LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046449.D
Acq On : 02 Jun 2025 17:09
Operator : JC/MD
Sample : Q2155-02
Misc : 3.40g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 447-SOLID

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\82X050525W.M
Title : SW846 8260

Signal : TIC: VX046449.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	34	rBV	7824	6724	1.59%	0.127%
2	1.636	70	90	92	rBV6	9172	40904	9.68%	0.775%
3	2.428	213	220	228	rBV2	1940	5370	1.27%	0.102%
4	3.416	375	382	389	rVB4	2146	5061	1.20%	0.096%
5	5.385	695	705	721	rBV	47644	138750	32.84%	2.630%
6	5.544	721	731	748	rVV	69698	199694	47.26%	3.785%
7	5.952	789	798	816	rBV	54784	150745	35.67%	2.858%
8	6.757	920	930	949	rBV	124171	304195	71.99%	5.766%
9	8.647	1233	1240	1253	rBV	270156	422558	100.00%	8.010%
10	10.049	1465	1470	1483	rBV	262036	382140	90.43%	7.244%
11	11.079	1634	1639	1648	rBV	208700	286814	67.88%	5.437%
12	11.481	1701	1705	1714	rVB5	2823	5523	1.31%	0.105%
13	11.969	1781	1785	1789	rBV6	5304	7246	1.71%	0.137%
14	12.024	1789	1794	1803	rVV	269841	347702	82.29%	6.591%
15	12.426	1854	1860	1862	rBV6	2966	4393	1.04%	0.083%
16	12.554	1873	1881	1882	rBV7	2151	5164	1.22%	0.098%
17	12.585	1882	1886	1895	rVV2	12786	25038	5.93%	0.475%
18	12.817	1919	1924	1929	rBV6	6214	10627	2.51%	0.201%
19	12.987	1945	1952	1955	rBV9	3144	6849	1.62%	0.130%
20	13.036	1955	1960	1964	rVV8	3529	6618	1.57%	0.125%
21	13.292	1999	2002	2007	rVB4	12233	17388	4.11%	0.330%
22	13.420	2016	2023	2031	rVV6	14502	36469	8.63%	0.691%
23	13.506	2033	2037	2040	rBV6	4968	7645	1.81%	0.145%
24	13.585	2046	2050	2054	rBV7	9337	16786	3.97%	0.318%
25	13.670	2061	2064	2071	rVB7	4993	7536	1.78%	0.143%
26	13.737	2071	2075	2076	rBV4	8116	9439	2.23%	0.179%
27	13.798	2082	2085	2089	rBV6	10983	13357	3.16%	0.253%
28	13.847	2089	2093	2099	rBV4	18763	37659	8.91%	0.714%
29	13.926	2100	2106	2111	rVV7	15510	34382	8.14%	0.652%
30	14.066	2125	2129	2133	rBV6	13084	23559	5.58%	0.447%
31	14.225	2148	2155	2161	rBV6	58418	119257	28.22%	2.261%
32	14.316	2168	2170	2173	rBV2	11724	15116	3.58%	0.287%
33	14.481	2193	2197	2205	rVB3	65252	106016	25.09%	2.010%
34	14.548	2205	2208	2210	rBV4	23618	29415	6.96%	0.558%
35	14.578	2210	2213	2215	rVV5	16529	17057	4.04%	0.323%
36	14.615	2215	2219	2225	rBV	114263	184720	43.71%	3.502%

LSC Area Percent Report

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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
447-SOLID

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

37	14.670	2225	2228	2231	rVV2	93875	105324	24.93%	1.997%
38	14.755	2239	2242	2244	rVB2	40856	42113	9.97%	0.798%
39	14.786	2244	2247	2250	rBV4	35249	47012	11.13%	0.891%
40	14.816	2250	2252	2254	rVV2	25524	29585	7.00%	0.561%
41	14.847	2254	2257	2261	rVB3	81707	104712	24.78%	1.985%
42	14.914	2266	2268	2271	rBV2	25436	33124	7.84%	0.628%
43	15.036	2284	2288	2293	rBV4	76785	135473	32.06%	2.568%
44	15.084	2294	2296	2300	rBV5	27670	45037	10.66%	0.854%
45	15.182	2307	2312	2314	rBV3	111010	180176	42.64%	3.415%
46	15.249	2320	2323	2330	rVB5	92088	146335	34.63%	2.774%
47	15.377	2340	2344	2347	rBV3	143683	205268	48.58%	3.891%
48	15.414	2347	2350	2354	rVB3	131882	167424	39.62%	3.174%
49	15.481	2358	2361	2364	rBV3	52452	88523	20.95%	1.678%
50	15.743	2400	2404	2407	rVV3	94692	136778	32.37%	2.593%
51	15.779	2407	2410	2414	rVB	87370	113025	26.75%	2.143%
52	15.859	2419	2423	2429	rVB7	86487	181436	42.94%	3.439%
53	15.987	2440	2444	2446	rBV4	68852	112234	26.56%	2.128%
54	16.084	2456	2460	2466	rBV5	133160	239025	56.57%	4.531%
55	16.414	2510	2514	2525	rBV5	47862	124845	29.55%	2.367%

