LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120823\
Data File : VN080424.D
Acq On : 08 Dec 2023 22:19
Operator : JC\MD
Sample : 05695-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

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\82N111623W.M
Title : SW846 8260

Signal : TIC: VN080424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.665	114	121	126	rBV2	12160	23801	1.54%	0.216%
2	8.171	1047	1057	1061	rBV	226716	549732	35.56%	4.999%
3	8.224	1061	1066	1077	rVB	345951	764345	49.45%	6.950%
4	8.582	1119	1127	1135	rBV	214123	484288	31.33%	4.403%
5	9.100	1207	1215	1226	rVB	512718	1060503	68.60%	9.643%
6	10.571	1457	1465	1474	rBV	853728	1545830	100.00%	14.056%
7	11.865	1678	1685	1694	rBV	798674	1436120	92.90%	13.058%
8	12.400	1770	1776	1783	rVB4	20107	39582	2.56%	0.360%
9	12.853	1845	1853	1861	rBV	680207	1187405	76.81%	10.797%
10	13.100	1890	1895	1898	rBV2	17613	28348	1.83%	0.258%
11	13.176	1903	1908	1914	rVB3	32920	57850	3.74%	0.526%
12	13.341	1930	1936	1942	rVB2	34433	61453	3.98%	0.559%
13	13.482	1954	1960	1965	rBV2	25846	46780	3.03%	0.425%
14	13.670	1987	1992	1997	rBV5	18905	36693	2.37%	0.334%
15	13.794	2006	2013	2024	rBV	836964	1492098	96.52%	13.567%
16	13.953	2032	2040	2043	rBV8	13284	29699	1.92%	0.270%
17	13.994	2043	2047	2048	rVV4	35006	52350	3.39%	0.476%
18	14.017	2049	2051	2058	rVB2	46062	69135	4.47%	0.629%
19	14.117	2062	2068	2074	rBV4	25218	46320	3.00%	0.421%
20	14.188	2074	2080	2084	rBV	24417	34564	2.24%	0.314%
21	14.247	2086	2090	2092	rBV4	13365	20527	1.33%	0.187%
22	14.276	2092	2095	2099	rVB3	12629	18662	1.21%	0.170%
23	14.329	2099	2104	2109	rVB2	37366	59755	3.87%	0.543%
24	14.441	2119	2123	2128	rBV3	48249	78019	5.05%	0.709%
25	14.576	2141	2146	2151	rBV3	24544	36095	2.33%	0.328%
26	14.629	2151	2155	2156	rBV4	14325	15925	1.03%	0.145%
27	14.659	2157	2160	2162	rVB3	14752	15945	1.03%	0.145%
28	14.694	2162	2166	2170	rVB	36426	49259	3.19%	0.448%
29	14.735	2170	2173	2176	rBV3	27146	27568	1.78%	0.251%
30	14.770	2176	2179	2183	rBV3	15963	25687	1.66%	0.234%
31	14.876	2190	2197	2201	rBV8	19024	44433	2.87%	0.404%
32	14.935	2201	2207	2210	rVV5	25686	51393	3.32%	0.467%
33	14.964	2210	2212	2216	rVV4	26447	34995	2.26%	0.318%
34	15.053	2219	2227	2234	rVV3	76083	214860	13.90%	1.954%
35	15.106	2234	2236	2243	rVB8	18068	39270	2.54%	0.357%
36	15.211	2248	2254	2261	rBV3	62429	110811	7.17%	1.008%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

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\82N111623W.M
Title : SW846 8260

