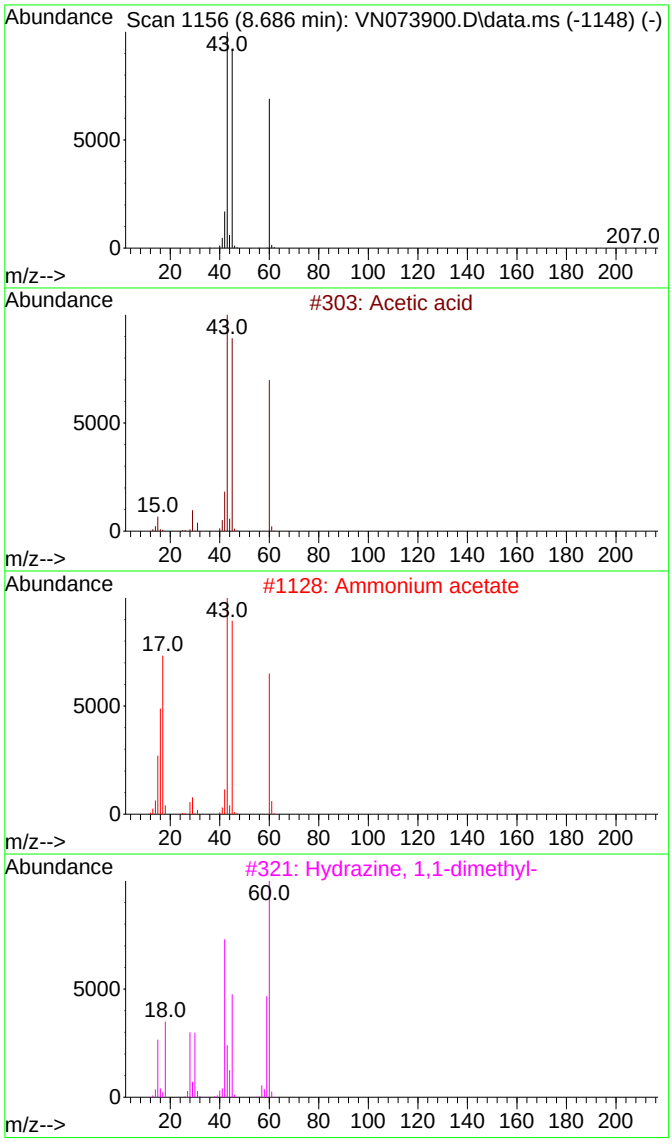
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

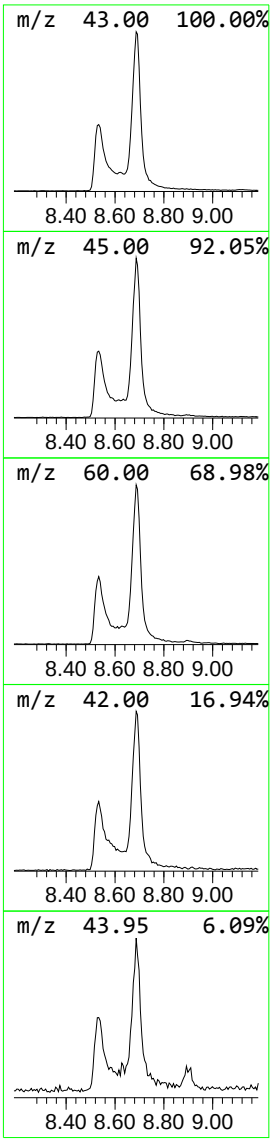
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ammonium acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.686	51.39 ug/l	1891340	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	91
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	5
5	Carbonyl sulfide	60	COS	000463-58-1	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