Sum of corrected areas: 5275365

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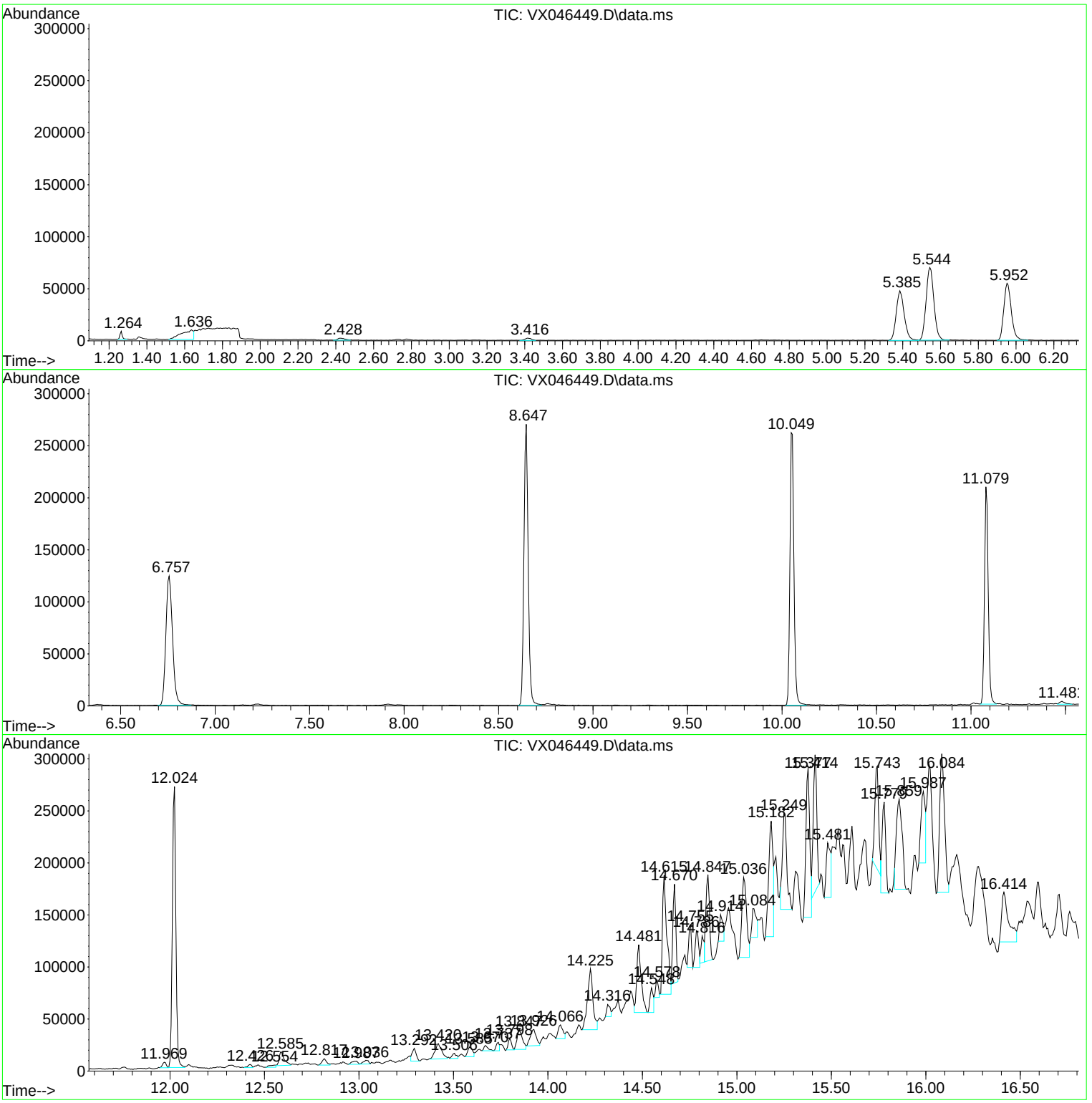
Instrument :
MSVOA_X
ClientSampleId :
447-SOLID

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
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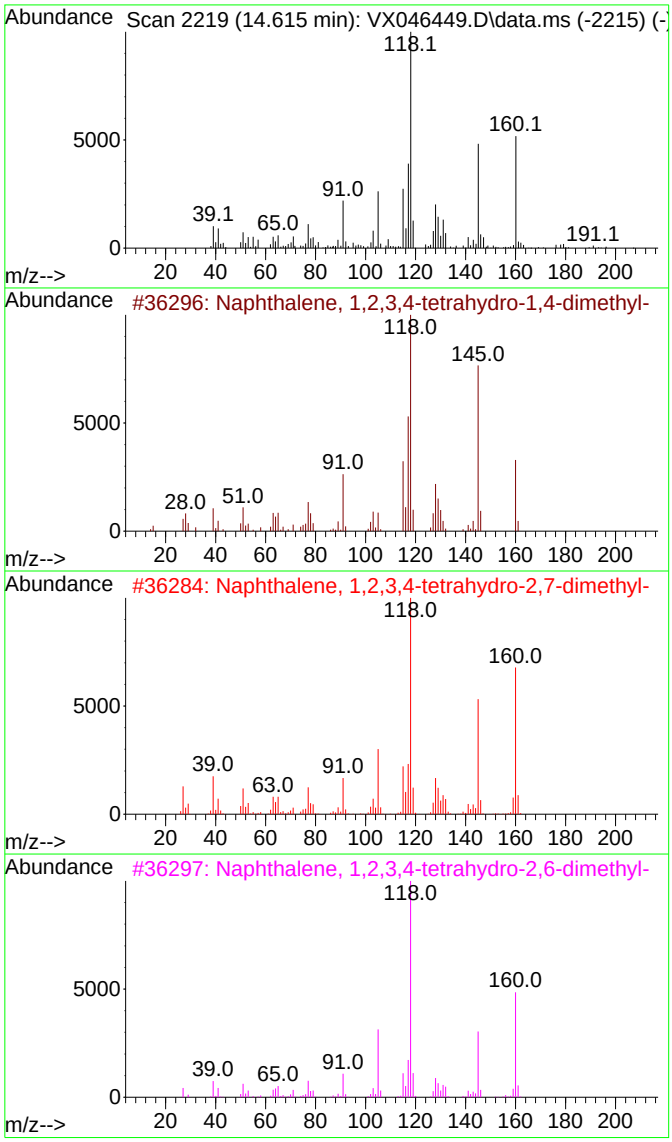
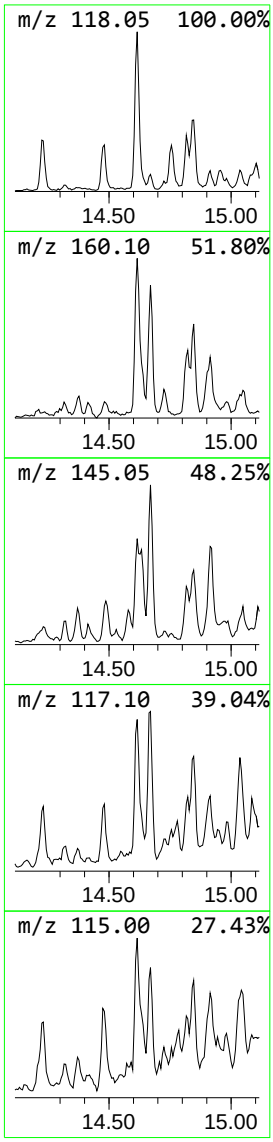
****
Peak Number 1 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	26.56 ug/l	184720	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	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	93
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	74
4	3-Phenylcyclopentanecarboxylic acid	190	C12H14O2	091495-75-9	50
5	2,5-Dimethylbenzyl cyanide	145	C10H11N	016213-85-7	50





