LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

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_X\Method\82X053122W.M
Title : SW846 8260

Signal : TIC: VX029128.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	24	28	51	rBV	298669	800595	1.30%	0.308%
2	5.391	692	706	716	rBV	213792	618872	1.00%	0.238%
3	5.556	717	733	743	rBV	342086	1080733	1.75%	0.416%
4	6.763	920	931	952	rBV	537205	1266494	2.05%	0.487%
5	8.653	1235	1241	1248	rVB	1133938	1724073	2.79%	0.663%
6	10.055	1466	1471	1477	rBV	1210408	1587257	2.57%	0.610%
7	10.195	1489	1494	1504	rVB	489322	633000	1.03%	0.243%
8	10.963	1614	1620	1634	rBV	2804025	3442975	5.58%	1.324%
9	11.085	1634	1640	1645	rBV	1020187	1320339	2.14%	0.508%
10	11.305	1671	1676	1682	rVB	2596681	3073057	4.98%	1.182%
11	11.402	1684	1692	1696	rVV	1471980	1829437	2.96%	0.703%
12	11.451	1696	1700	1707	rVB	905302	1107916	1.79%	0.426%
13	11.616	1719	1727	1737	rBV	5618102	6784457	10.99%	2.609%
14	11.756	1738	1750	1755	rBV	17720638	22571326	36.55%	8.679%
15	11.811	1755	1759	1764	rVB	669479	784211	1.27%	0.302%
16	11.975	1780	1786	1789	rBV	493114	676784	1.10%	0.260%
17	12.024	1789	1794	1799	rVB2	1905008	2766294	4.48%	1.064%
18	12.091	1799	1805	1809	rBV	6684082	8128844	13.16%	3.126%
19	12.250	1824	1831	1838	rBV	14385507	19899600	32.22%	7.652%
20	12.317	1838	1842	1848	rVV2	2071040	2933690	4.75%	1.128%
21	12.463	1861	1866	1873	rVB	472816	634009	1.03%	0.244%
22	12.536	1873	1878	1879	rBV	1222755	1522254	2.46%	0.585%
23	12.554	1879	1881	1886	rVV	1533982	1770040	2.87%	0.681%
24	12.615	1886	1891	1894	rVV	3284364	4046421	6.55%	1.556%
25	12.701	1900	1905	1911	rBV	6562540	8914108	14.43%	3.428%
26	12.847	1925	1929	1934	rVB	708759	906295	1.47%	0.348%
27	12.926	1934	1942	1945	rBV	1117962	1528273	2.47%	0.588%
28	12.963	1945	1948	1953	rVV	2383123	3123908	5.06%	1.201%
29	13.067	1960	1965	1968	rVV2	709090	1129176	1.83%	0.434%
30	13.170	1977	1982	1987	rVB	4556914	5401882	8.75%	2.077%
31	13.292	1997	2002	2006	rBV2	4717037	6031910	9.77%	2.319%
32	13.347	2006	2011	2018	rVB	3770671	4816527	7.80%	1.852%
33	13.426	2018	2024	2030	rVB	13444721	17667135	28.61%	6.793%
34	13.505	2030	2037	2041	rBV	2189859	2710070	4.39%	1.042%
35	13.548	2041	2044	2048	rVB	814752	960470	1.56%	0.369%
36	13.676	2058	2065	2070	rVB2	681752	1079640	1.75%	0.415%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

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_X\Method\82X053122W.M
Title : SW846 8260

37	13.792	2074	2084	2089	rBV2	35777990	61755411	100.00%	23.745%
38	14.225	2150	2155	2158	rBV2	1152117	1816036	2.94%	0.698%
39	14.322	2165	2171	2177	rVB	1480097	2636921	4.27%	1.014%
40	14.524	2200	2204	2212	rVB	731062	1108540	1.80%	0.426%
41	14.639	2218	2223	2233	rVB	13791724	17271976	27.97%	6.641%
42	14.786	2241	2247	2252	rBV	15032791	19465321	31.52%	7.485%
43	15.206	2308	2316	2321	rBV	924292	1254268	2.03%	0.482%
44	15.377	2332	2344	2347	rBV	1003073	1537441	2.49%	0.591%
45	15.481	2354	2361	2366	rBV	864997	1327218	2.15%	0.510%
46	15.615	2376	2383	2387	rBV	1559030	2430790	3.94%	0.935%
47	15.651	2387	2389	2395	rVB	604779	746329	1.21%	0.287%
48	15.840	2410	2420	2431	rVB	412109	1168777	1.89%	0.449%
49	16.328	2492	2500	2510	rBV	1248648	2281214	3.69%	0.877%

