LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121423\
Data File : VN080488.D
Acq On : 14 Dec 2023 17:26
Operator : JC\MD
Sample : 05831-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6931

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\82N121223W.M
Title : SW846 8260

Signal : TIC: VN080488.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.783	304	311	319	rBV3	9756	24768	1.91%	0.237%
2	7.559	941	953	966	rBV	245058	601788	46.40%	5.768%
3	8.165	1046	1056	1061	rBV	186532	448712	34.60%	4.300%
4	8.224	1061	1066	1077	rVB	312924	692921	53.43%	6.641%
5	8.576	1116	1126	1139	rBV	173313	401010	30.92%	3.843%
6	9.100	1204	1215	1230	rVB	464537	944405	72.82%	9.051%
7	9.271	1237	1244	1250	rBV4	10604	23733	1.83%	0.227%
8	10.565	1456	1464	1471	rBV	646897	1204115	92.85%	11.540%
9	10.629	1471	1475	1483	rVB2	23388	43891	3.38%	0.421%
10	11.288	1580	1587	1596	rBV	325040	512833	39.54%	4.915%
11	11.865	1676	1685	1696	rVB	718091	1271324	98.03%	12.184%
12	11.965	1696	1702	1706	rBV2	22088	35741	2.76%	0.343%
13	12.023	1706	1712	1716	rVV	74339	123238	9.50%	1.181%
14	12.064	1716	1719	1730	rVB	41602	76171	5.87%	0.730%
15	12.400	1769	1776	1783	rBV2	32261	53820	4.15%	0.516%
16	12.847	1844	1852	1864	rBV	525926	915243	70.57%	8.772%
17	13.035	1878	1884	1889	rBV2	14526	22743	1.75%	0.218%
18	13.094	1889	1894	1899	rVV	49702	92859	7.16%	0.890%
19	13.129	1899	1900	1904	rVV2	23006	25750	1.99%	0.247%
20	13.176	1904	1908	1915	rVB2	34615	52494	4.05%	0.503%
21	13.335	1929	1935	1942	rVB2	39301	65774	5.07%	0.630%
22	13.482	1953	1960	1966	rBV	59357	96338	7.43%	0.923%
23	13.676	1988	1993	1998	rVB4	9808	15181	1.17%	0.145%
24	13.794	2005	2013	2024	rVB	721775	1296854	100.00%	12.429%
25	13.988	2041	2046	2048	rVV2	27886	49509	3.82%	0.474%
26	14.023	2048	2052	2064	rVB3	28513	63695	4.91%	0.610%
27	14.182	2074	2079	2085	rBV	16617	27353	2.11%	0.262%
28	14.247	2085	2090	2092	rVV2	19959	31799	2.45%	0.305%
29	14.276	2092	2095	2100	rVV3	19225	28956	2.23%	0.278%
30	14.329	2100	2104	2111	rVB	23645	34728	2.68%	0.333%
31	14.400	2111	2116	2119	rBV2	10398	17879	1.38%	0.171%
32	14.447	2119	2124	2129	rVB2	36540	59738	4.61%	0.573%
33	14.576	2140	2146	2152	rVB3	14479	22856	1.76%	0.219%
34	14.653	2152	2159	2162	rBV2	17580	28314	2.18%	0.271%
35	14.694	2162	2166	2171	rVV	31168	47442	3.66%	0.455%
36	14.876	2189	2197	2201	rBV7	7729	14828	1.14%	0.142%

LSC Area Percent Report

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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