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Data File : VX046449.D
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Operator : JC/MD
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Misc : 3.40g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
447-SOLID

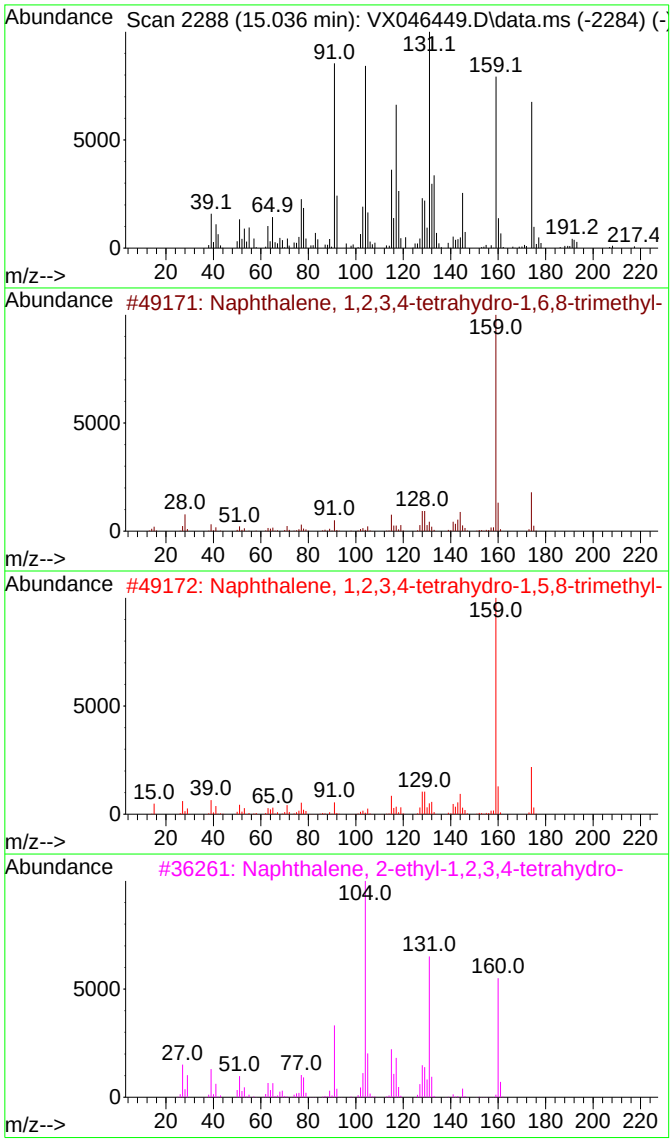
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

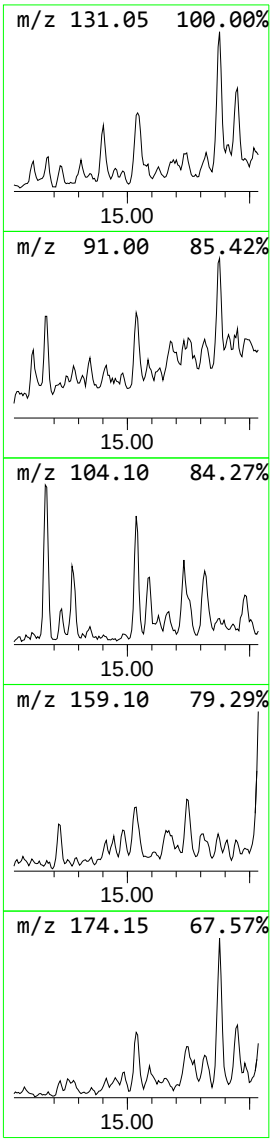
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Naphthalene, 2-ethyl-1,2,3,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.036	19.48 ug/l	135473	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	80
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	80
3	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	55
4	Cyclohexanone, 3-phenyl-	174	C12H14O	020795-53-3	45
5	2-Ethylindane-1,3-dione	174	C11H10O2	027606-61-7	42