Sum of corrected areas: 260072314

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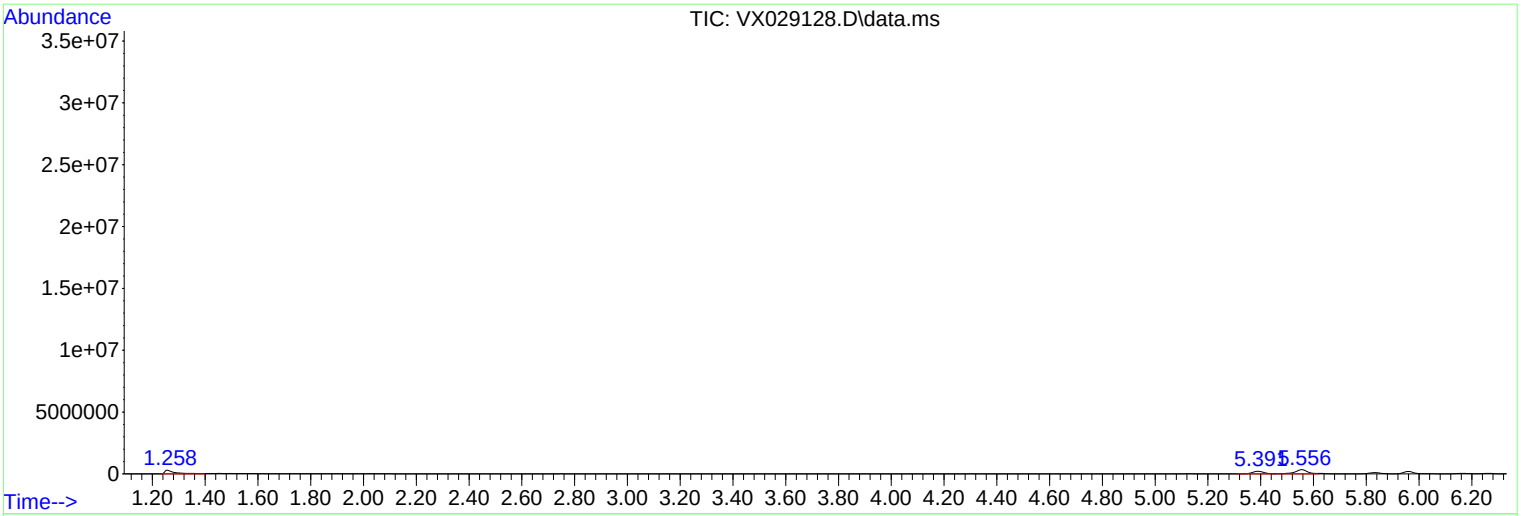
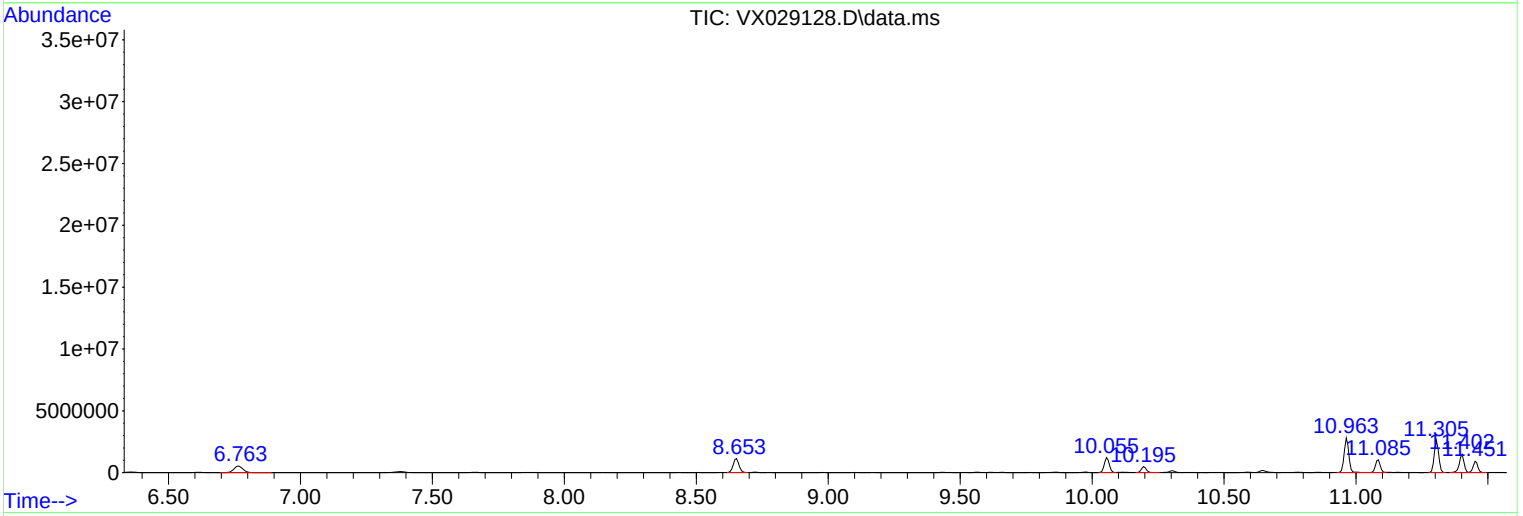
ALS Vial : 24 Sample Multiplier: 1

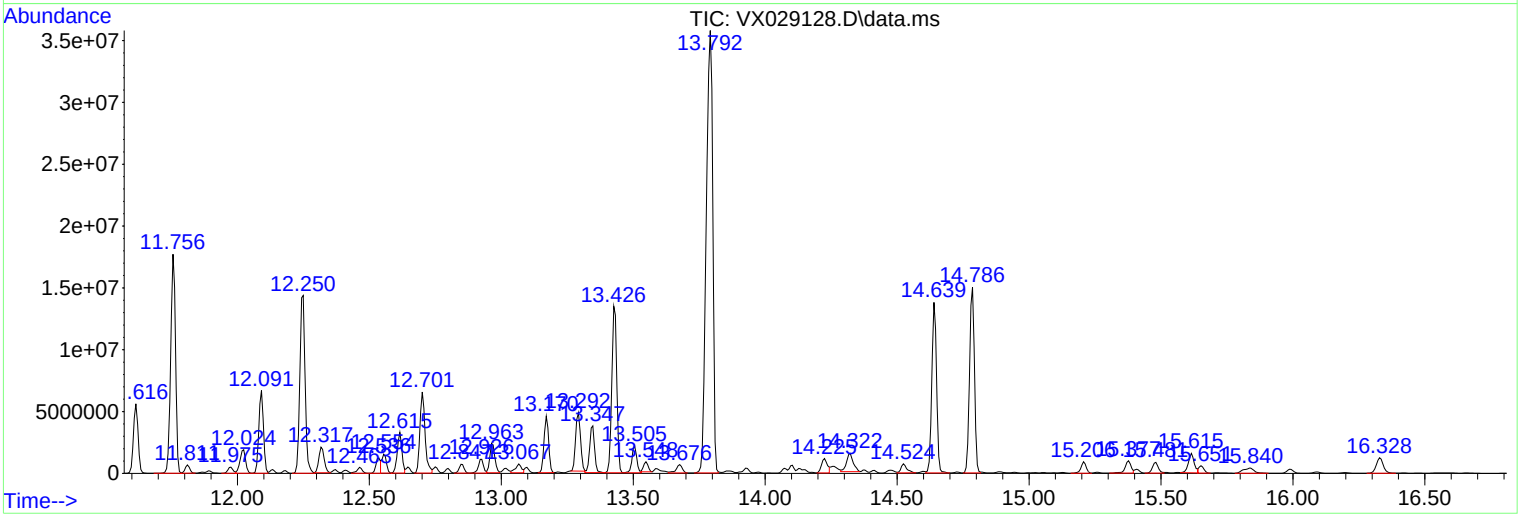
Instrument :
MSVOA_X
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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