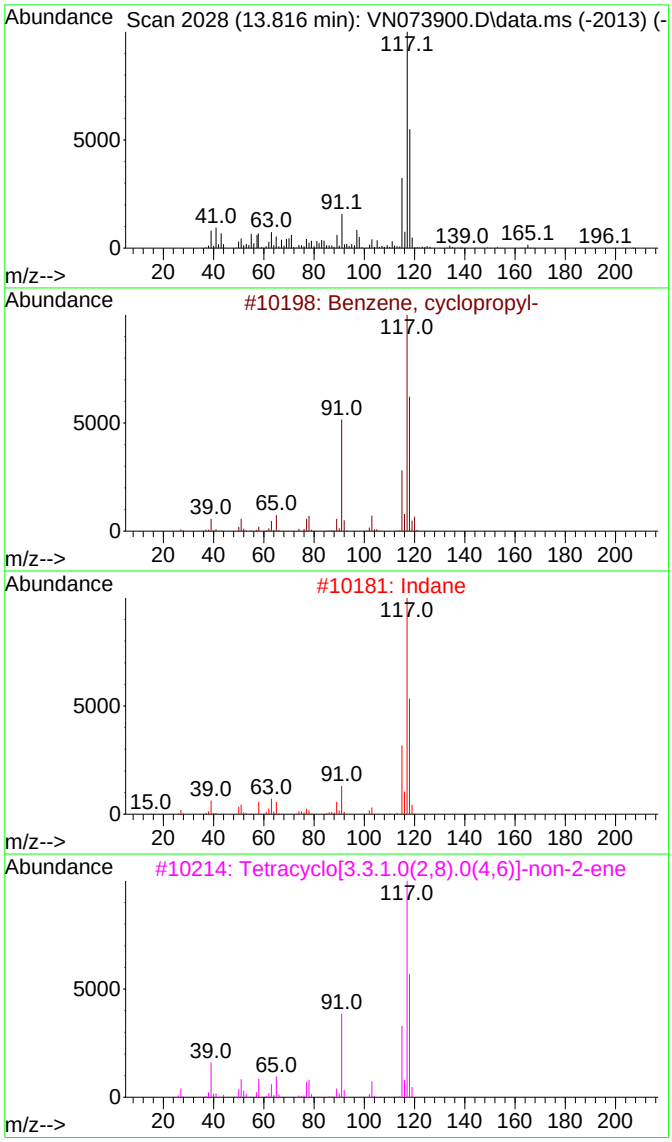
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

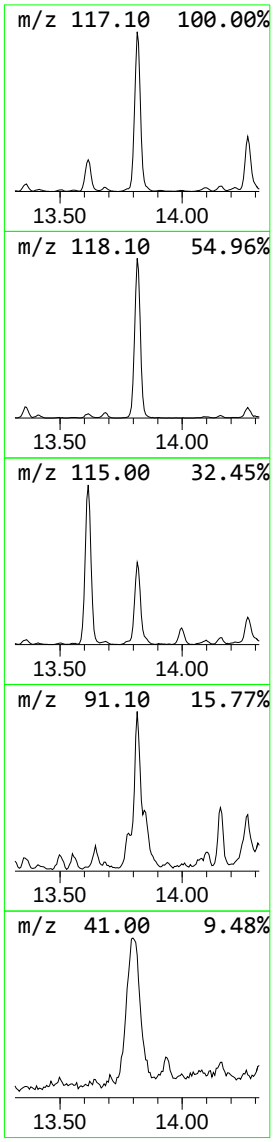
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, cyclopropyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	54.01 ug/l	3264600	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2	Indane	118	C9H10	000496-11-7	81
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	74
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Deltacyclene	118	C9H10	007785-10-6	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

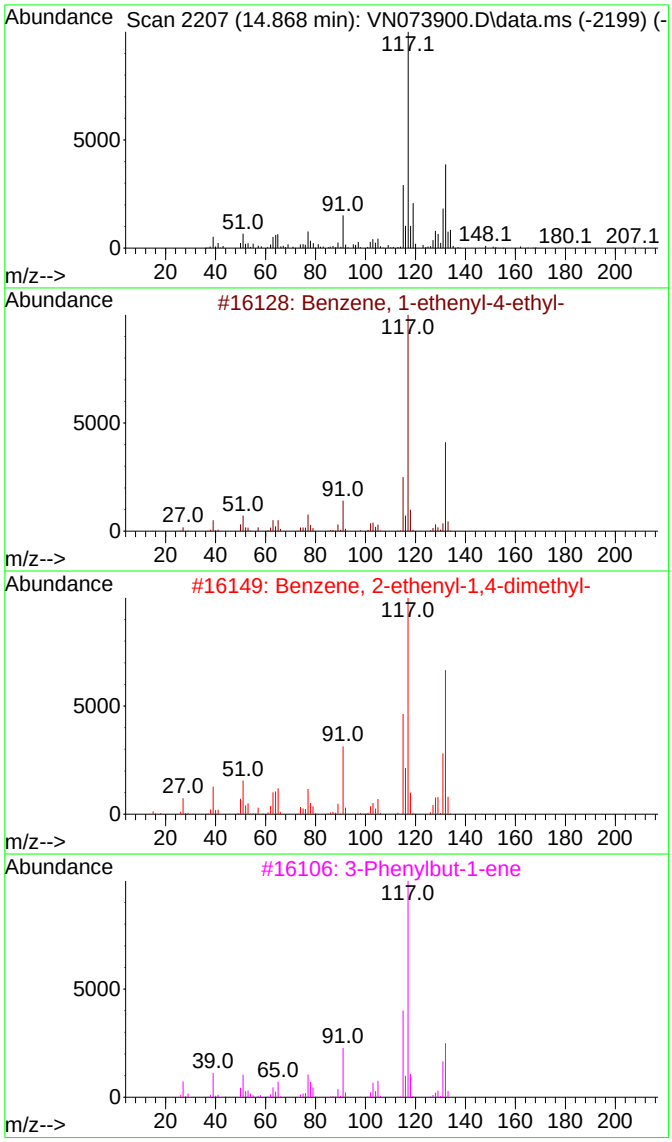
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