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ClientSampleId :
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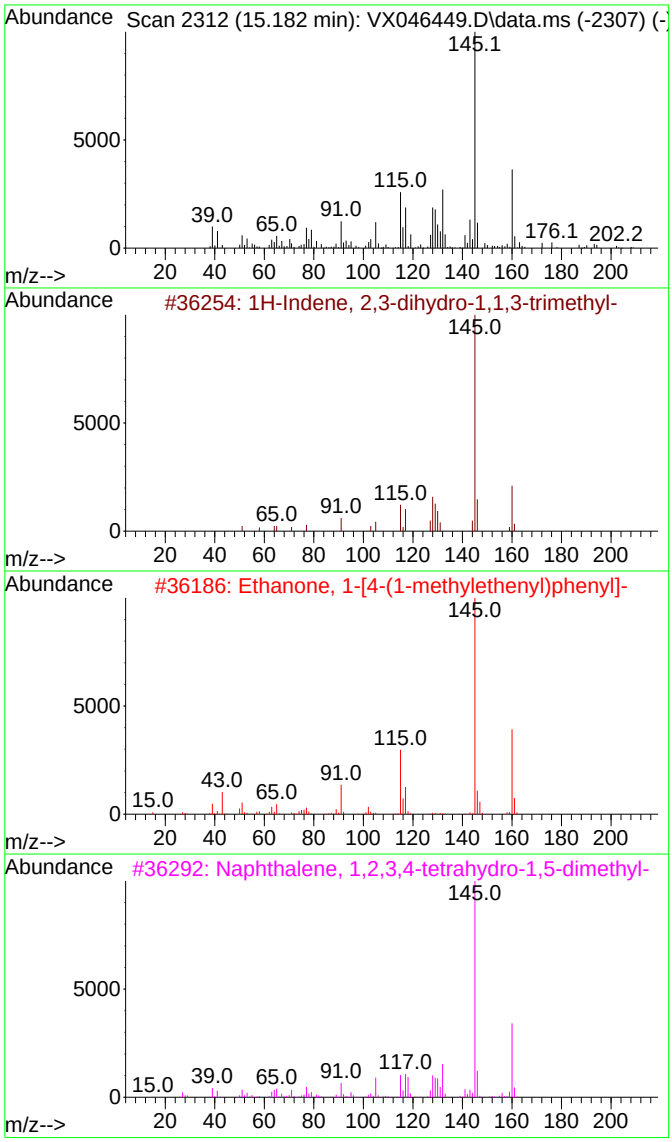
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

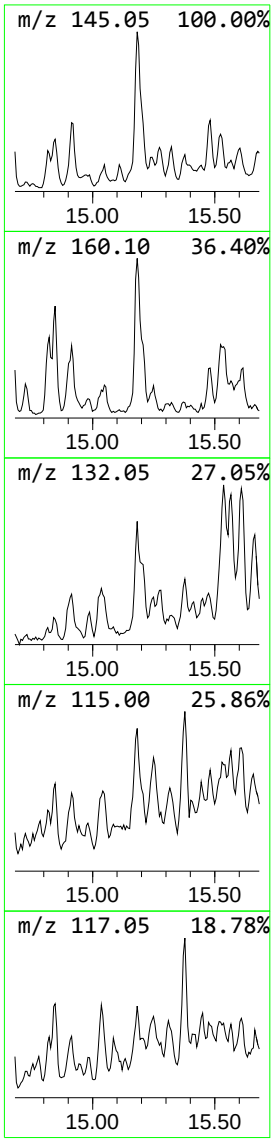
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	25.91 ug/l	180176	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	93
2	Ethanone, 1-[4-(1-methylethenyl)...	160	C11H12O	005359-04-6	92
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	90
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	89
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	83





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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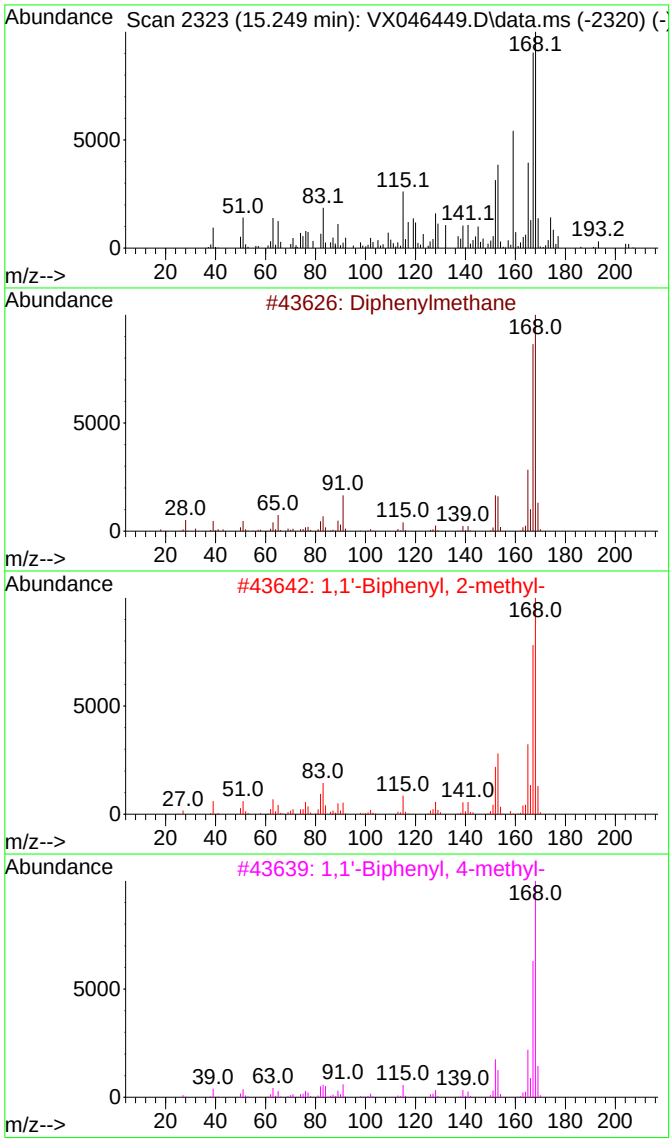
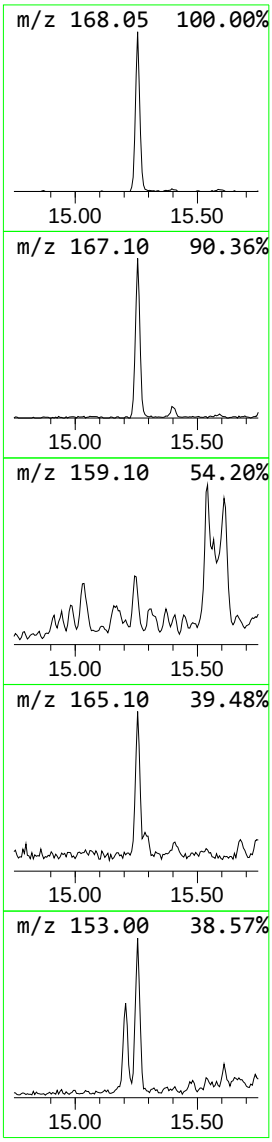
****
Peak Number 4 Diphenylmethane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	21.04 ug/l	146335	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenylmethane	168	C13H12	000101-81-5	93
2	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	92
3	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	92
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	64
5	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	64