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Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
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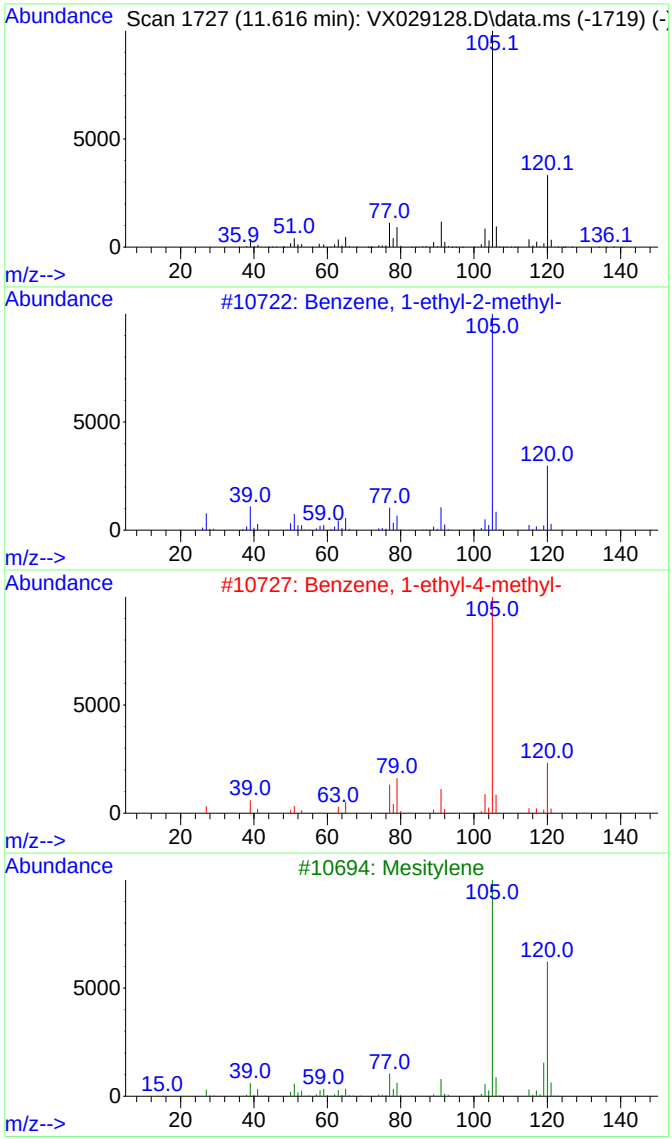
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

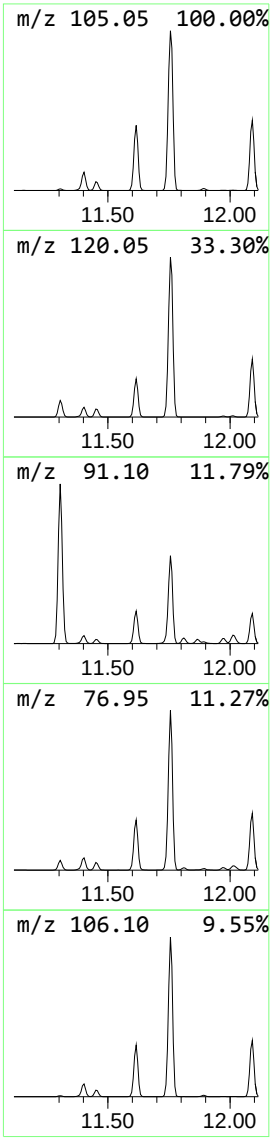
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	122.63 ug/l	6784460	1,4-Dichlorobenzene-d4	12.024

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-4-methyl-	120	C9H12	000622-96-8	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

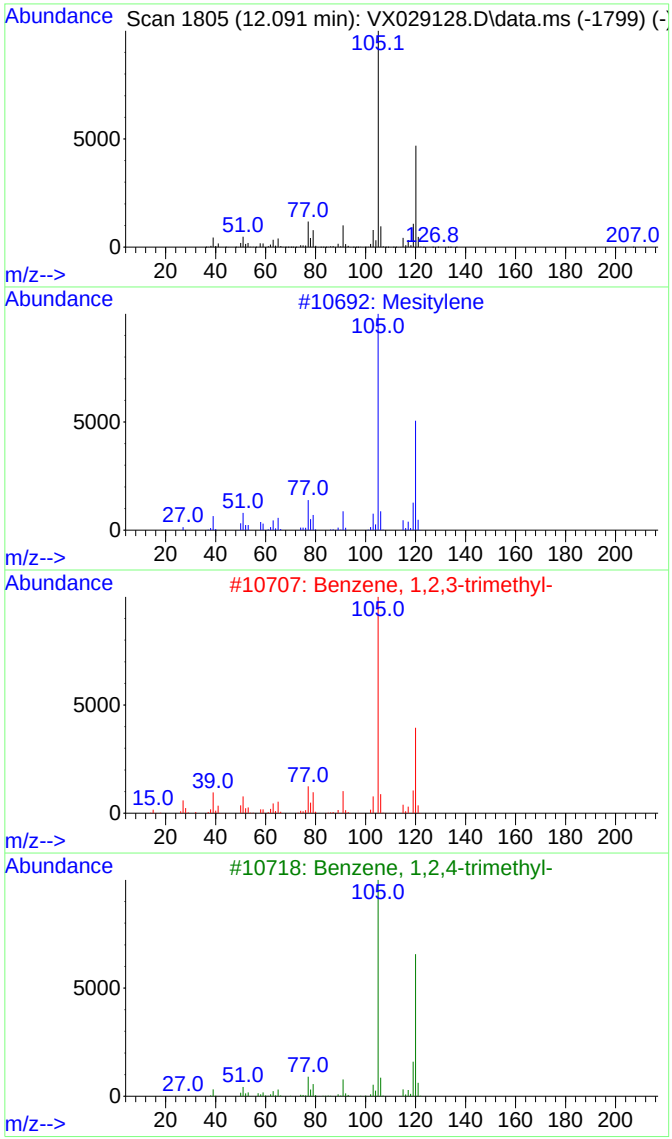
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