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Title : SW846 8260

37	14.929	2201	2206	2211	rBV2	19000	38282	2.95%	0.367%
38	15.053	2217	2227	2233	rBV2	89918	195135	15.05%	1.870%
39	15.211	2247	2254	2261	rBV	57067	100190	7.73%	0.960%
40	15.317	2261	2272	2278	rVV7	21851	71269	5.50%	0.683%
41	15.364	2278	2280	2285	rVV4	13225	20505	1.58%	0.197%
42	15.441	2285	2293	2301	rVB4	25673	66047	5.09%	0.633%
43	15.700	2331	2337	2342	rBV4	19279	38565	2.97%	0.370%
44	15.752	2342	2346	2347	rVV4	9445	13548	1.04%	0.130%
45	15.788	2347	2352	2364	rVB6	18089	53477	4.12%	0.513%
46	15.947	2372	2379	2385	rBV3	21249	43285	3.34%	0.415%
47	16.164	2401	2416	2425	rBV2	51322	151336	11.67%	1.450%
48	16.252	2425	2431	2439	rBV2	12664	22590	1.74%	0.217%
49	16.347	2439	2447	2452	rBV5	14326	33514	2.58%	0.321%
50	16.505	2460	2474	2486	rBV3	38047	89558	6.91%	0.858%
51	16.711	2503	2509	2515	rVB7	13177	27895	2.15%	0.267%

Sum of corrected areas: 10433999

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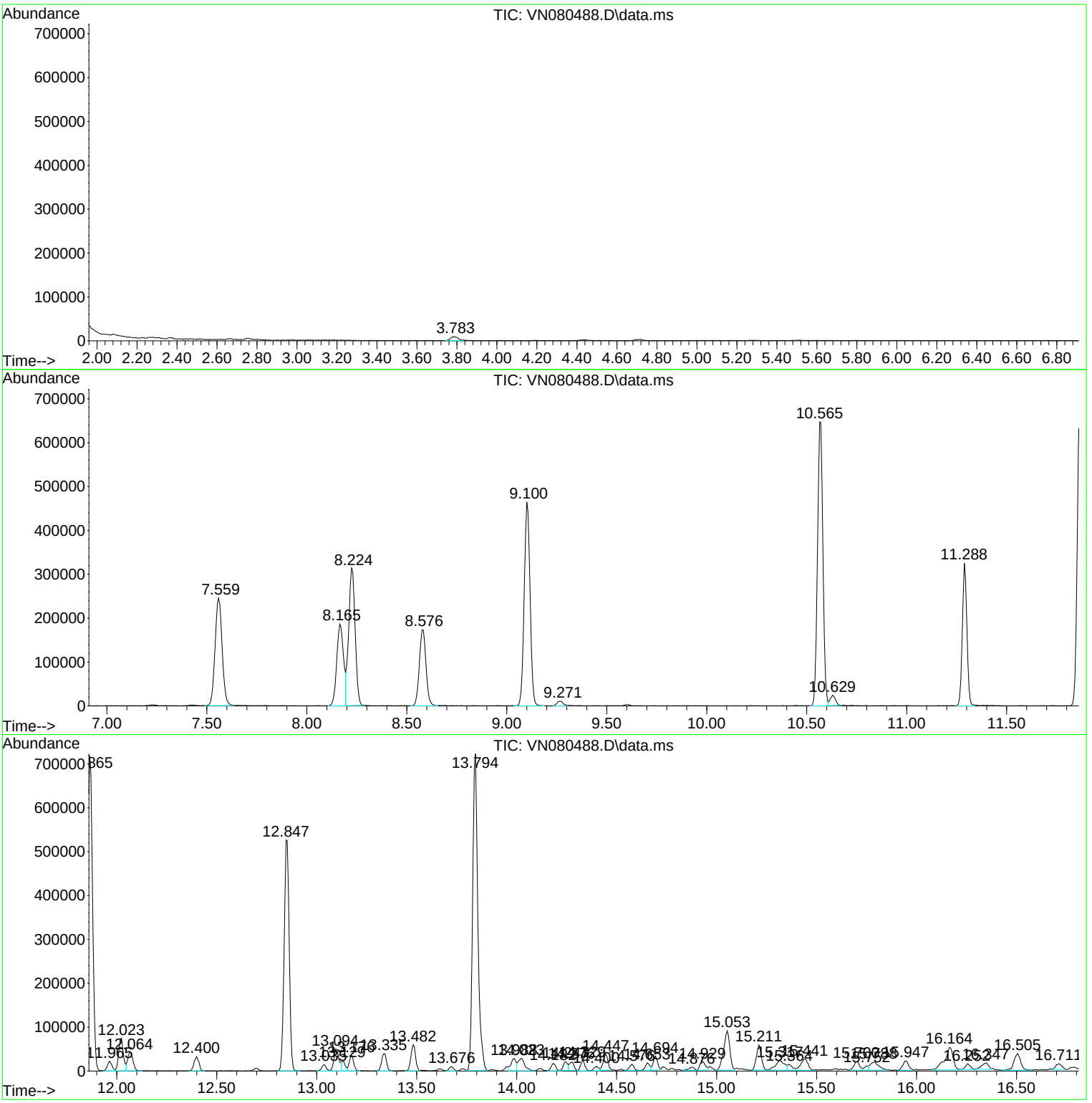
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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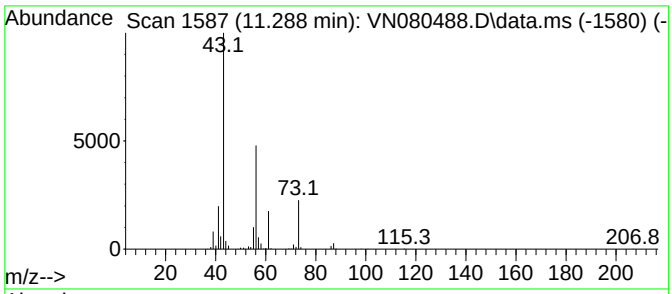
Quant Title : SW846 8260