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
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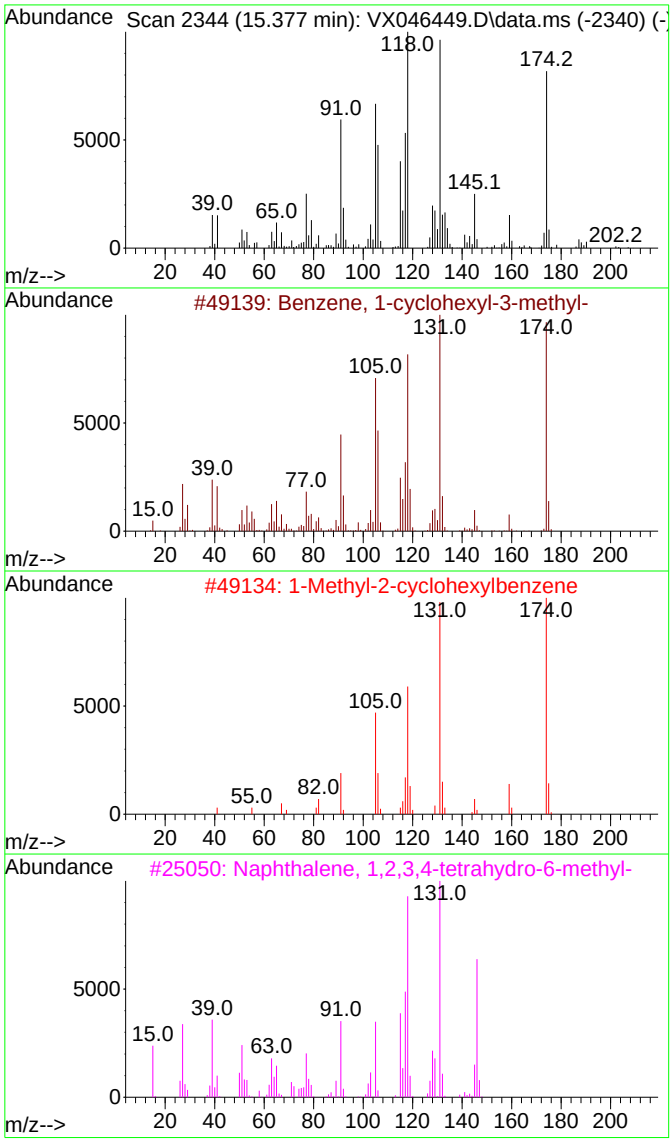
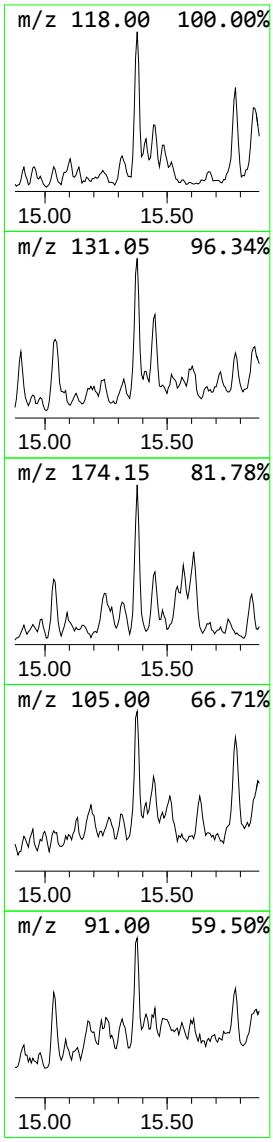
****
Peak Number 5 Benzene, 1-cyclohexyl-3-met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.377	29.52 ug/l	205268	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	76
2	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	47
4	3-Amino-6-methoxyquinoline	174	C10H10N2O	029507-86-6	38
5	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	35





