LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032023\
Data File : VX034628.D
Acq On : 20 Mar 2023 15:21
Operator : JC/MD
Sample : 01939-04
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034628.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.624	67	88	92	rBV4	29276	132679	3.12%	0.311%
2	2.416	211	218	226	rBV	20578	42626	1.00%	0.100%
3	5.385	694	705	717	rBV2	133581	393853	9.27%	0.922%
4	5.544	717	731	755	rVB	259698	769411	18.10%	1.801%
5	5.952	788	798	815	rBV	167709	443818	10.44%	1.039%
6	6.757	921	930	944	rBV	424986	1037629	24.41%	2.428%
7	8.647	1225	1240	1249	rBV	890520	1411515	33.21%	3.303%
8	9.275	1335	1343	1352	rBV	62140	99361	2.34%	0.233%
9	10.055	1464	1471	1484	rBV	847827	1203075	28.31%	2.816%
10	11.085	1634	1640	1651	rBV	676242	956594	22.51%	2.239%
11	11.311	1669	1677	1684	rBV2	32883	46856	1.10%	0.110%
12	12.024	1788	1794	1802	rVB	883811	1107587	26.06%	2.592%
13	12.311	1837	1841	1850	rVB5	28856	59095	1.39%	0.138%
14	12.725	1902	1909	1913	rBV4	37849	81808	1.92%	0.191%
15	12.811	1918	1923	1927	rBV3	83104	134469	3.16%	0.315%
16	12.920	1933	1941	1945	rBV2	67552	116683	2.75%	0.273%
17	12.963	1945	1948	1950	rBV	46218	57922	1.36%	0.136%
18	13.030	1955	1959	1964	rVV4	38987	75758	1.78%	0.177%
19	13.158	1975	1980	1986	rBV7	36549	87804	2.07%	0.205%
20	13.213	1986	1989	1991	rBV2	49896	58505	1.38%	0.137%
21	13.250	1991	1995	1998	rVV2	70565	102351	2.41%	0.240%
22	13.292	1998	2002	2007	rVB3	201684	299954	7.06%	0.702%
23	13.420	2016	2023	2034	rBV4	296529	727878	17.13%	1.703%
24	13.512	2034	2038	2040	rBV4	89955	157160	3.70%	0.368%
25	13.585	2046	2050	2054	rBV3	172764	312589	7.35%	0.732%
26	13.664	2061	2063	2069	rVB3	161912	262485	6.18%	0.614%
27	13.756	2074	2078	2082	rVV2	119888	250570	5.90%	0.586%
28	13.798	2082	2085	2089	rVB2	171607	204305	4.81%	0.478%
29	13.853	2089	2094	2099	rBV3	475097	737154	17.34%	1.725%
30	13.926	2099	2106	2111	rBV3	453580	849284	19.98%	1.988%
31	13.981	2111	2115	2117	rVV3	99538	163596	3.85%	0.383%
32	14.006	2117	2119	2125	rVB5	113474	203715	4.79%	0.477%
33	14.067	2125	2129	2133	rBV4	265768	400907	9.43%	0.938%
34	14.164	2142	2145	2149	rBV5	144371	193958	4.56%	0.454%
35	14.225	2149	2155	2161	rBV3	1252153	2228066	52.42%	5.214%
36	14.323	2167	2171	2175	rBV2	383526	551776	12.98%	1.291%

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Integration Parameters: RTEINT.P
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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Title : SW846 8260

37	14.371	2176	2179	2184	rVV3	429064	500070	11.77%	1.170%
38	14.420	2184	2187	2193	rVB4	298837	539146	12.69%	1.262%
39	14.481	2193	2197	2205	rBV2	1323643	1990803	46.84%	4.659%
40	14.548	2205	2208	2210	rBV3	179341	226858	5.34%	0.531%
41	14.579	2210	2213	2215	rBV	184391	172649	4.06%	0.404%
42	14.615	2215	2219	2225	rBV2	1893478	2995529	70.48%	7.011%
43	14.670	2225	2228	2232	rVB2	1496367	1680282	39.54%	3.932%
44	14.725	2233	2237	2239	rBV3	388774	495559	11.66%	1.160%
45	14.756	2239	2242	2244	rVV3	353908	341653	8.04%	0.800%
46	14.786	2244	2247	2250	rVV3	266721	365907	8.61%	0.856%
47	14.816	2250	2252	2254	rVV2	430445	480226	11.30%	1.124%
48	14.847	2254	2257	2262	rVB2	969852	1188454	27.96%	2.781%
49	14.914	2263	2268	2273	rBV2	660683	1295264	30.48%	3.031%
50	15.042	2284	2289	2293	rBV3	598541	1172750	27.59%	2.745%
51	15.182	2307	2312	2315	rBV	1042318	1663512	39.14%	3.893%
52	15.249	2319	2323	2330	rVB5	538353	1030192	24.24%	2.411%
53	15.316	2331	2334	2340	rVB4	313686	548456	12.90%	1.284%
54	15.377	2340	2344	2347	rBV2	677105	911674	21.45%	2.134%
55	15.414	2347	2350	2354	rVB3	324061	388876	9.15%	0.910%
56	15.481	2358	2361	2364	rBV3	399715	571149	13.44%	1.337%
57	15.560	2369	2374	2379	rVV	2553140	4250039	100.00%	9.947%
58	15.609	2379	2382	2386	rVB2	586070	829731	19.52%	1.942%
59	15.664	2387	2391	2397	rVB7	274270	666468	15.68%	1.560%
60	15.743	2399	2404	2408	rVB4	399923	670392	15.77%	1.569%
61	15.847	2418	2421	2429	rVB6	343306	756344	17.80%	1.770%
62	15.987	2441	2444	2447	rBV3	201990	320036	7.53%	0.749%
63	16.085	2457	2460	2471	rVB4	384138	713801	16.80%	1.671%