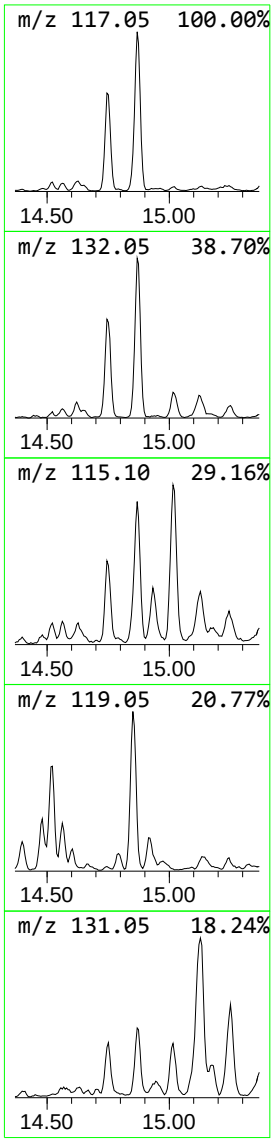
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	28.24 ug/l	1707150	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

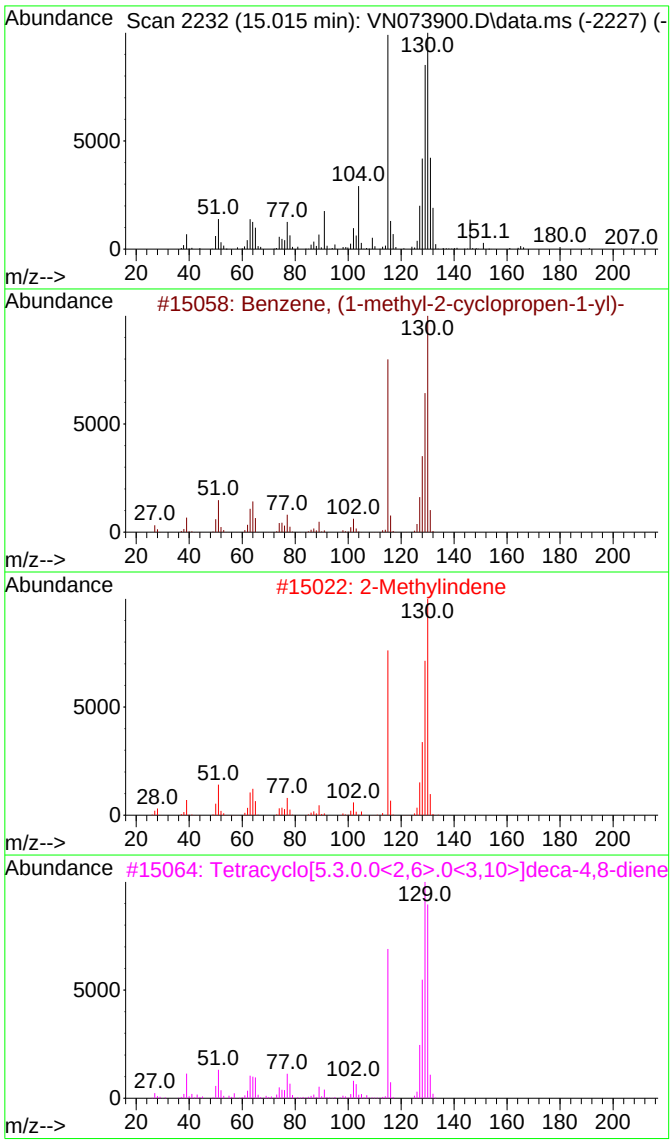
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