37	15.323	2267	2273	2276	rBV6	49628	97426	6.30%	0.886%
38	15.435	2286	2292	2299	rVB3	60280	145242	9.40%	1.321%
39	15.600	2315	2320	2324	rBV7	19614	38162	2.47%	0.347%
40	15.706	2332	2338	2342	rBV6	40879	90691	5.87%	0.825%
41	15.788	2348	2352	2367	rVB6	49979	161863	10.47%	1.472%
42	15.947	2372	2379	2383	rBV4	41088	91499	5.92%	0.832%
43	16.129	2402	2410	2413	rBV6	26165	65734	4.25%	0.598%
44	16.164	2413	2416	2422	rVB3	52020	88407	5.72%	0.804%
45	16.258	2428	2432	2437	rBV6	18724	36349	2.35%	0.331%
46	16.500	2464	2473	2481	rBV4	55743	167633	10.84%	1.524%
47	16.711	2502	2509	2516	rBV7	46376	102973	6.66%	0.936%
48	16.782	2517	2521	2522	rBV3	18777	21854	1.41%	0.199%

Sum of corrected areas: 10997933

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ClientSampleId :
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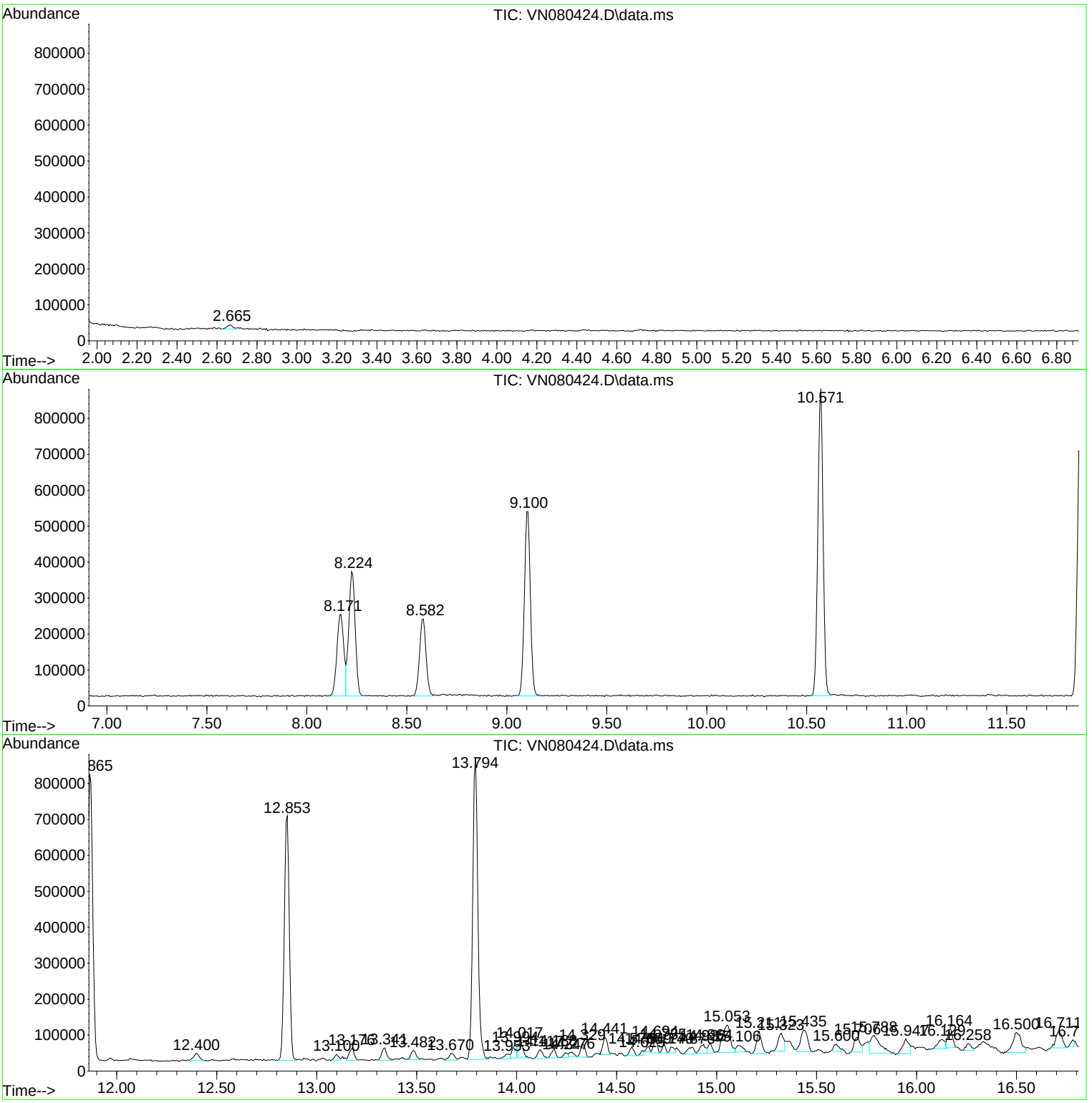
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