Sum of corrected areas: 42728616

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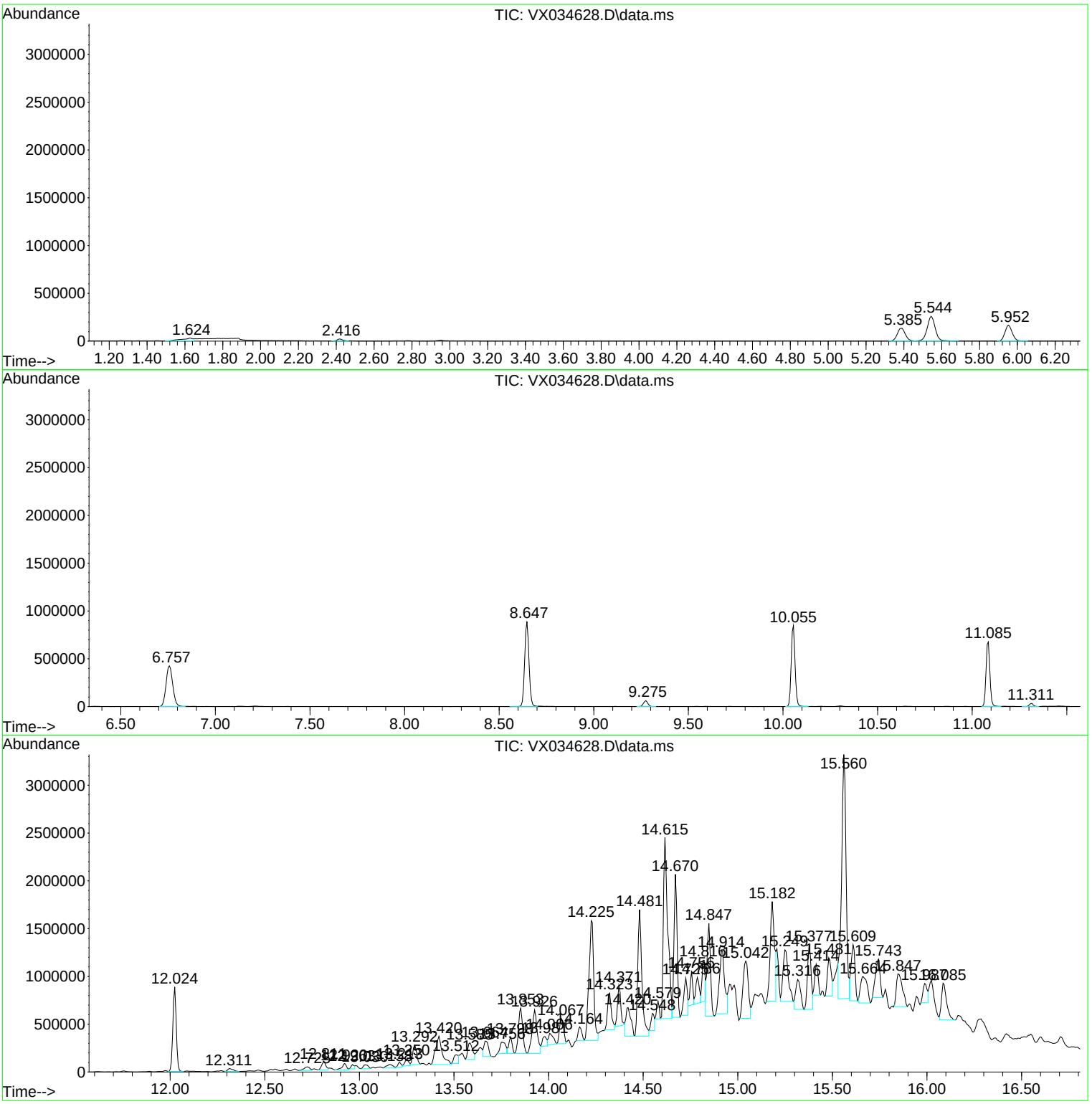
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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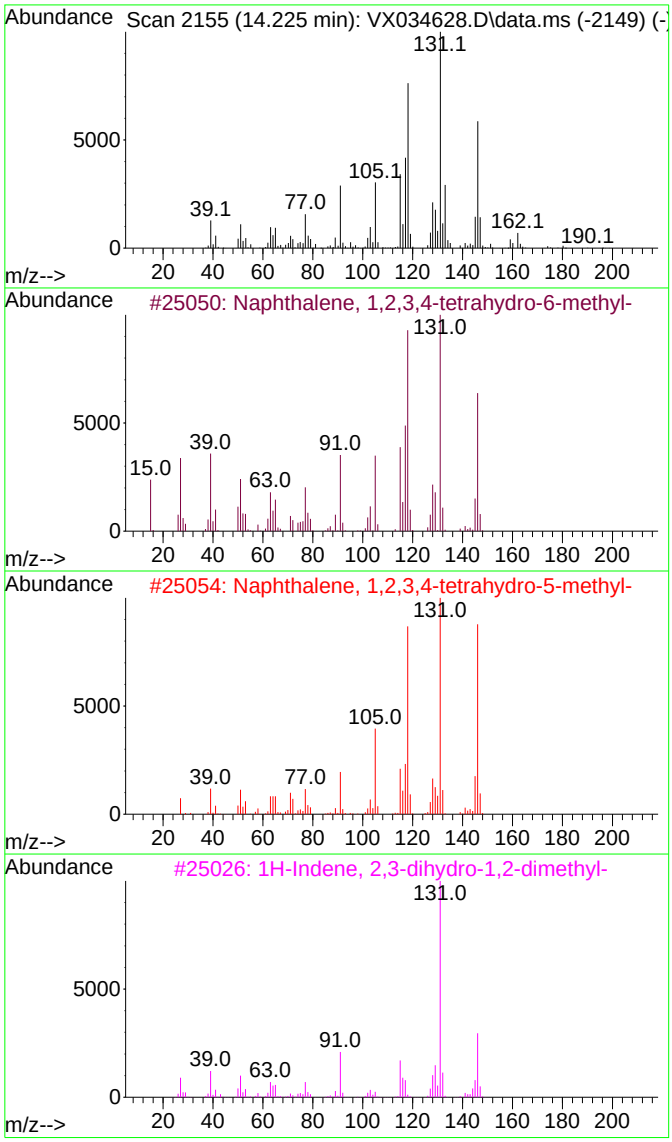
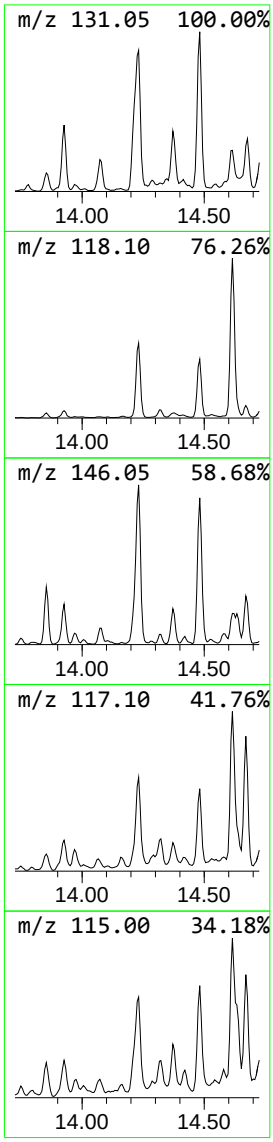
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	100.58 ug/l	2228070	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	55
4	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	55
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	50