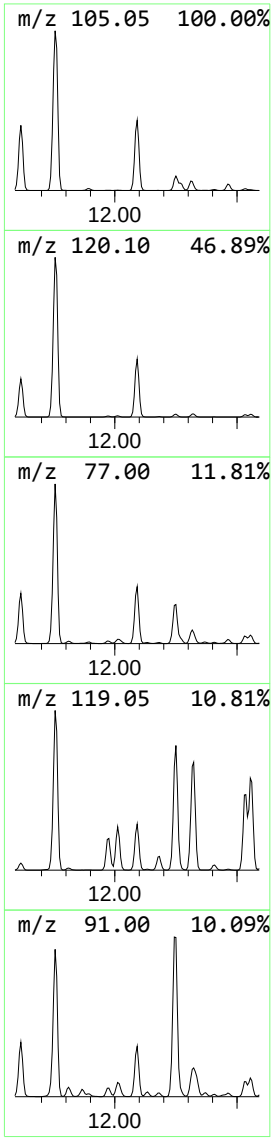
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	146.93 ug/l	8128840	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

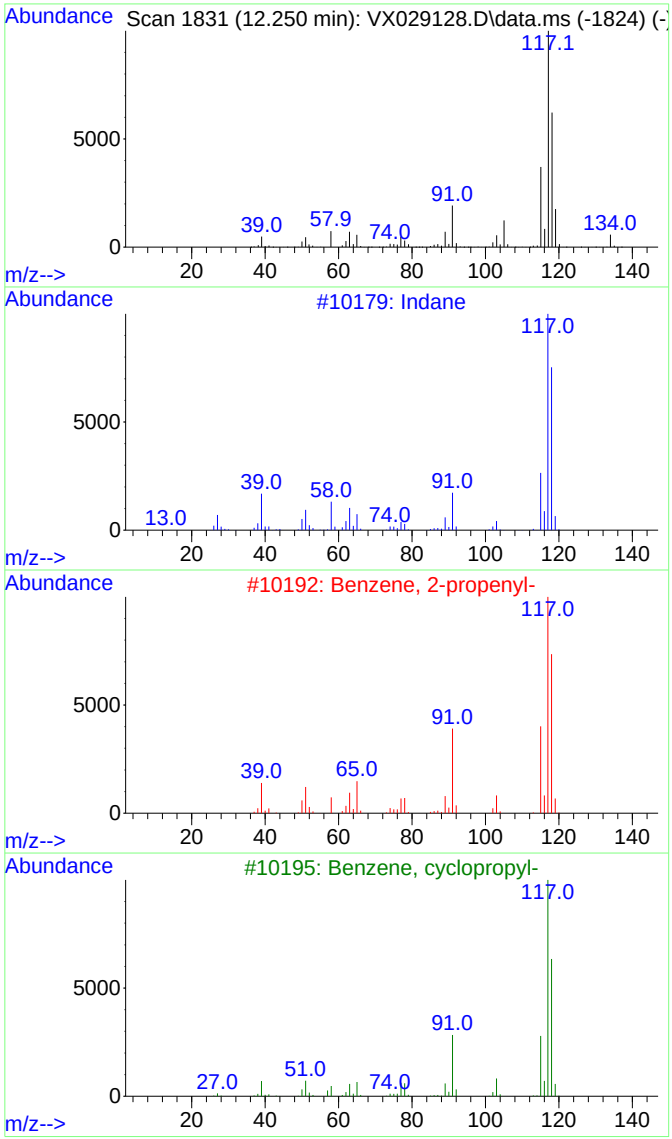
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

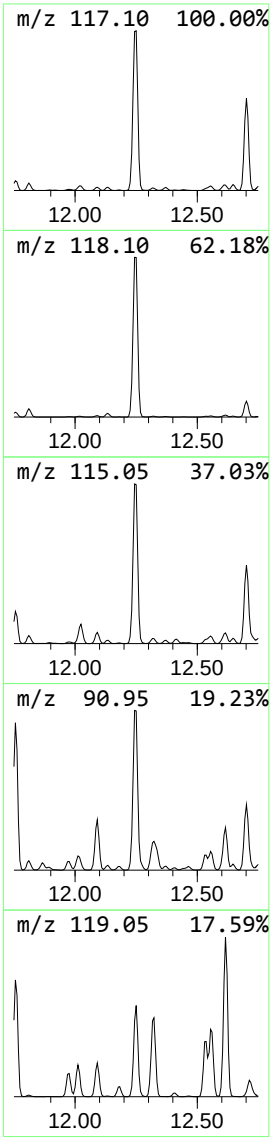
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	359.68 ug/l	19899600	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	68
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

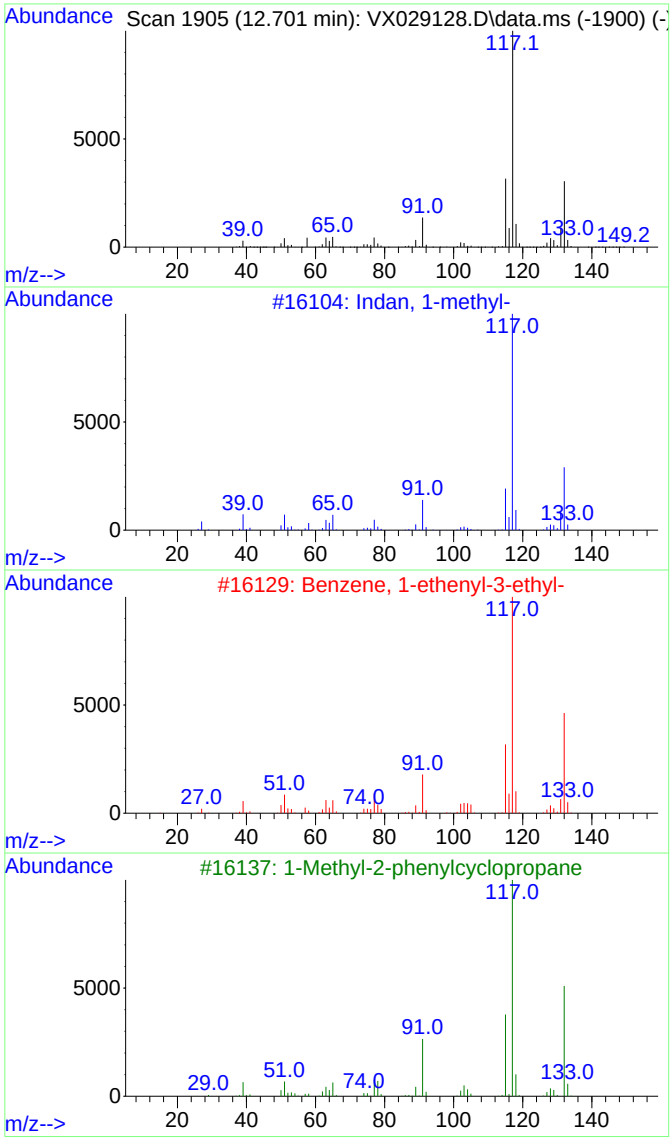
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