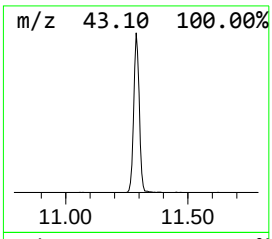
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

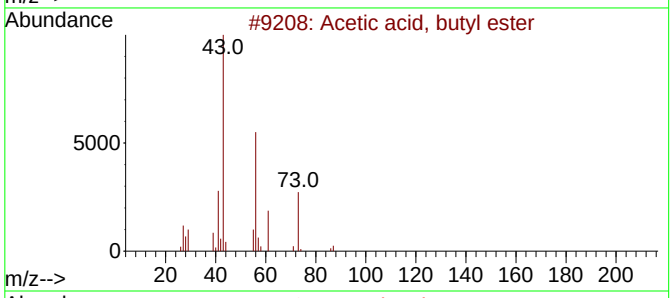
****
Peak Number 1 Acetic acid, butyl ester Concentration Rank 1

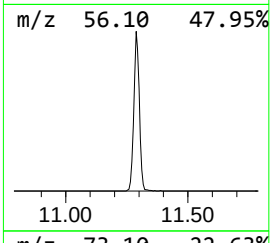
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.288	20.17 ug/l	512833	Chlorobenzene-d5	11.865

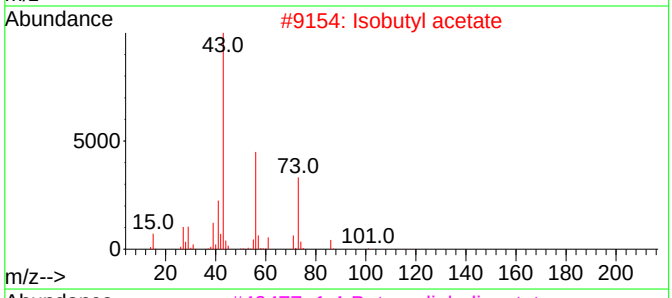
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2	Isobutyl acetate	116	C6H12O2	000110-19-0	56
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	25
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9