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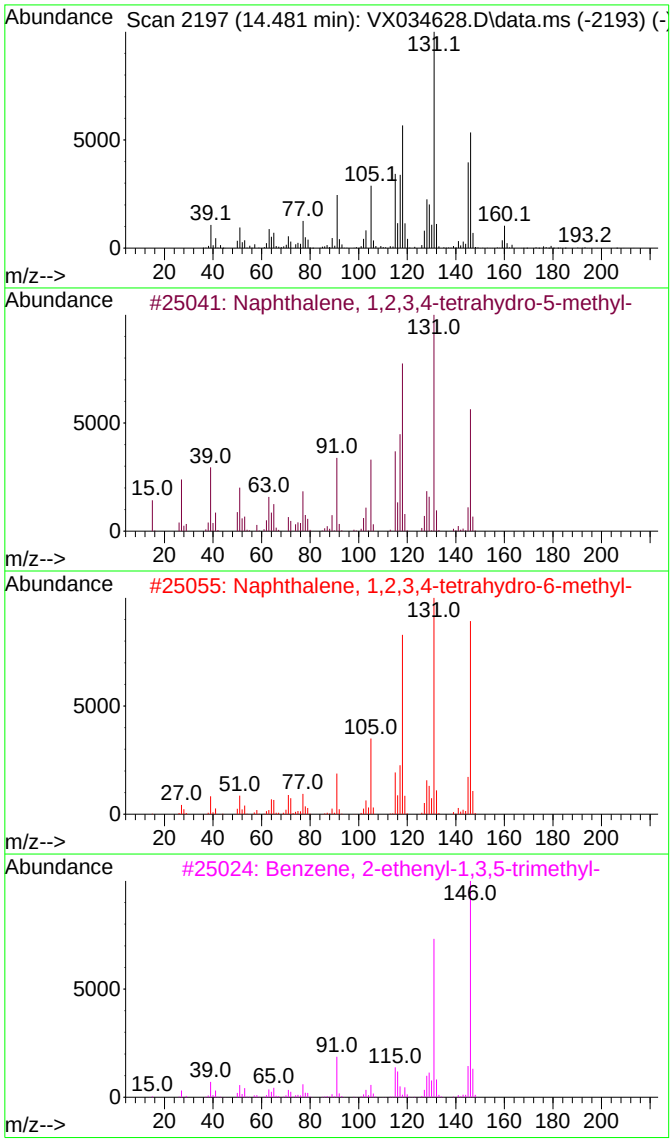
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

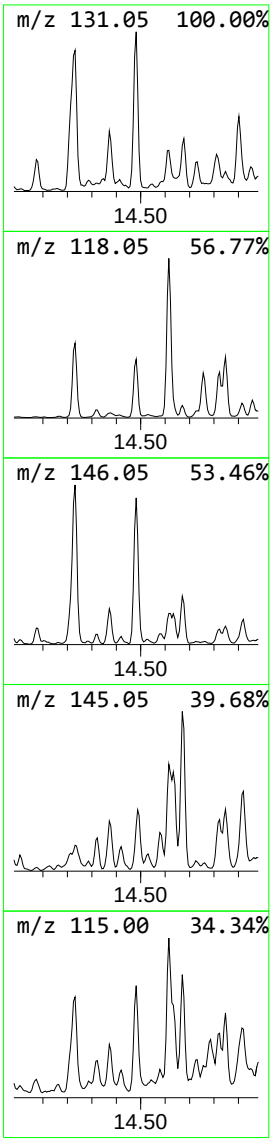
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	89.87 ug/l	1990800	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	89
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	76
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
4	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	60
5	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58