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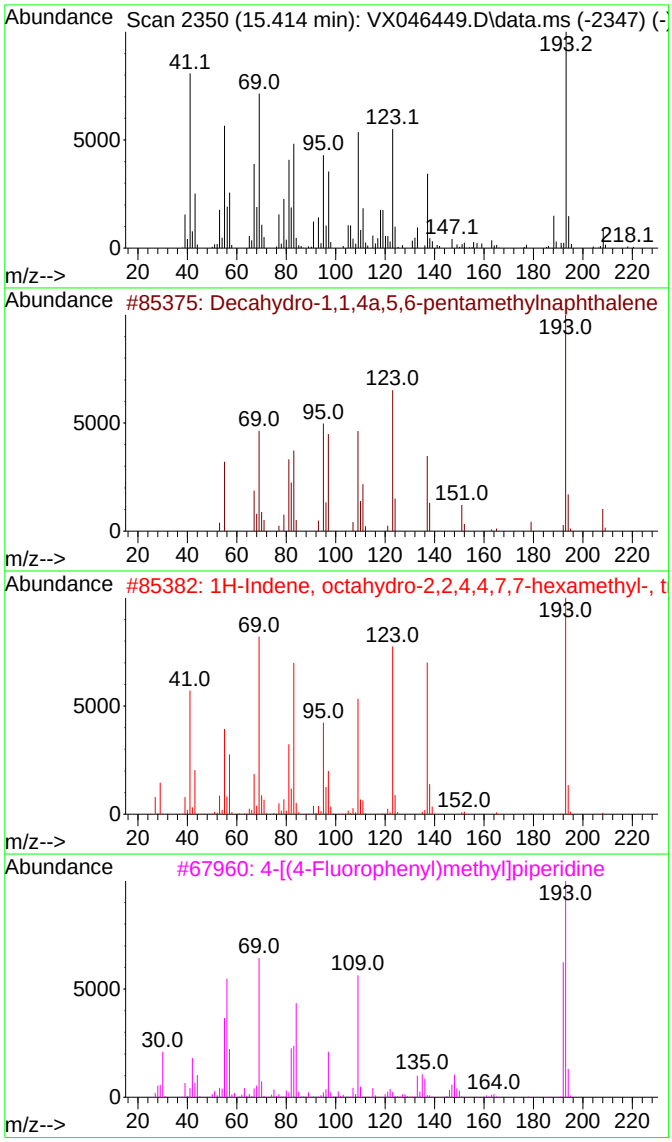
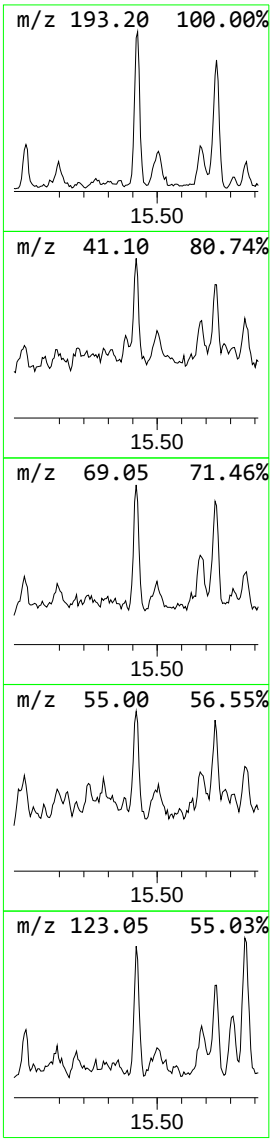
****
Peak Number 6 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	24.08 ug/l	167424	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	90
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	59
3	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	35
4	1,3-Bis(bromomethyl)cyclohexane	268	C8H14Br2	1000216-89-9	22
5	9-Phenanthrenamine	193	C14H11N	000947-73-9	22





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Instrument :
MSVOA_X
ClientSampleId :
447-SOLID

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

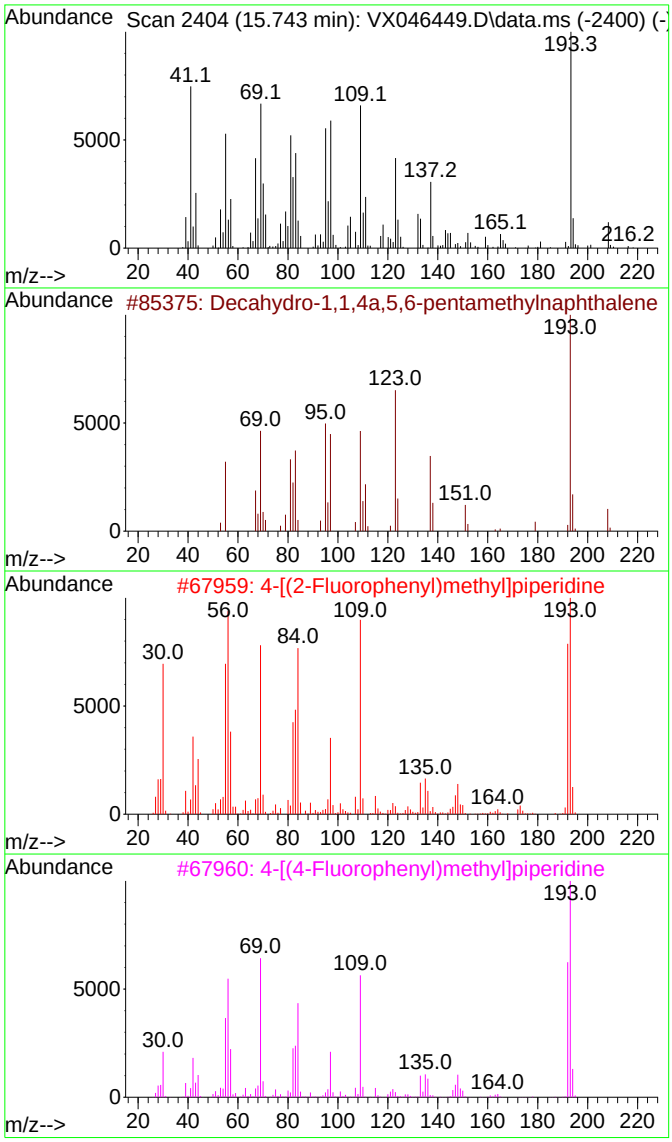
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