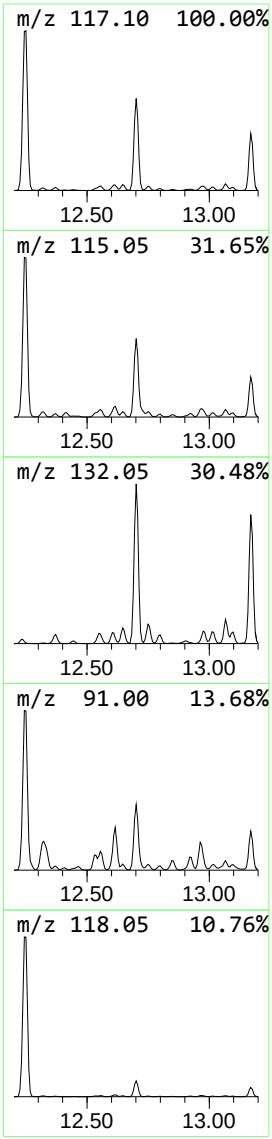
****

Peak Number 4 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	161.12 ug/l	8914110	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87





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Data File : VX029128.D
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

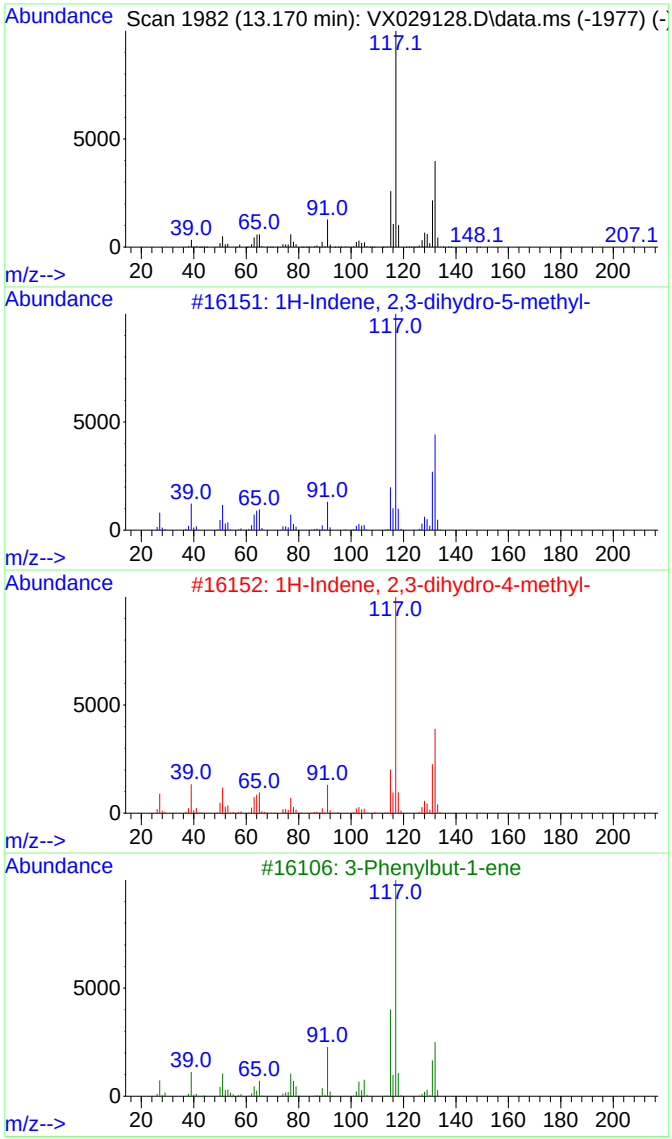
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

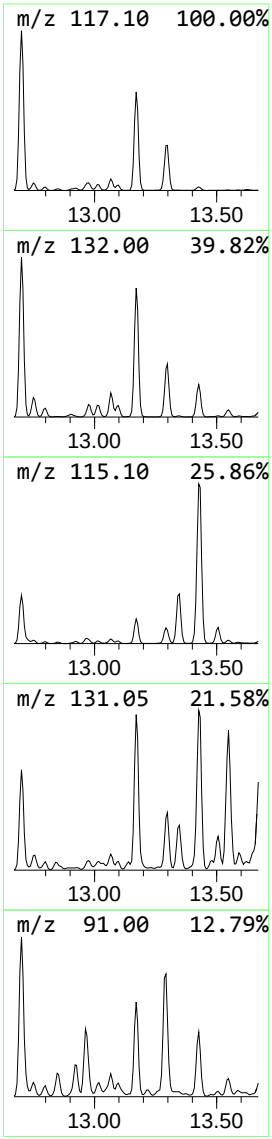
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	97.64 ug/l	5401880	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5	Indan, 1-methyl-	132	C10H12	000767-58-8	83





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Instrument :
MSVOA_X
ClientSampleId :
MW-14