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Instrument :
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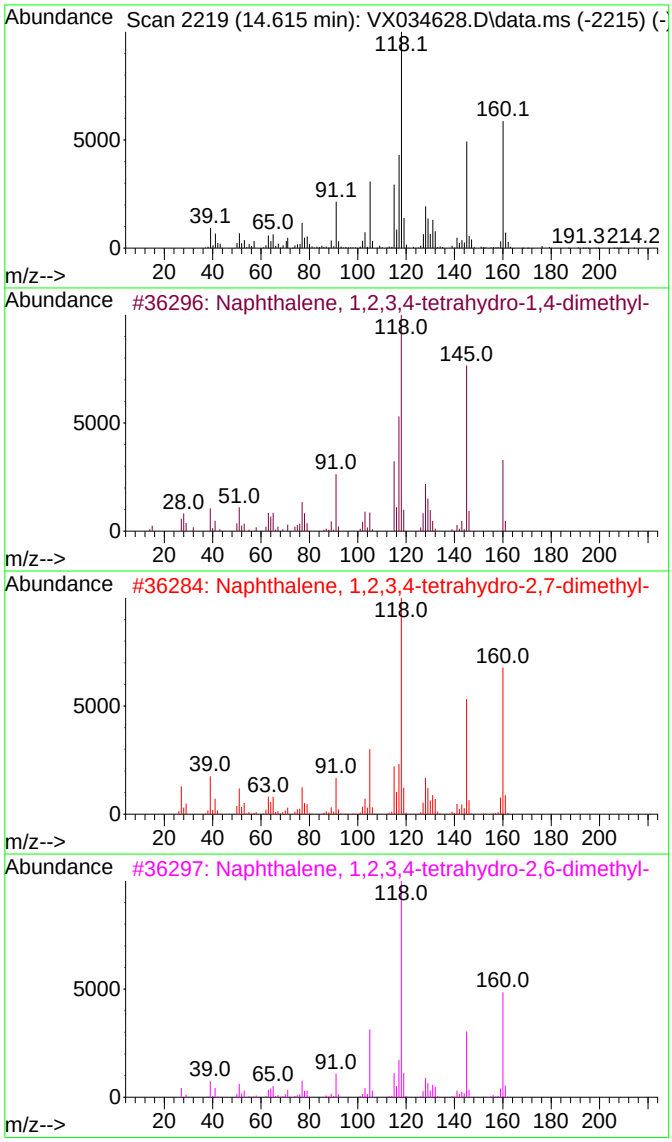
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

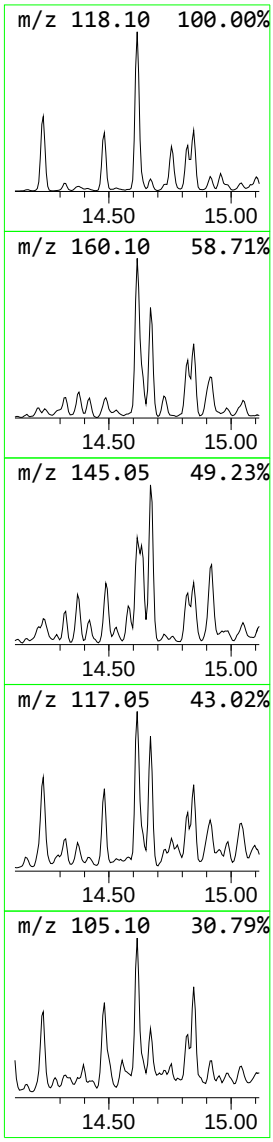
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	135.23 ug/l	2995530	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	81
4	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	62
5	Benzene, 1,2,4-trimethyl-5-(1-me...	160	C12H16	054340-84-0	50