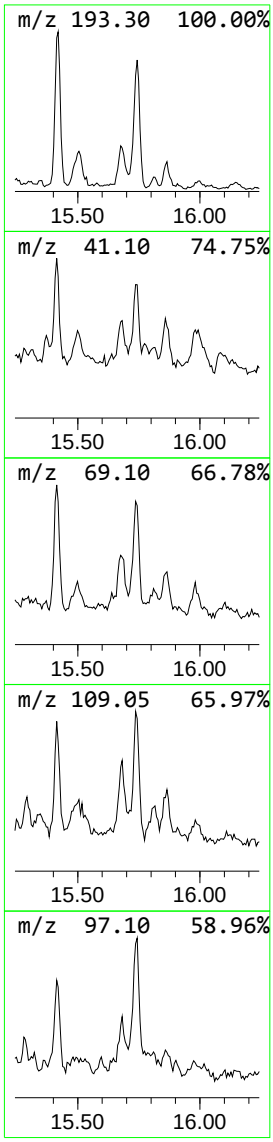
****

Peak Number 7 unknown15.743 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	19.67 ug/l	136778	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	76
2	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	46
3	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	35
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	30
5	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
Data File : VX046449.D
Acq On : 02 Jun 2025 17:09
Operator : JC/MD
Sample : Q2155-02
Misc : 3.40g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
447-SOLID

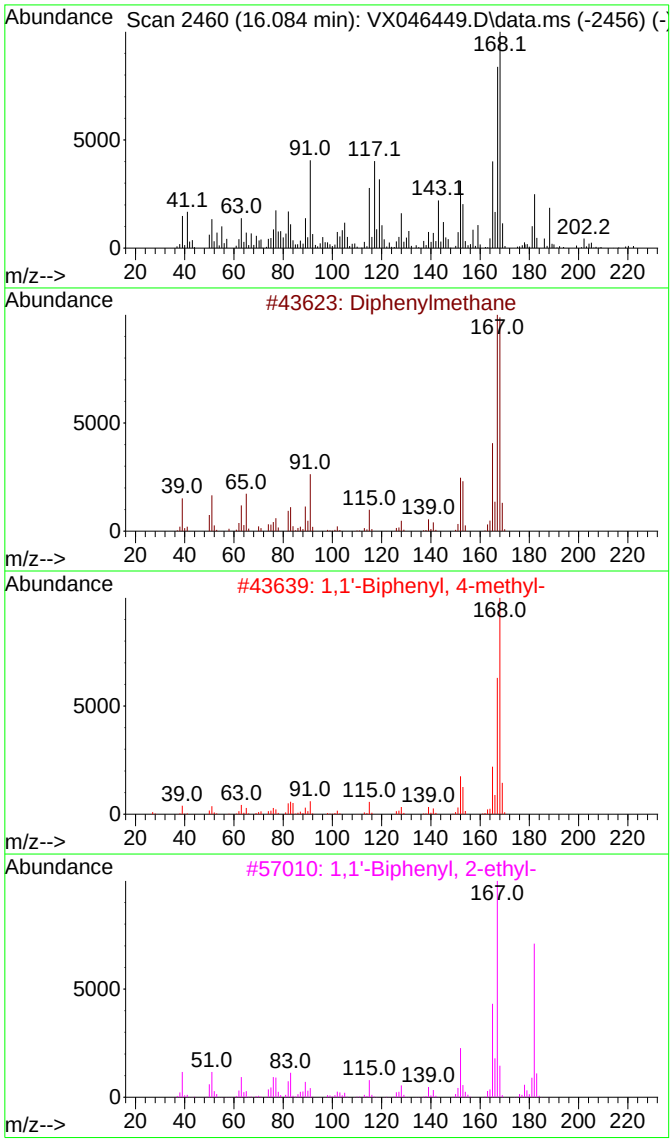
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

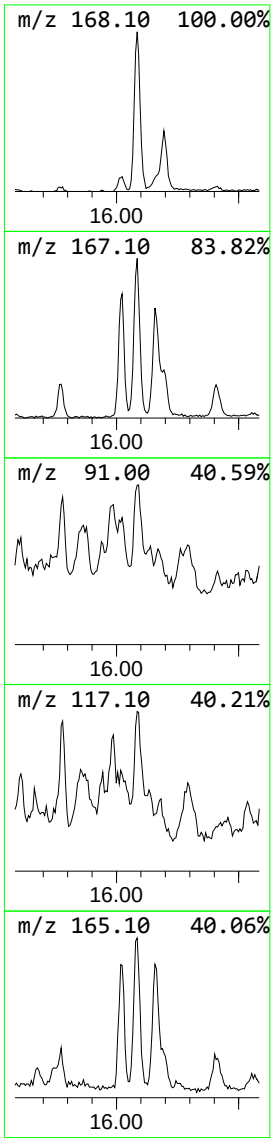
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,1'-Biphenyl, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.084	34.37 ug/l	239025	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenylmethane	168	C13H12	000101-81-5	91
2	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	90
3	1,1'-Biphenyl, 2-ethyl-	182	C14H14	001812-51-7	89
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	55
5	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	55