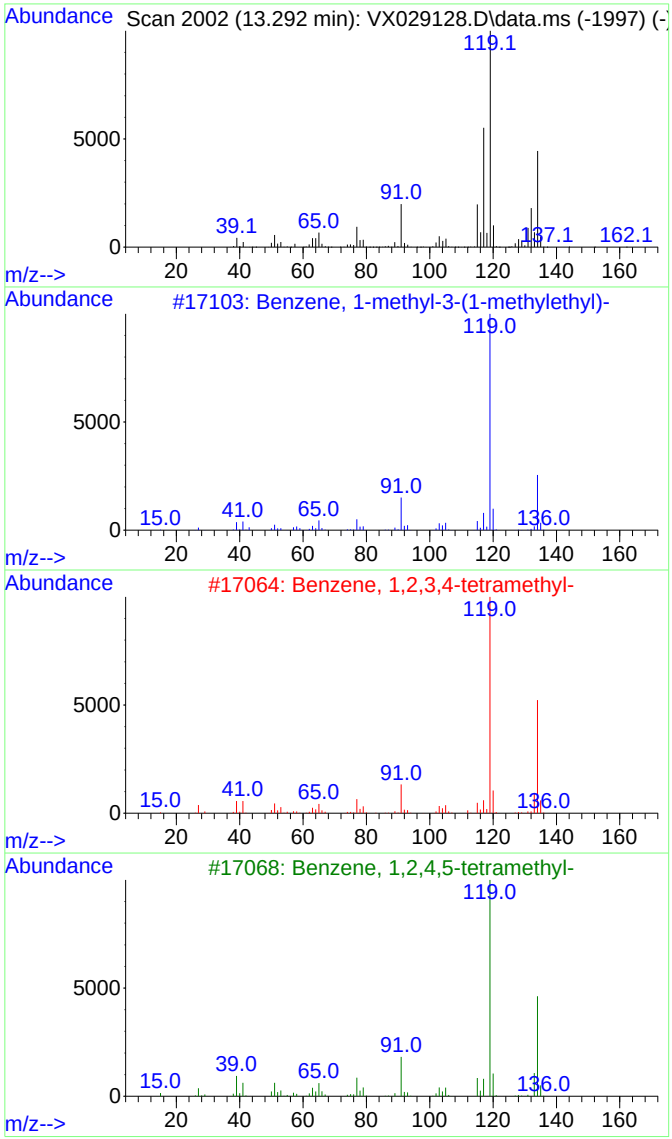
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

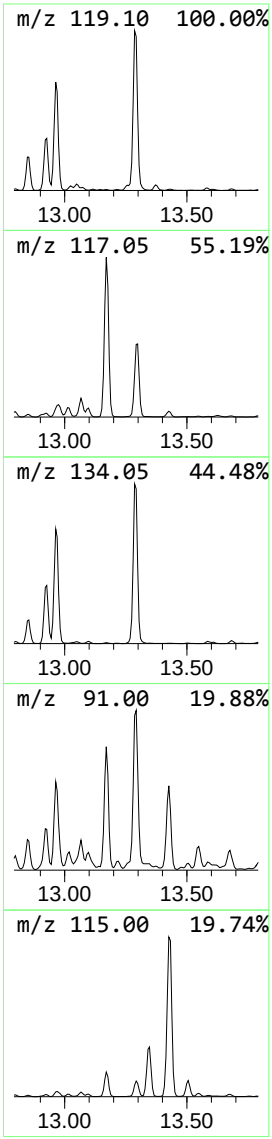
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	109.03 ug/l	6031910	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
4	o-Cymene	134	C10H14	000527-84-4	64
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	58





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Data File : VX029128.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

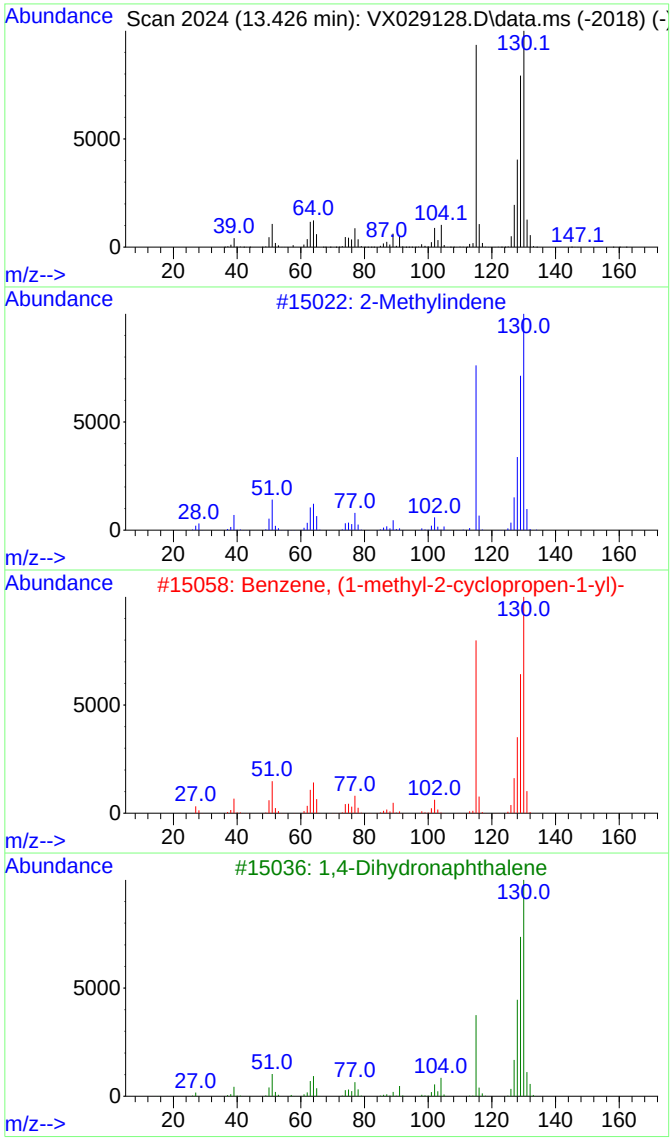
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

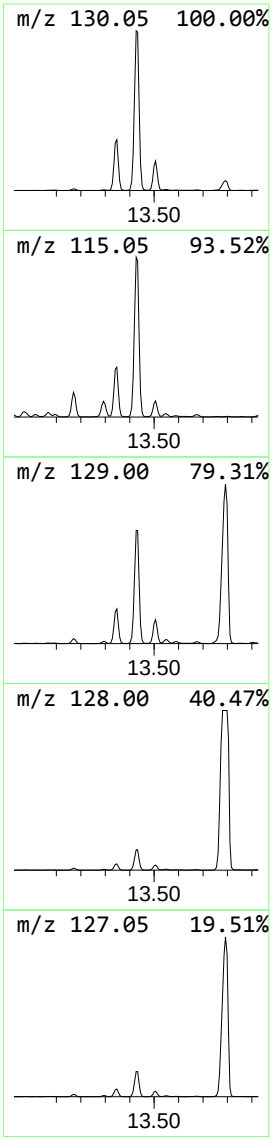
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Methylindene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	319.33 ug/l	17667100	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	95
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
3	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94





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Data File : VX029128.D
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Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