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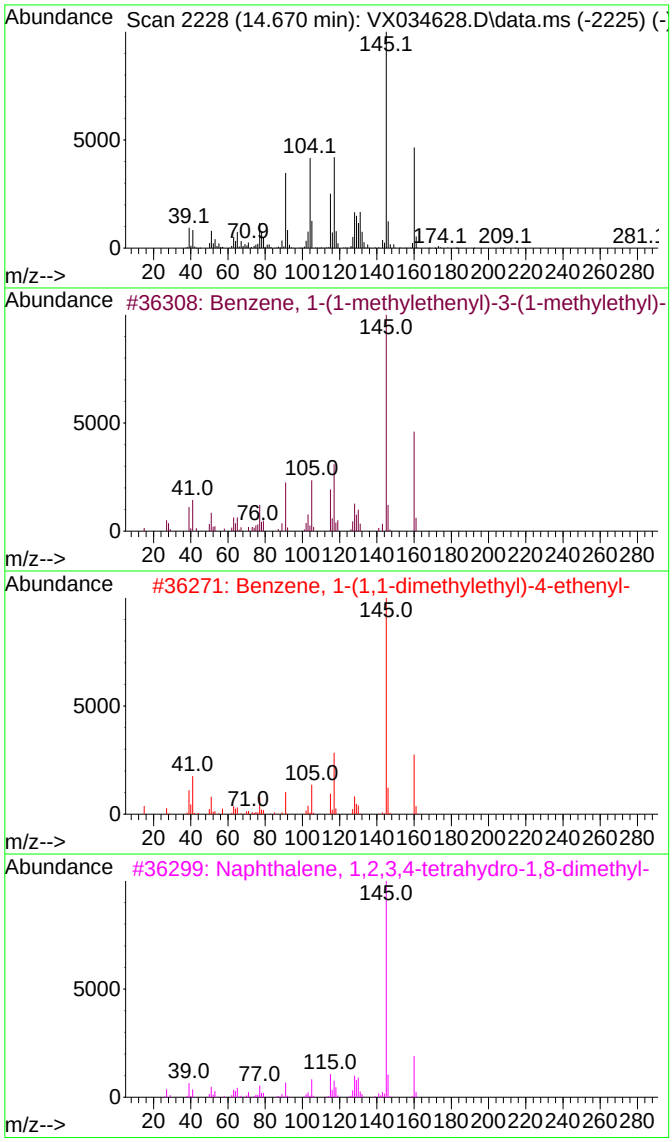
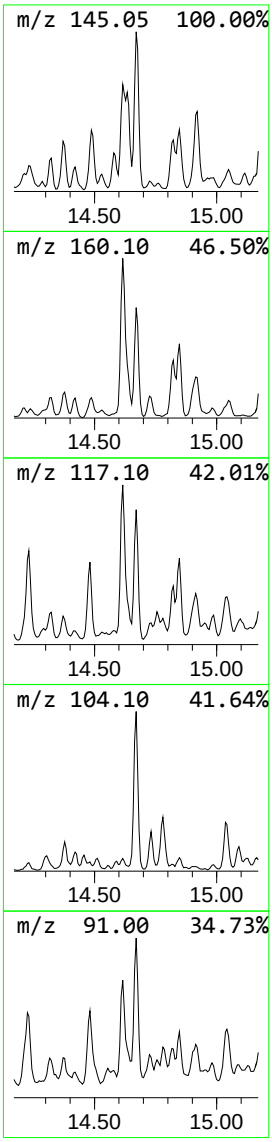
****
Peak Number 4 Benzene, 1-(1-methylethenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	75.85 ug/l	1680280	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	81
2	Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	64
5	1H-Indene, 2,3-dihydro-1,1,4-tri...	160	C12H16	016204-72-1	64





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TIC Library : C:\Database\NIST20.L
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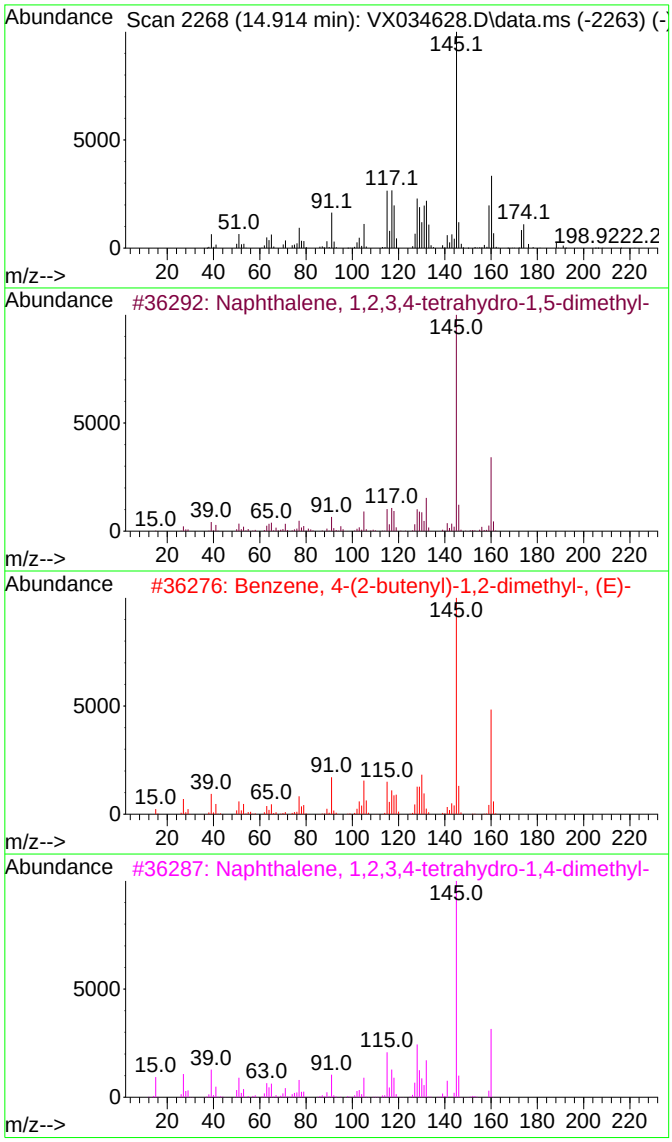
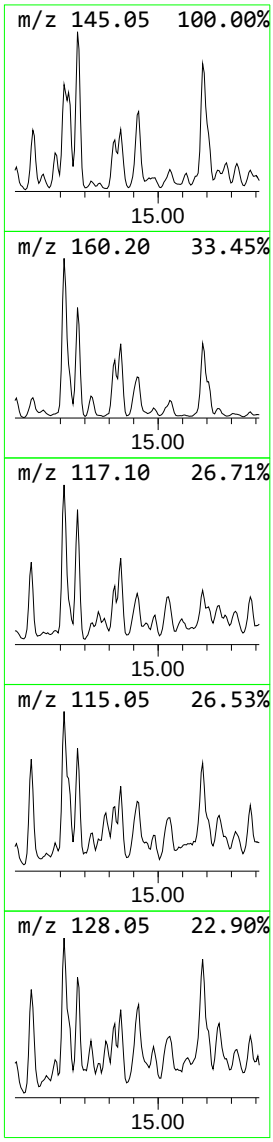
****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.914	58.47 ug/l	1295260	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	89
2	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	70
4	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	60
5	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	60