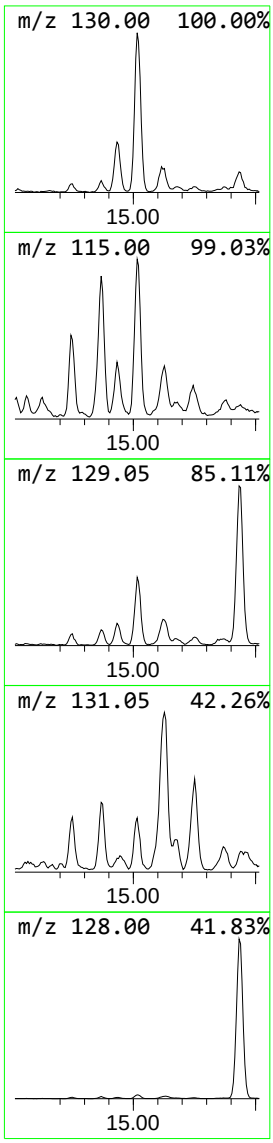
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (1-methyl-2-cyclop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.015	11.99 ug/l	724968	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
2	2-Methylindene	130	C10H10	002177-47-1	95
3	Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	91
4	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	86
5	Benzene, 1-butynyl-	130	C10H10	000622-76-4	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

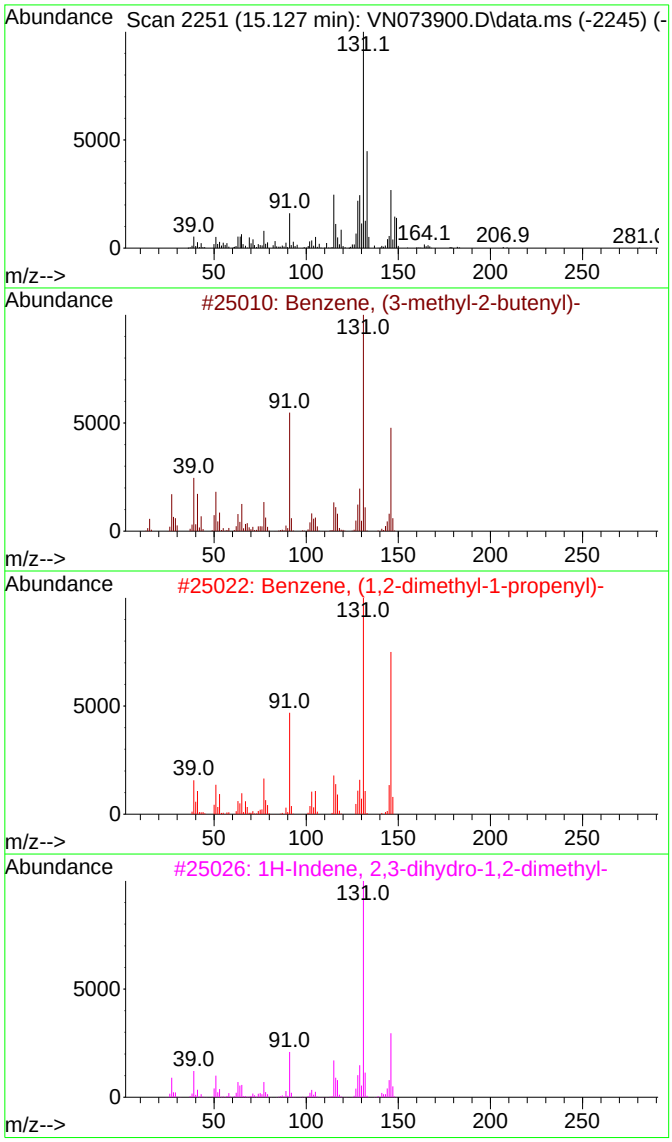
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