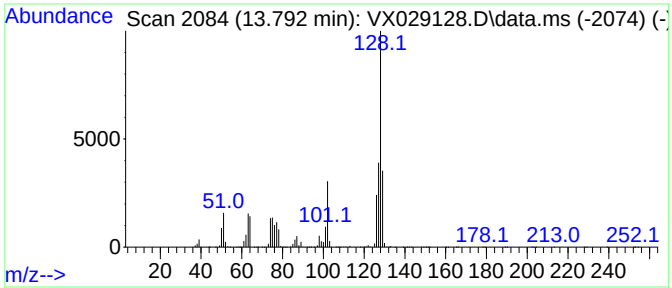
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

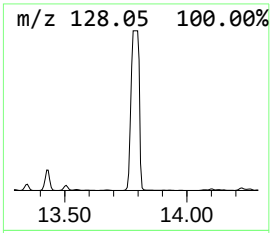
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

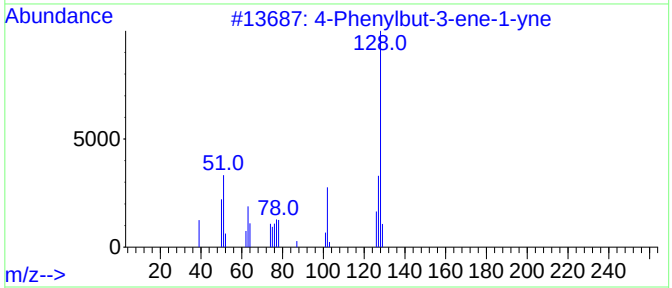
****
Peak Number 8 4-Phenylbut-3-ene-1-yne Concentration Rank 1

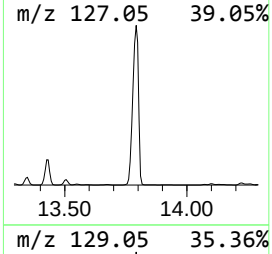
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	1116.21 ug/l	61755400	1,4-Dichlorobenzene-d4	12.024

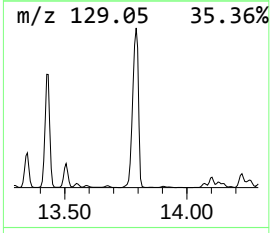
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	90
2	Naphthalene	128	C10H8	000091-20-3	86
3	Azulene	128	C10H8	000275-51-4	76
4	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	52
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	47

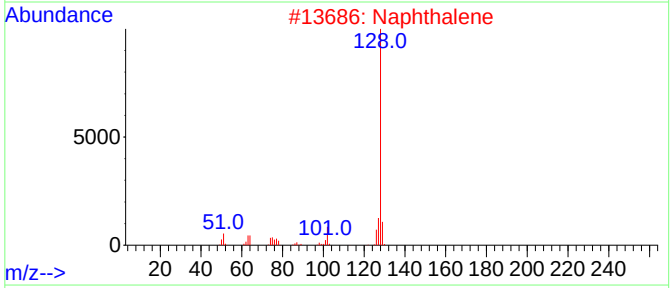


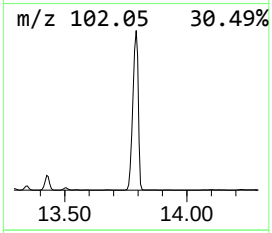


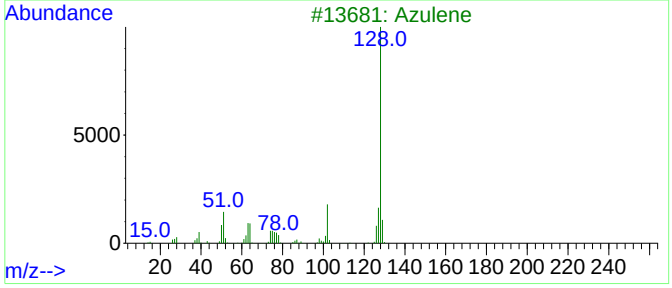


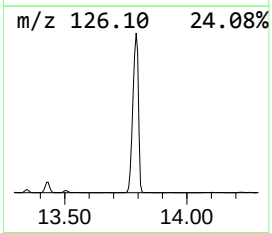












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

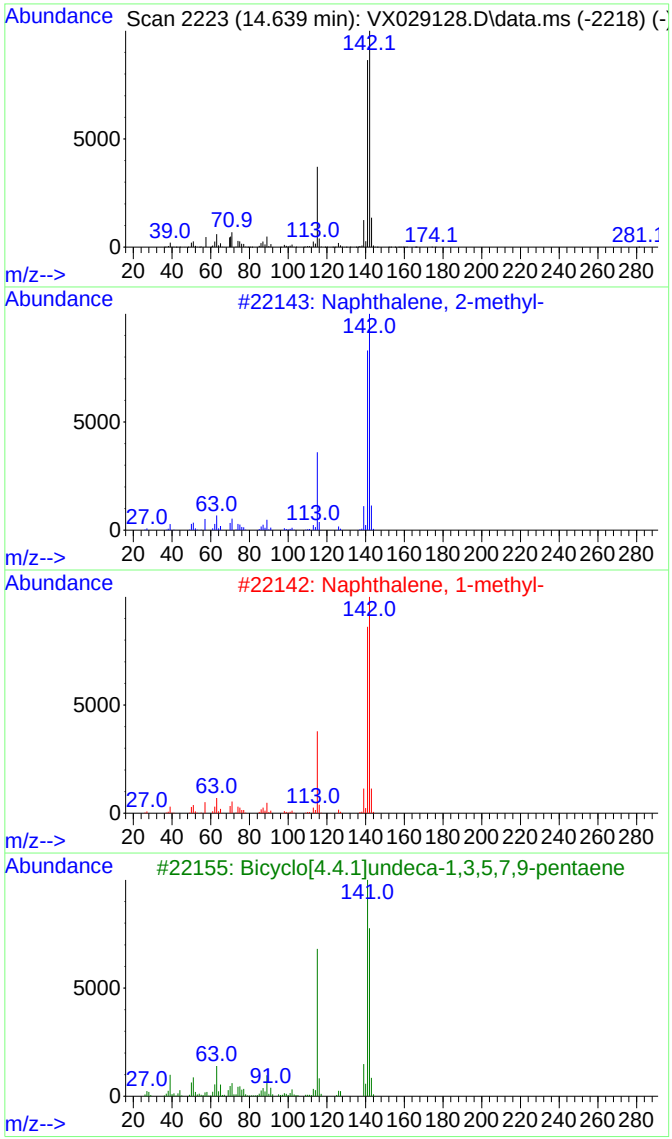
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