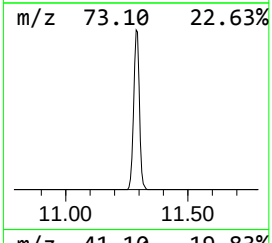


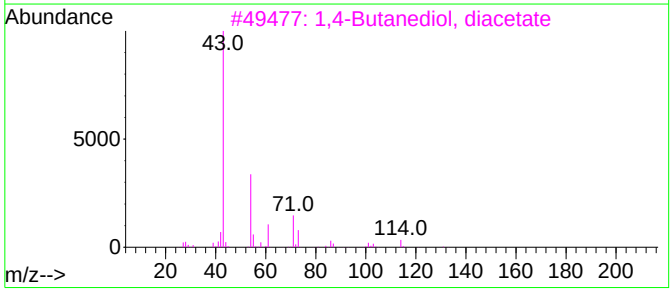


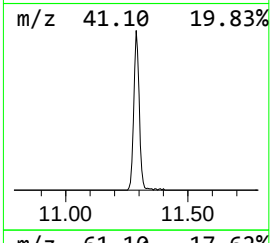


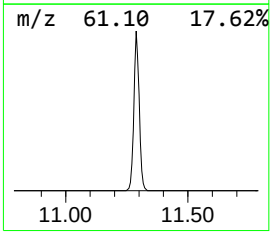












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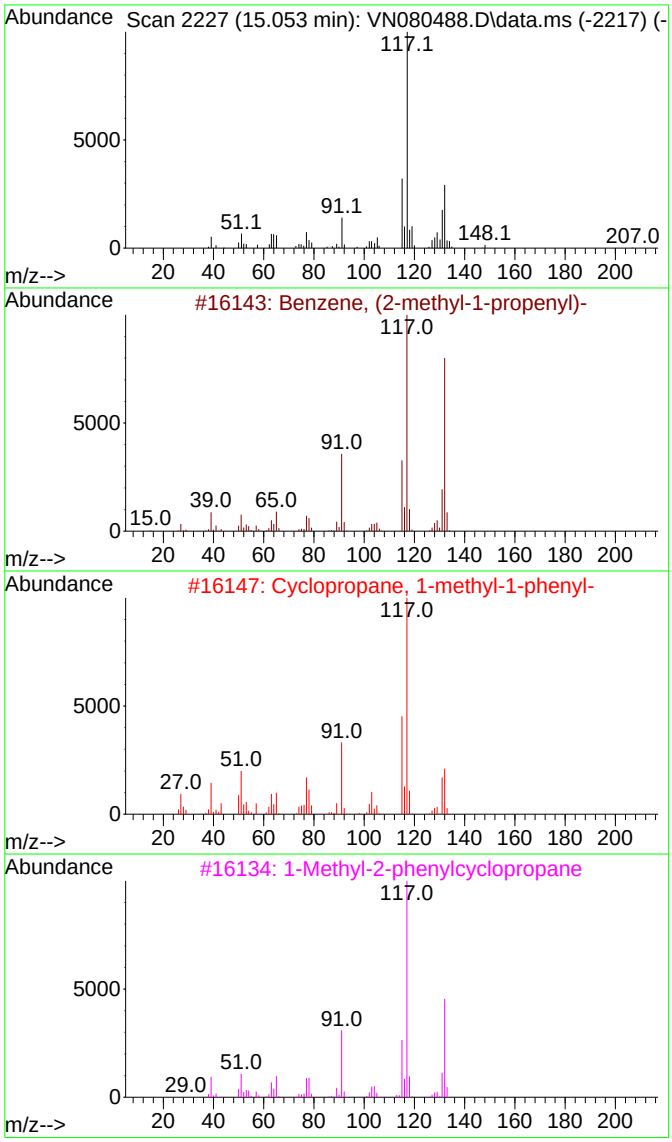
Quant Title : SW846 8260

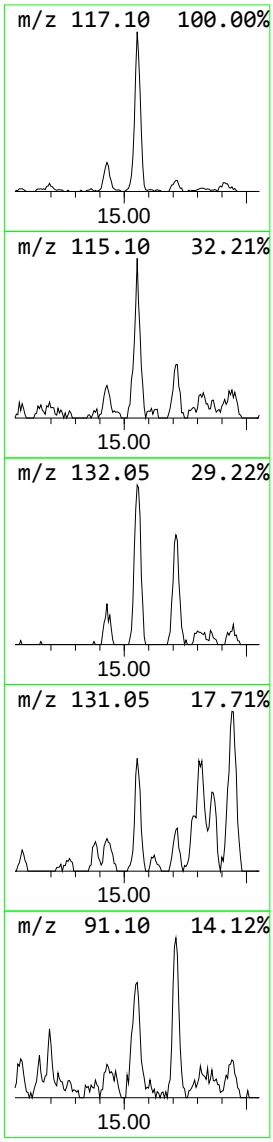
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, (2-methyl-1-propen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	7.52 ug/l	195135	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
2	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	81
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	72
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	68