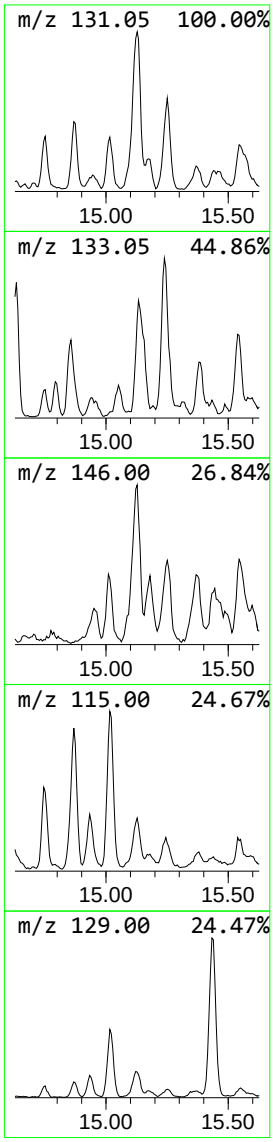
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (3-methyl-2-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	12.16 ug/l	734849	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	64
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	60
4	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	58
5	1,2,3,4-Tetrahydro-1-naphthalene...	164	C10H12S	103324-34-1	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

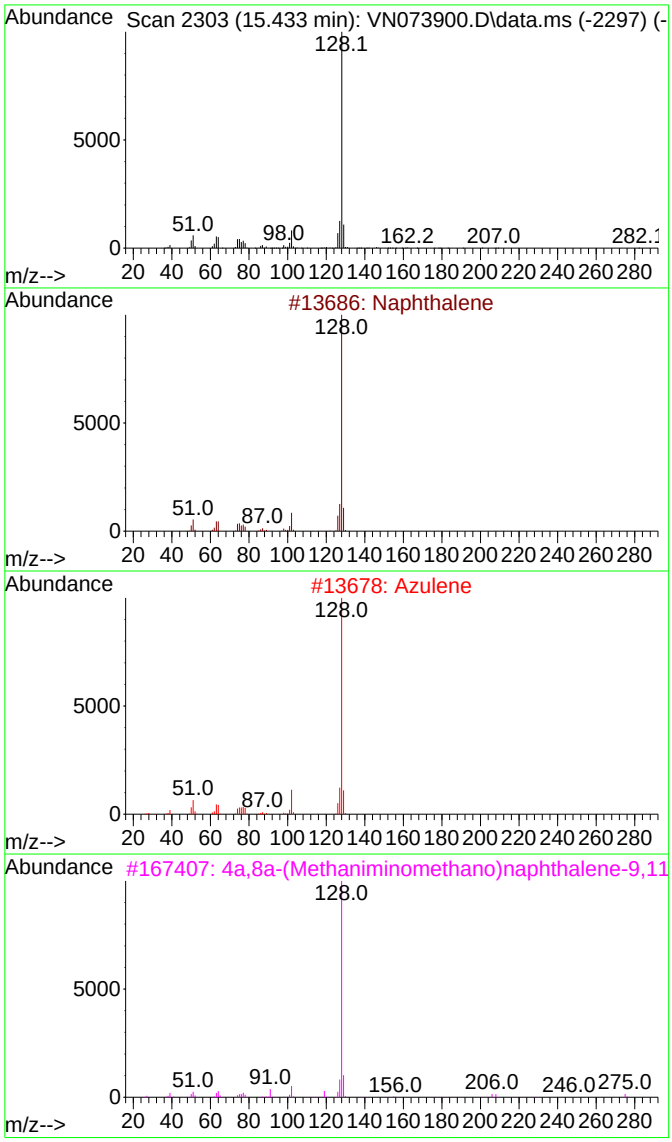
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

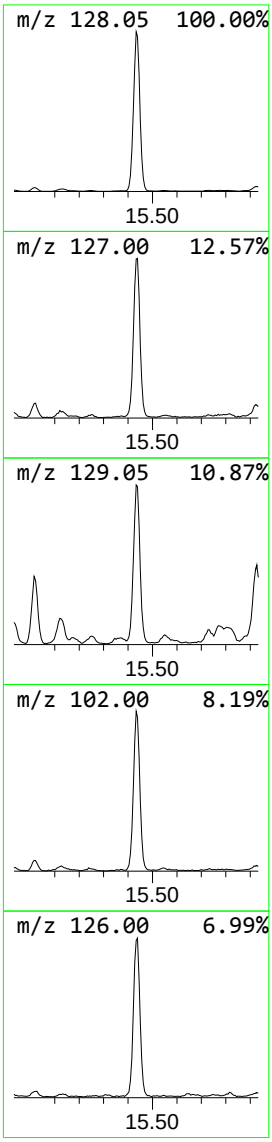
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4a,8a-(Methaniminomethano)n... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	67.72 ug/l	4093300	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	93
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