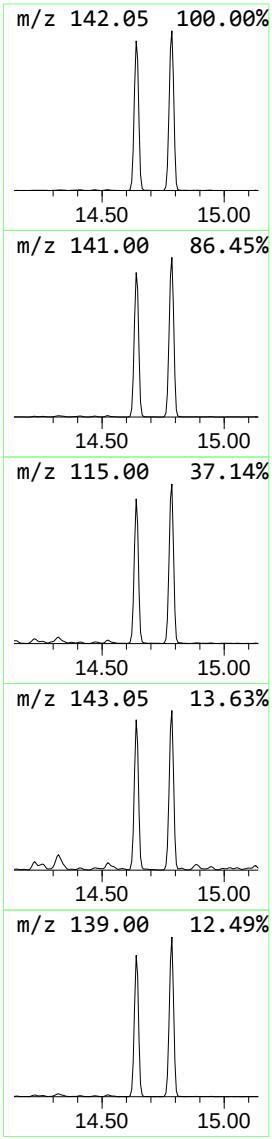
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	312.19 ug/l	17272000	1,4-Dichlorobenzene-d4	12.024

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	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	Benzocycloheptatriene	142	C11H10	000264-09-5	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

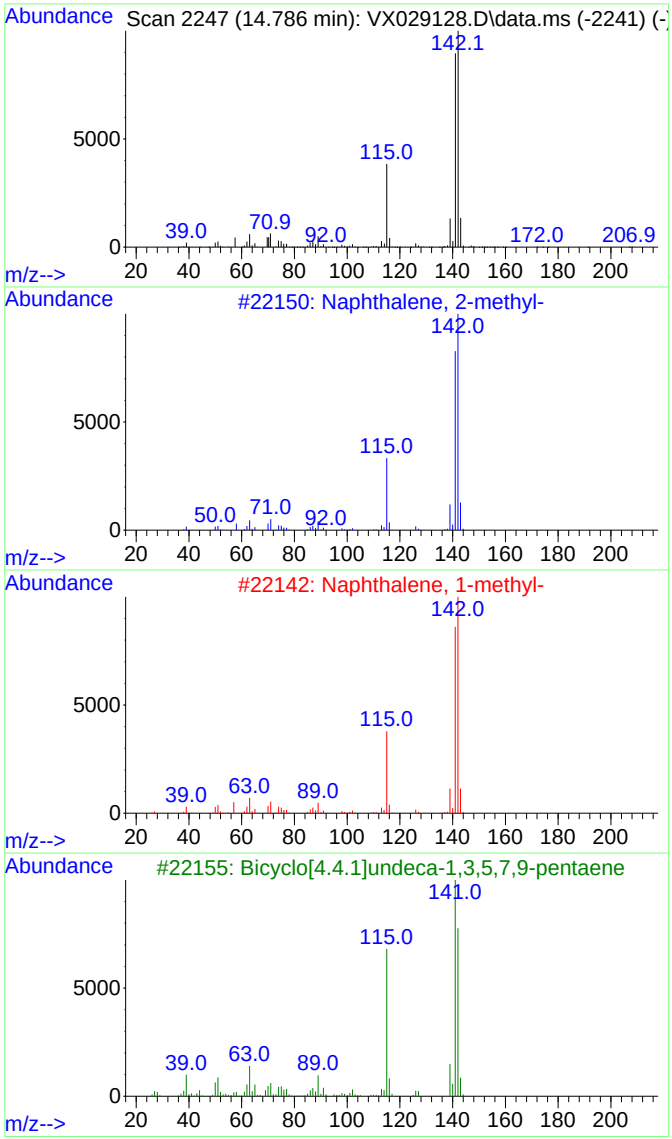
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

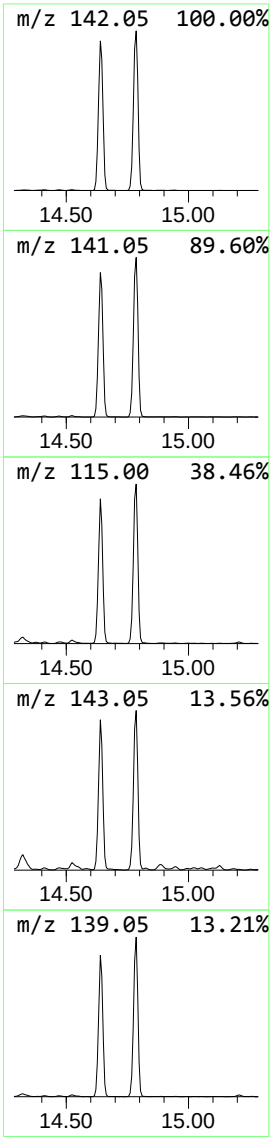
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	351.83 ug/l	19465300	1,4-Dichlorobenzene-d4	12.024

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	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	Benzocycloheptatriene	142	C11H10	000264-09-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060122\
Data File : VX029128.D
Acq On : 01 Jun 2022 19:04
Operator : JC/MD
Sample : N3087-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.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
Benzene, 1-ethy...	11.616	122.6	ug/l	6784460	4	12.024	2766290	50.0
Benzene, 1,2,3-...	12.091	146.9	ug/l	8128840	4	12.024	2766290	50.0
Indane	12.250	359.7	ug/l	19899600	4	12.024	2766290	50.0
Indan, 1-methyl-	12.701	161.1	ug/l	8914110	4	12.024	2766290	50.0
1H-Indene, 2,3-...	13.170	97.6	ug/l	5401880	4	12.024	2766290	50.0
Benzene, 1-meth...	13.292	109.0	ug/l	6031910	4	12.024	2766290	50.0
2-Methylindene	13.426	319.3	ug/l	17667100	4	12.024	2766290	50.0
4-Phenylbut-3-e...	13.792	1116.2	ug/l	61755400	4	12.024	2766290	50.0
Bicyclo[4.4.1]u...	14.639	312.2	ug/l	17272000	4	12.024	2766290	50.0
1,4-Methanonaph...	14.786	351.8	ug/l	19465300	4	12.024	2766290	50.0