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Data File : VX046449.D
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Instrument :
MSVOA_X
ClientSampleId :
447-SOLID

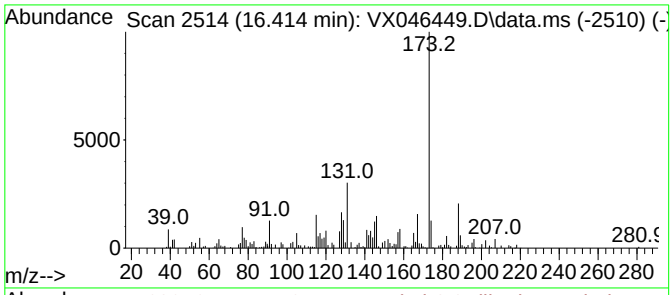
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

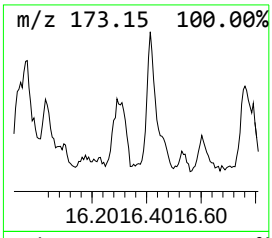
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

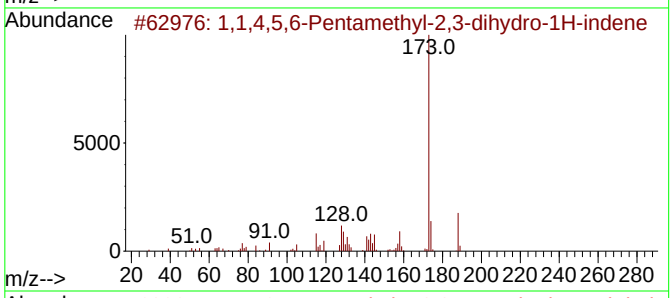
****
Peak Number 10 1,1,4,5,6-Pentamethyl-2,3-d... Concentration Rank 10

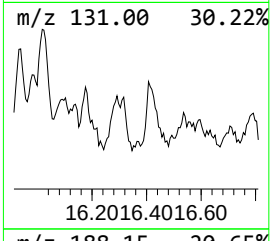
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.413	17.95 ug/l	124845	1,4-Dichlorobenzene-d4	12.024

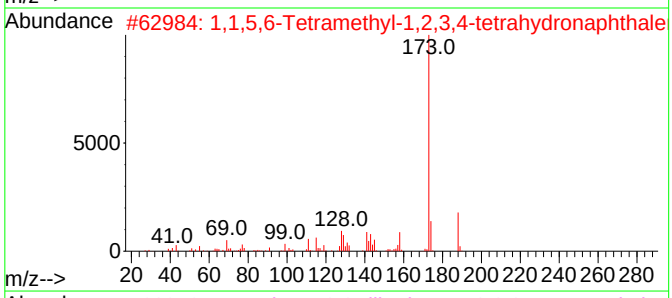
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4,5,6-Pentamethyl-2,3-dihydr...	188	C14H20	016204-67-4	93
2	1,1,5,6-Tetramethyl-1,2,3,4-tetr...	188	C14H20	031197-54-3	76
3	1H-Indene, 2,3-dihydro-1,1,2,3,3...	188	C14H20	001203-17-4	74
4	1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	056298-98-7	68
5	1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	055255-42-0	68

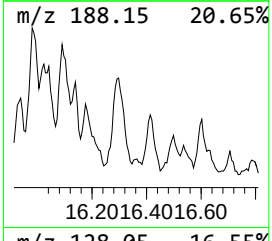


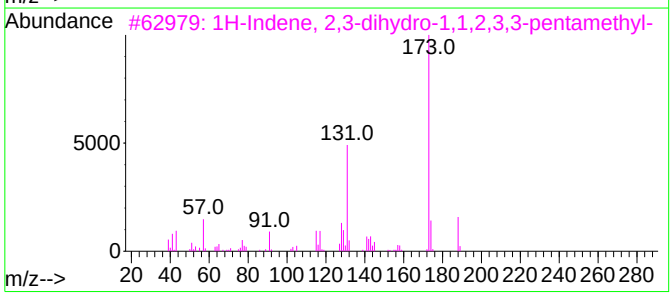


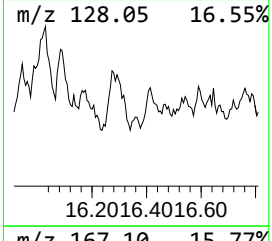


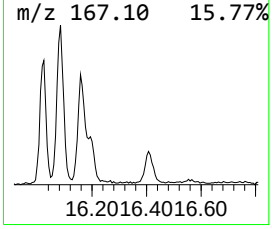












Tentatively Identified Compound (LSC) summary

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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,...	14.615	26.6	ug/l	184720	4	12.024	347702	50.0
Naphthalene, 2-...	15.036	19.5	ug/l	135473	4	12.024	347702	50.0
1H-Indene, 2,3-...	15.182	25.9	ug/l	180176	4	12.024	347702	50.0
Diphenylmethane	15.249	21.0	ug/l	146335	4	12.024	347702	50.0
Benzene, 1-cycl...	15.377	29.5	ug/l	205268	4	12.024	347702	50.0
Decahydro-1,1,4...	15.414	24.1	ug/l	167424	4	12.024	347702	50.0
unknown15.743	15.743	19.7	ug/l	136778	4	12.024	347702	50.0
1,1'-Biphenyl, ...	16.084	34.4	ug/l	239025	4	12.024	347702	50.0
1,1,4,5,6-Penta...	16.413	17.9	ug/l	124845	4	12.024	347702	50.0