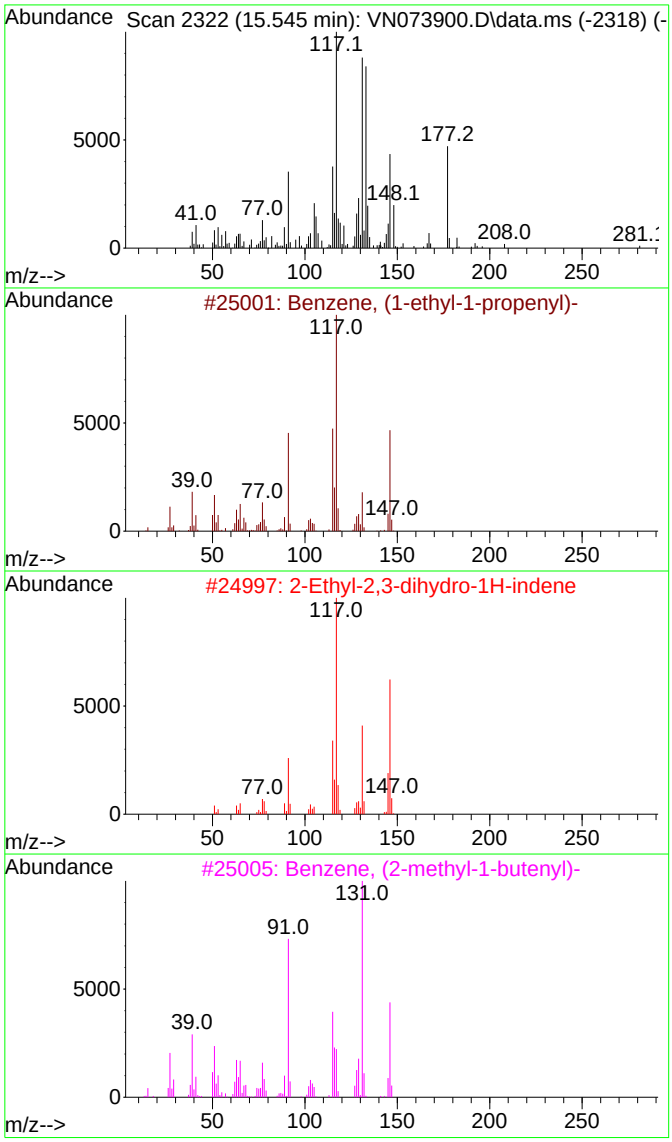
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

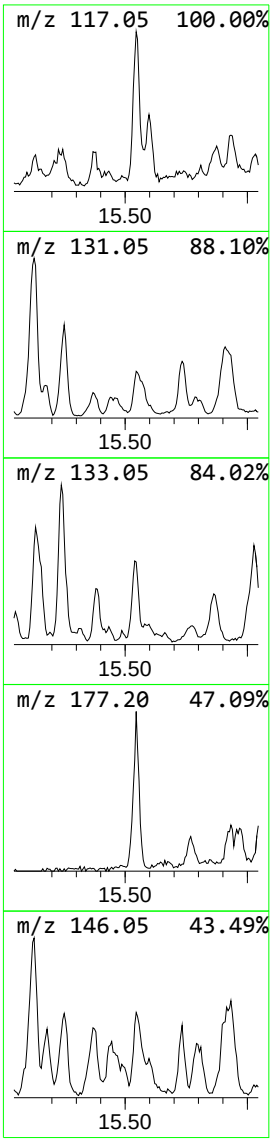
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (1-ethyl-1-propenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	12.44 ug/l	751608	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethyl-1-propenyl)-	146	C11H14	004701-36-4	70
2	2-Ethyl-2,3-dihydro-1H-indene	146	C11H14	056147-63-8	42
3	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	42
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	42
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