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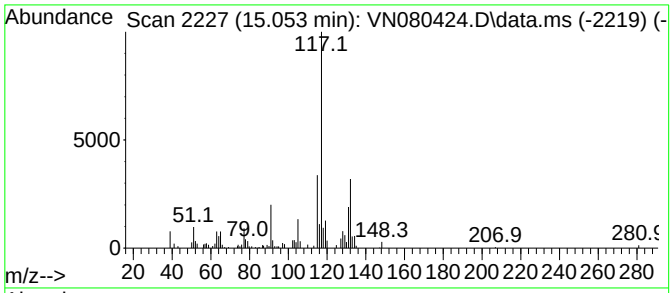
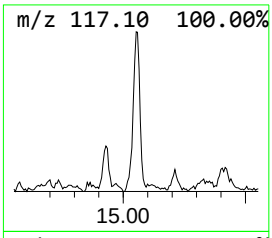
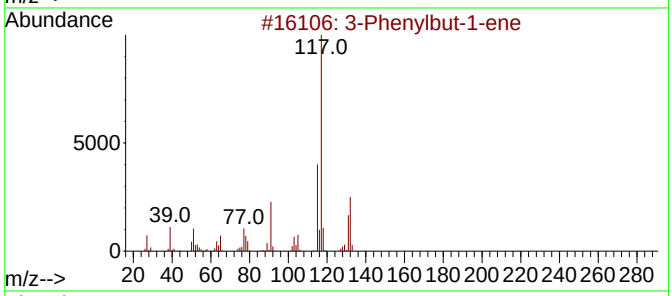
****
Peak Number 1 3-Phenylbut-1-ene Concentration Rank 1

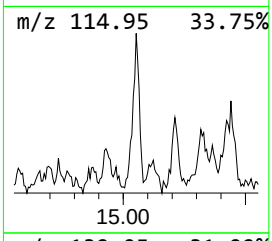
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	7.20 ug/l	214860	1,4-Dichlorobenzene-d4	13.794

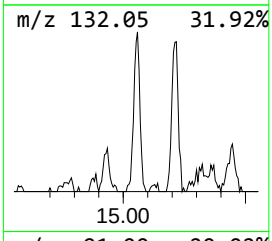
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
5	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	83