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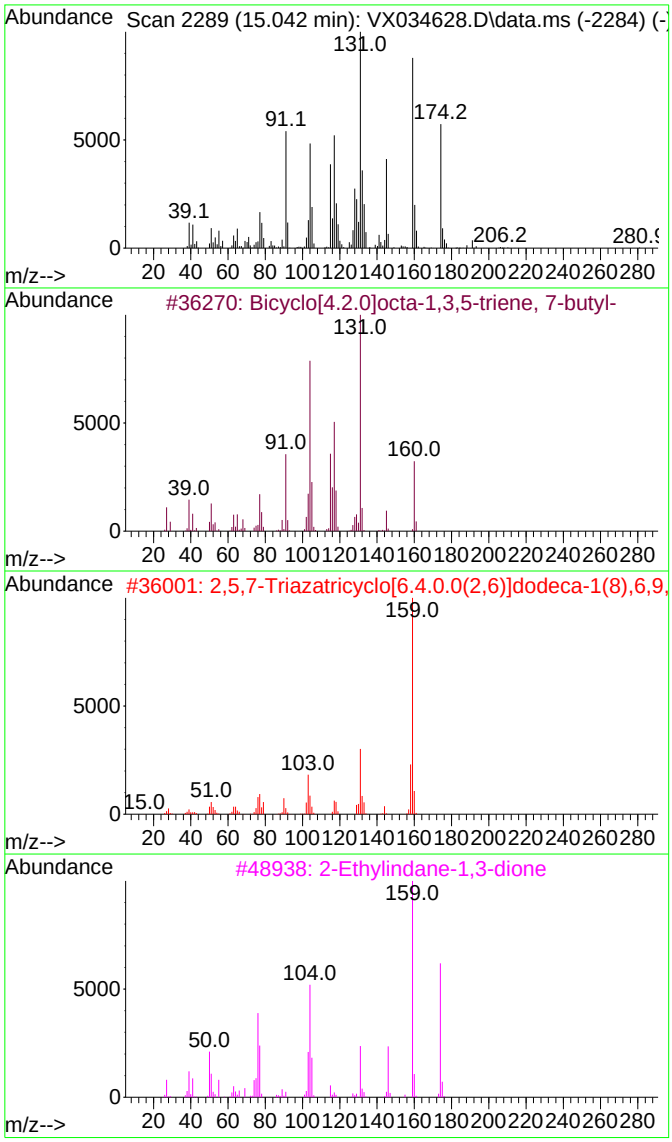
Quant Title : SW846 8260

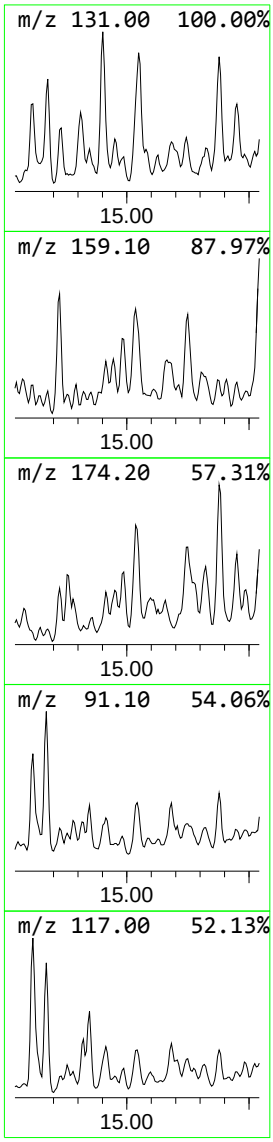
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.042	52.94 ug/l	1172750	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene,...	160	C12H16	078920-29-3	50
2	2,5,7-Triazatricyclo[6.4.0.0(2,6...	159	C9H9N3	024134-26-7	46
3	2-Ethylindane-1,3-dione	174	C11H10O2	027606-61-7	46
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-17-7	38
5	2-Benzylidenecyclopentanol, (E)-	174	C12H14O	058738-53-7	38