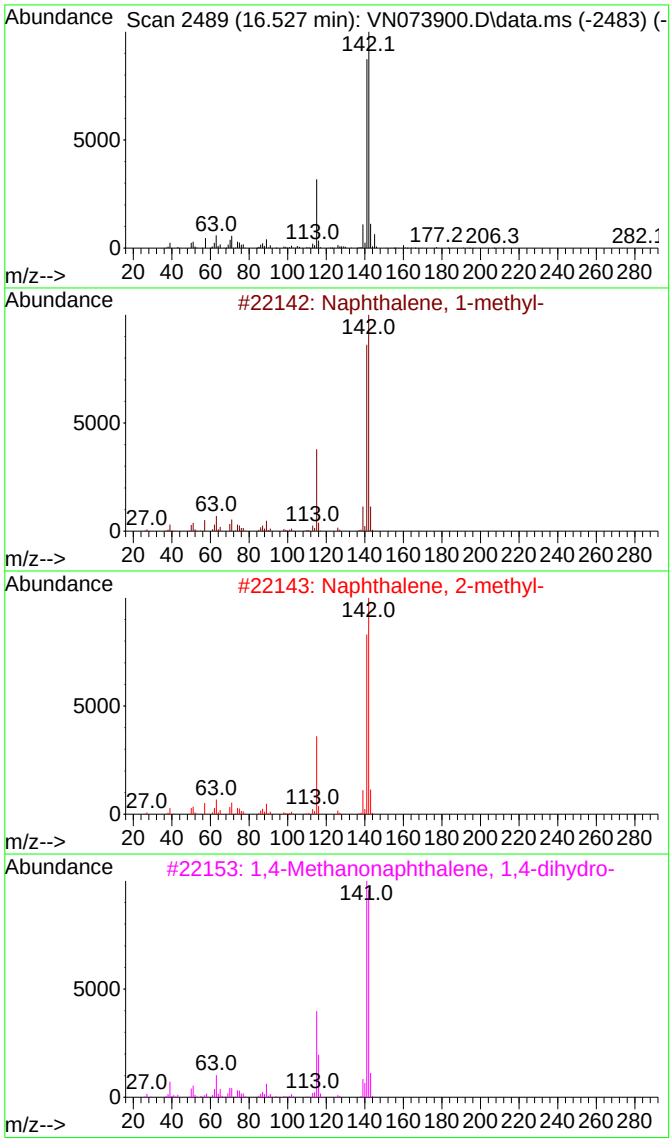
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

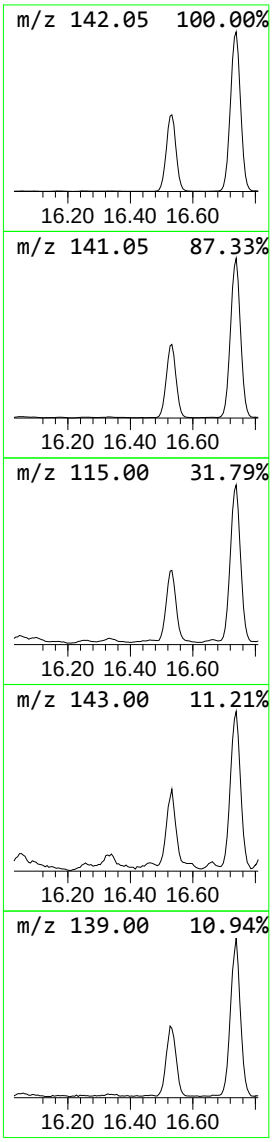
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,4-Methanonaphthalene, 1,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	48.29 ug/l	2918770	1,4-Dichlorobenzene-d4	13.616

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	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