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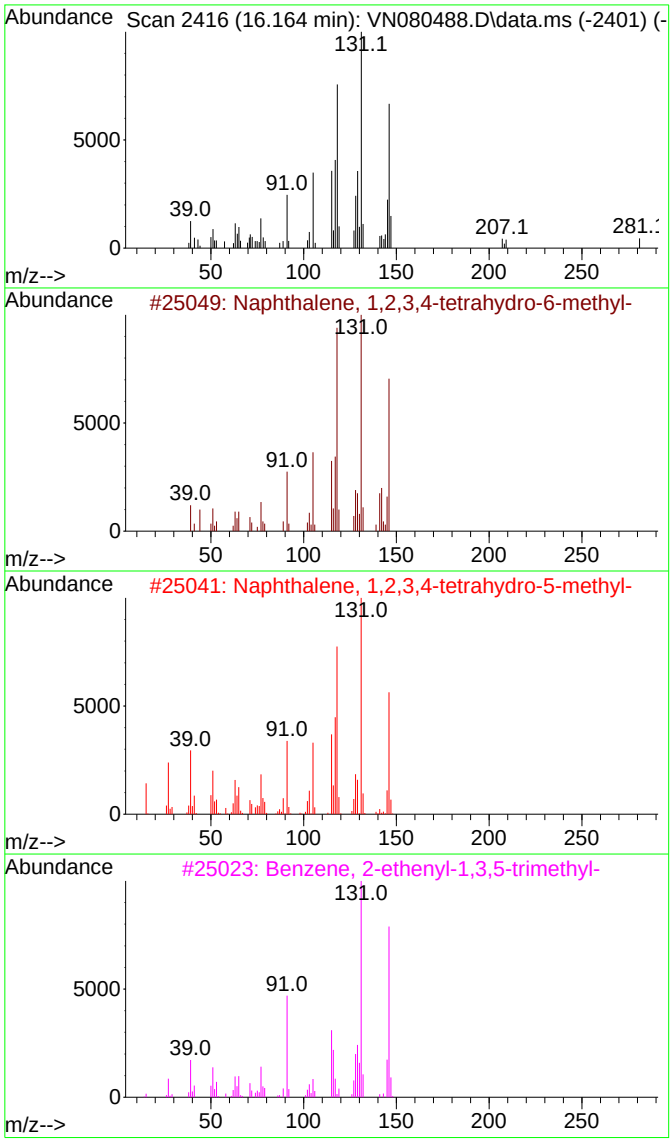
Quant Title : SW846 8260

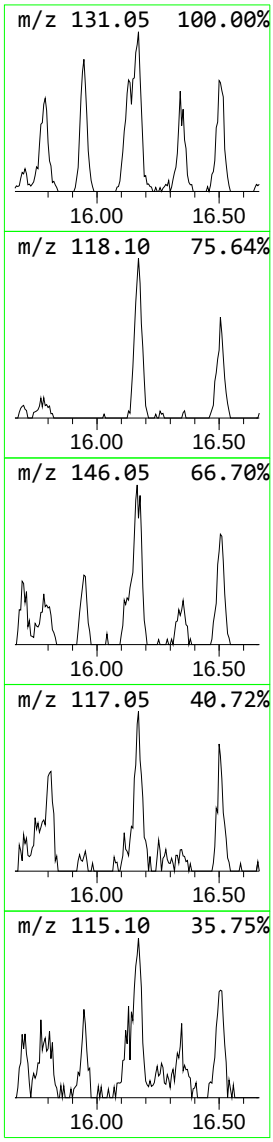
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.164	5.83 ug/l	151336	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
4	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	52
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	50





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetic acid, bu...	11.288	20.2	ug/l	512833	3	11.865	1271320	50.0
Benzene, (2-met...	15.053	7.5	ug/l	195135	4	13.794	1296850	50.0
Naphthalene, 1,...	16.164	5.8	ug/l	151336	4	13.794	1296850	50.0