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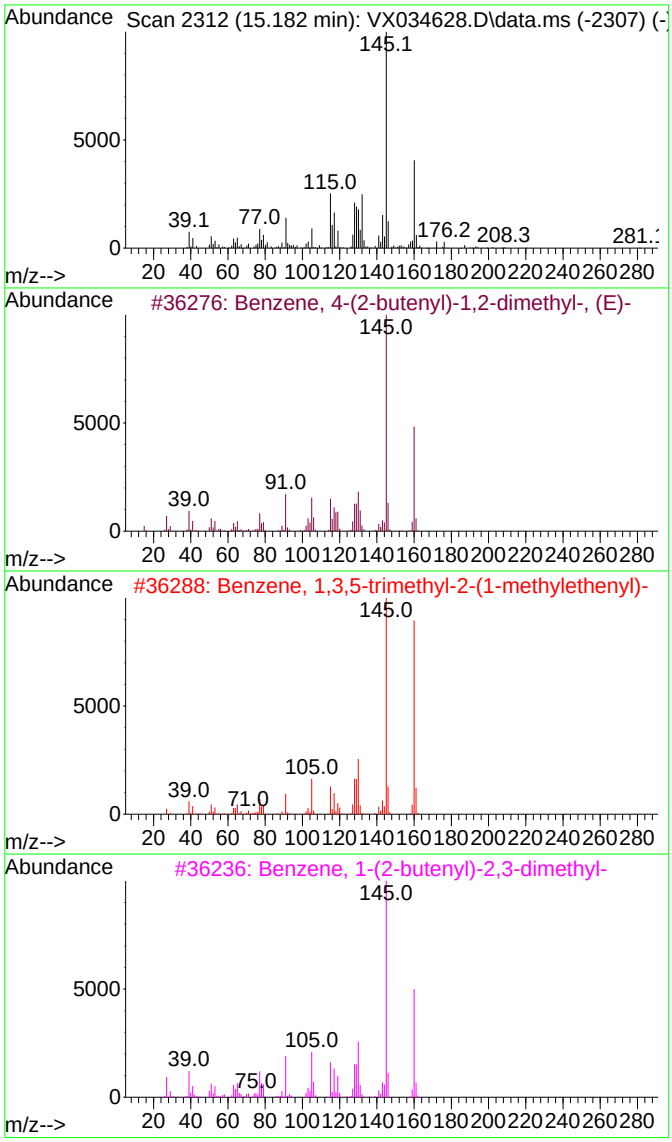
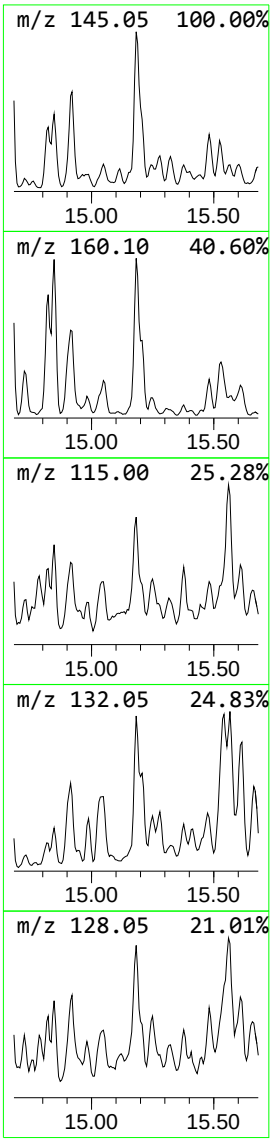
****
Peak Number 8 Benzene, 4-(2-butenyl)-1,2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	75.10 ug/l	1663510	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	93
2	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	89
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	76
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	74
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	74





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Data File : VX034628.D
Acq On : 20 Mar 2023 15:21
Operator : JC/MD
Sample : 01939-04
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071

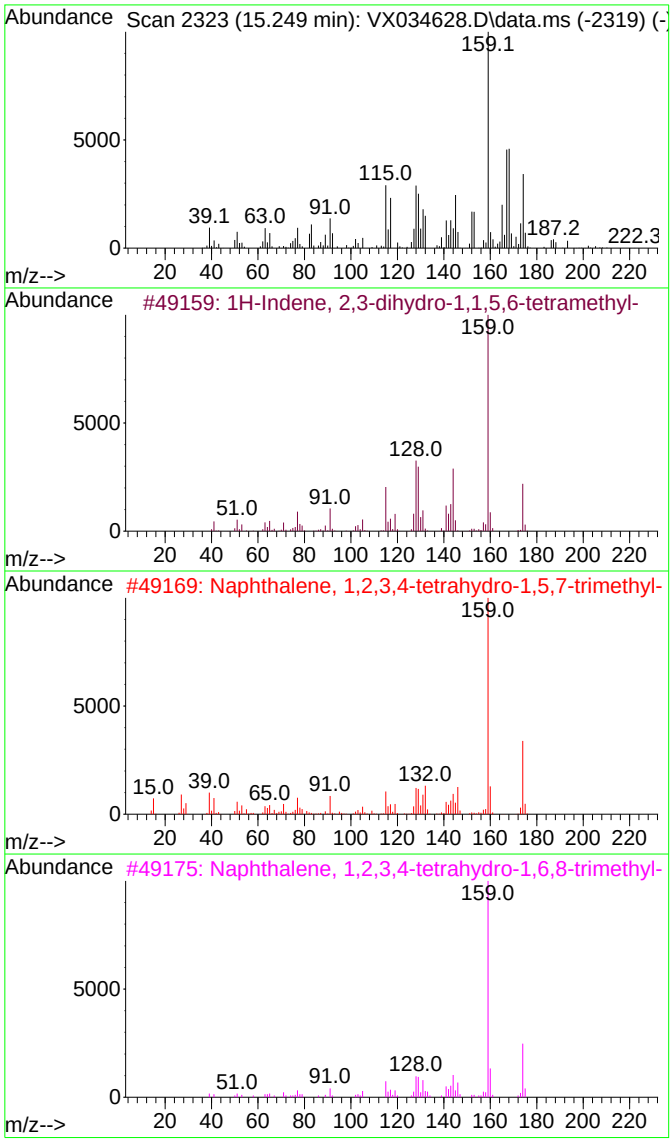
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