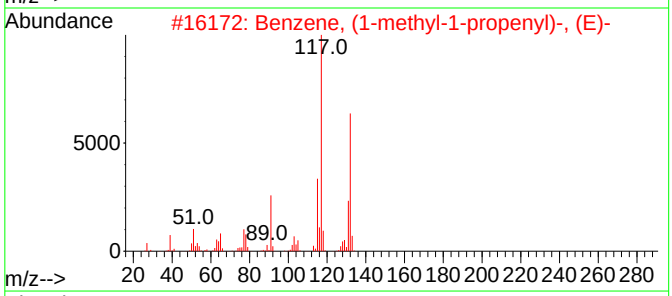


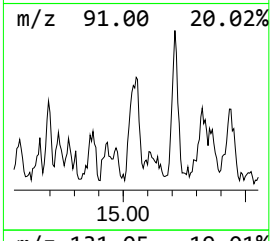


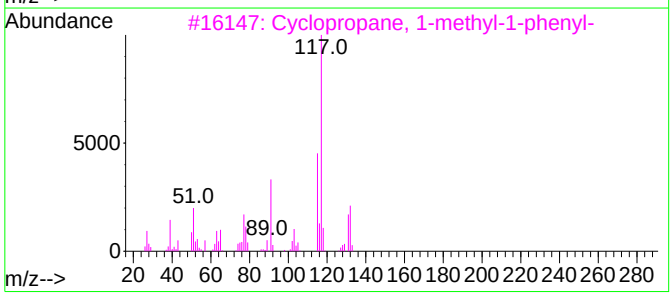


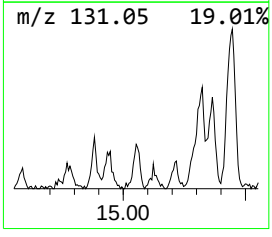












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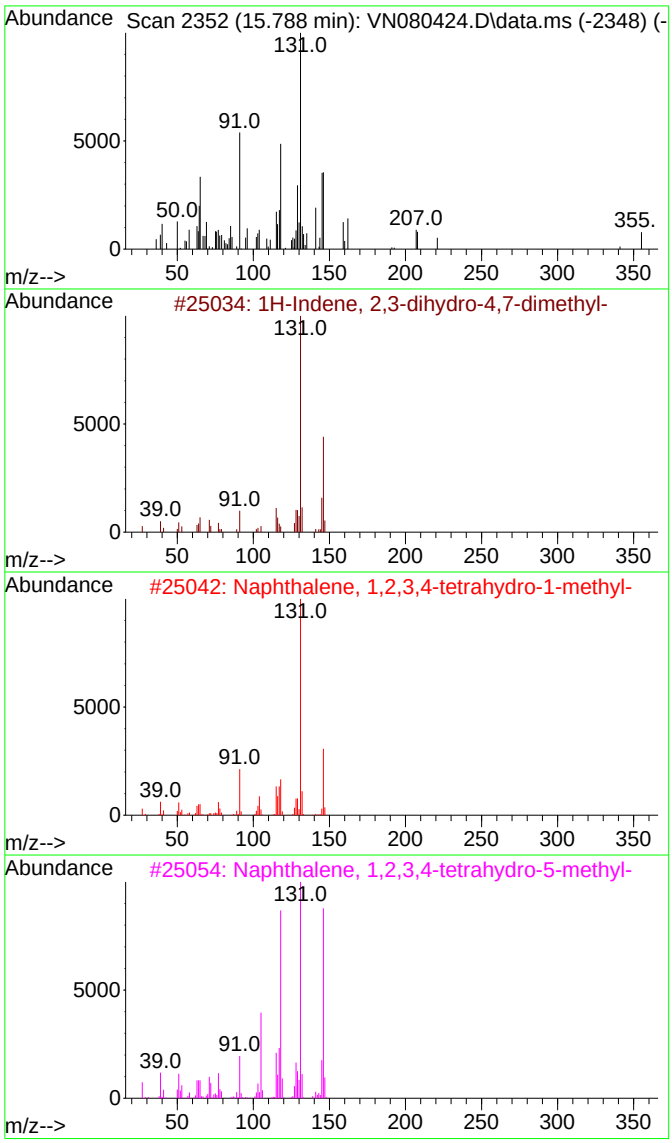
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

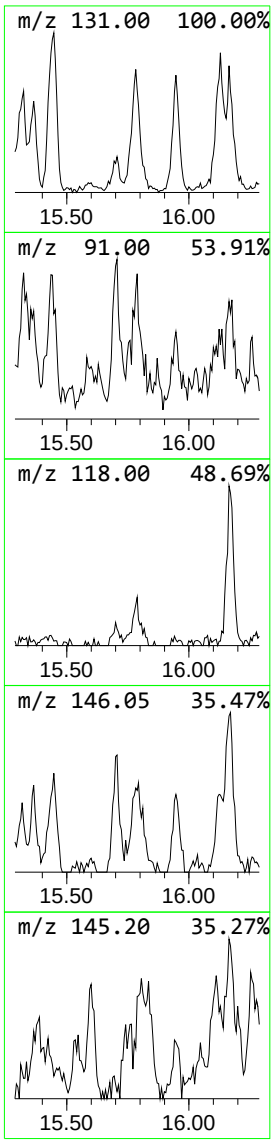
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.788	5.42 ug/l	161863	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	55
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	55
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	52
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	52
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	46