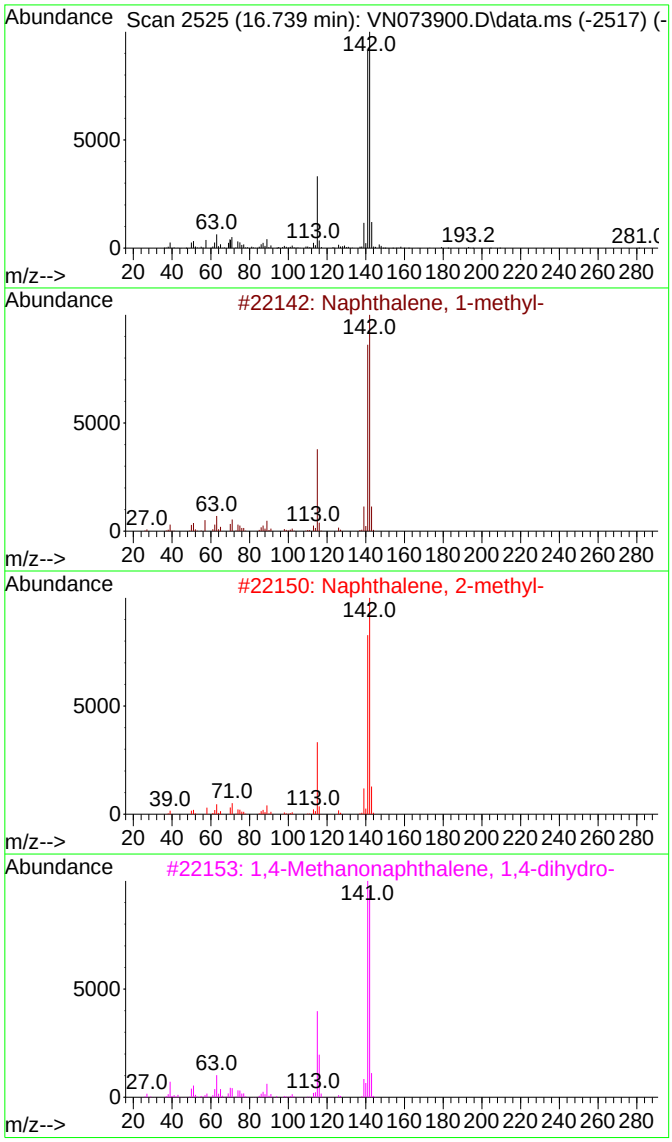
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

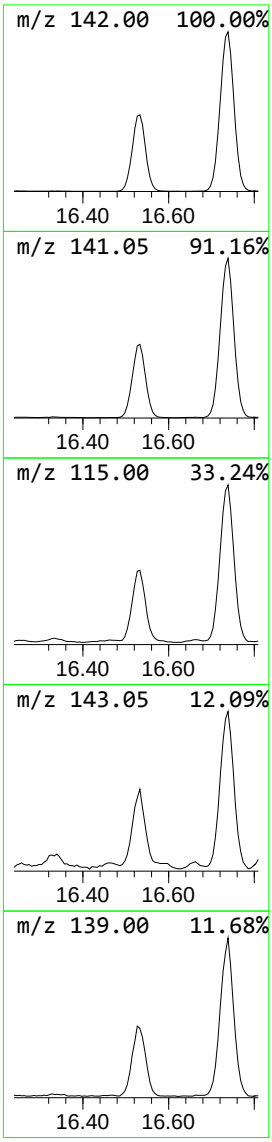
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzocycloheptatriene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	112.58 ug/l	6804410	1,4-Dichlorobenzene-d4	13.616

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	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Spiro(tricyclo[6.2.1.0(2,7)]unde...	186	C13H14O	1000210-02-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
Data File : VN073900.D
Acq On : 15 Aug 2022 17:06
Operator : JC\MD
Sample : N4102-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-DRUMS-0808

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.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
Acetic acid	8.533	29.2	ug/l	1073870	2	8.898	1840140	50.0
Ammonium acetate	8.686	51.4	ug/l	1891340	2	8.898	1840140	50.0
Benzene, cyclop...	13.816	54.0	ug/l	3264600	4	13.616	3022150	50.0
Benzene, 1-ethe...	14.868	28.2	ug/l	1707150	4	13.616	3022150	50.0
Benzene, (1-met...	15.015	12.0	ug/l	724968	4	13.616	3022150	50.0
Benzene, (3-met...	15.127	12.2	ug/l	734849	4	13.616	3022150	50.0
4a,8a-(Methanim...	15.433	67.7	ug/l	4093300	4	13.616	3022150	50.0
Benzene, (1-eth...	15.545	12.4	ug/l	751608	4	13.616	3022150	50.0
1,4-Methanonaph...	16.527	48.3	ug/l	2918770	4	13.616	3022150	50.0
Benzocyclohepta...	16.739	112.6	ug/l	6804410	4	13.616	3022150	50.0