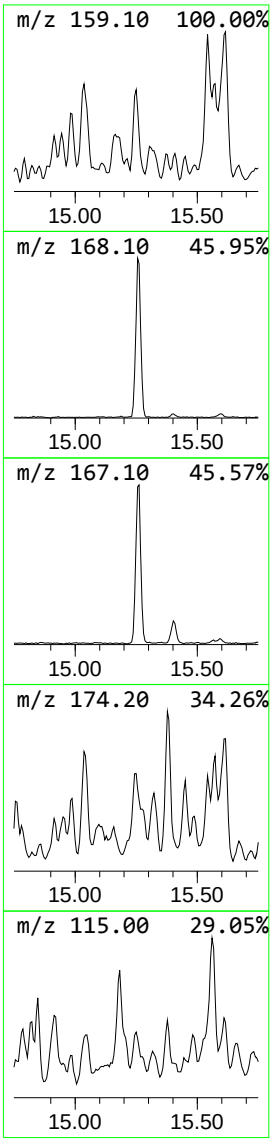
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	46.51 ug/l	1030190	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,5,6-t...	174	C13H18	000942-43-8	64
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-55-0	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	64
4	1H-Indene, 2,3-dihydro-1,1,4,7-t...	174	C13H18	001078-04-2	50
5	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-17-7	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032023\
Data File : VX034628.D
Acq On : 20 Mar 2023 15:21
Operator : JC/MD
Sample : 01939-04
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071

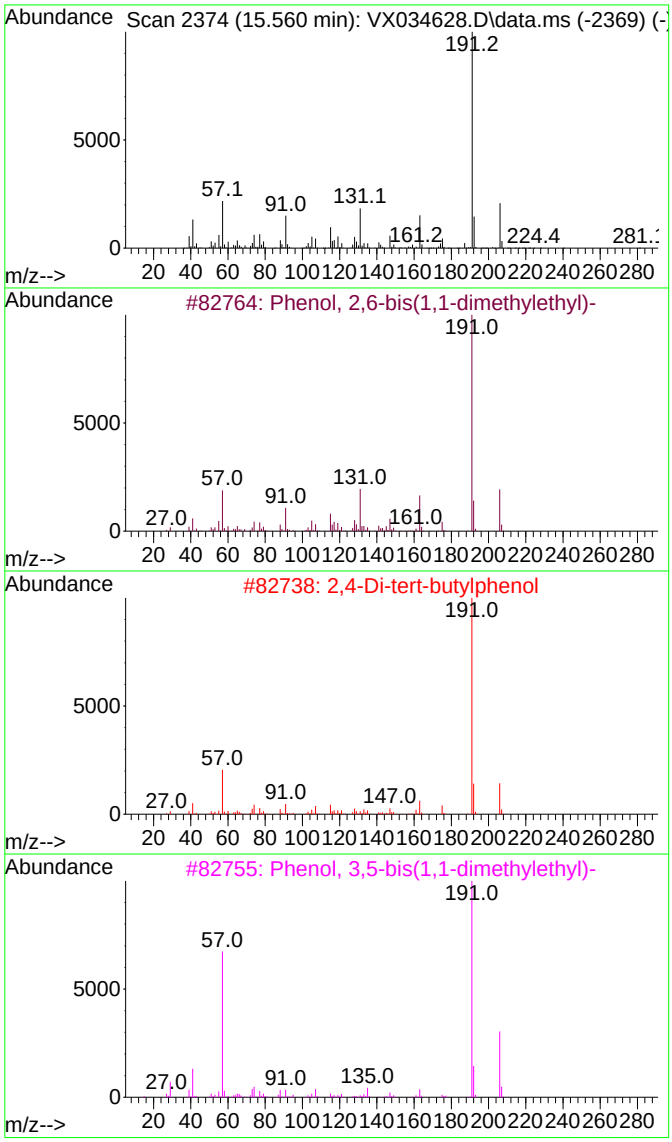
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

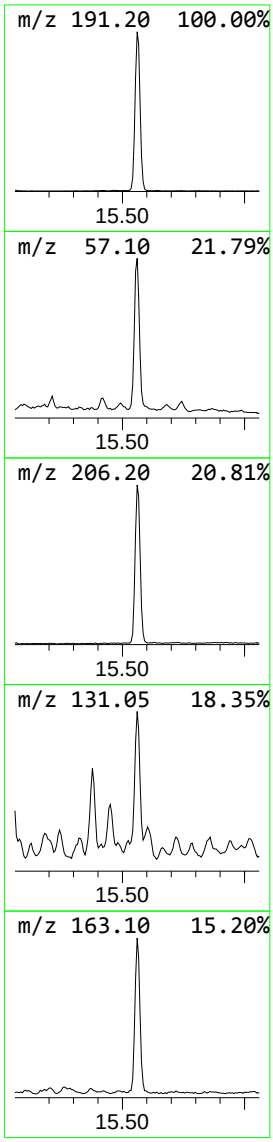
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	191.86 ug/l	4250040	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	90
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	81
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	80
5	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032023\
Data File : VX034628.D
Acq On : 20 Mar 2023 15:21
Operator : JC/MD
Sample : 01939-04
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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
Naphthalene, 1,...	14.225	100.6	ug/l	2228070	4	12.024	1107590	50.0
Naphthalene, 1,...	14.481	89.9	ug/l	1990800	4	12.024	1107590	50.0
Naphthalene, 1,...	14.615	135.2	ug/l	2995530	4	12.024	1107590	50.0
Benzene, 1-(1-m...	14.670	75.8	ug/l	1680280	4	12.024	1107590	50.0
Naphthalene, 1,...	14.914	58.5	ug/l	1295260	4	12.024	1107590	50.0
Bicyclo[4.2.0]o...	15.042	52.9	ug/l	1172750	4	12.024	1107590	50.0
Benzene, 4-(2-b...	15.182	75.1	ug/l	1663510	4	12.024	1107590	50.0
1H-Indene, 2,3-...	15.249	46.5	ug/l	1030190	4	12.024	1107590	50.0
Phenol, 2,6-bis...	15.560	191.9	ug/l	4250040	4	12.024	1107590	50.0