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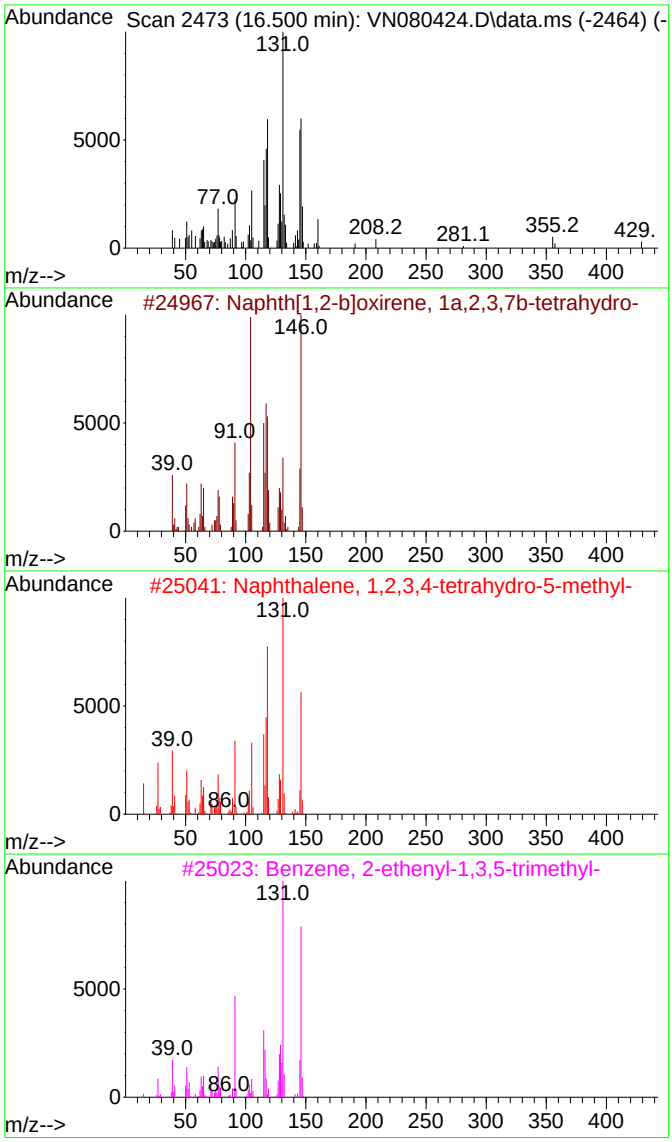
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

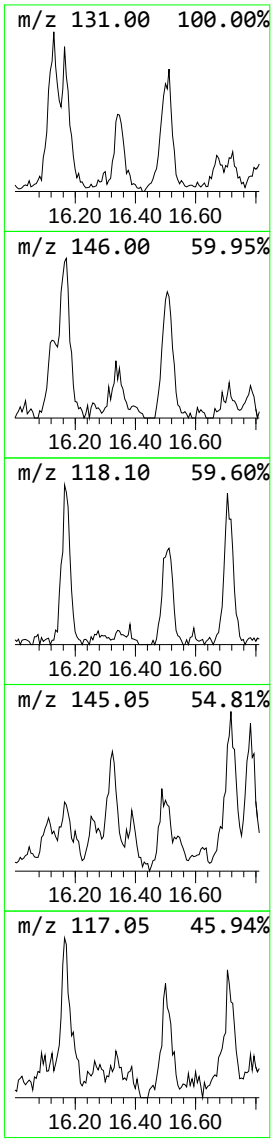
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphth[1,2-b]oxirene, 1a,2,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.500	5.62 ug/l	167633	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	86
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	68
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	49
5	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Phenylbut-1-ene	15.053	7.2	ug/l	214860	4	13.794	1492100	50.0
1H-Indene, 2,3-...	15.788	5.4	ug/l	161863	4	13.794	1492100	50.0
Naphth[1,2-b]ox...	16.500	5.6	ug/l	167633	4	13.794	1492100	50.0