

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN093020\
 Data File : VN063750.D
 Acq On : 30 Sep 2020 15:32
 Operator : JC/MD
 Sample : L4129-17
 Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRUM-COMP-2

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.435	195	216	217	rBV9	35518	81566	5.30%	0.539%
2	2.679	288	292	308	rVB9	11828	23572	1.53%	0.156%
3	3.049	395	407	420	rVB5	7968	18401	1.20%	0.122%
4	5.505	1155	1171	1181	rBV4	11164	31769	2.06%	0.210%
5	6.807	1559	1576	1579	rBV5	7283	15481	1.01%	0.102%
6	7.547	1785	1806	1817	rBV2	175202	459484	29.86%	3.039%
7	7.621	1817	1829	1847	rVB	305228	754606	49.04%	4.991%
8	7.833	1880	1895	1906	rBV5	13225	33837	2.20%	0.224%
9	7.987	1925	1943	1963	rBV2	240371	591002	38.40%	3.909%
10	8.399	2054	2071	2085	rBV3	38801	83000	5.39%	0.549%
11	8.547	2102	2117	2136	rBV2	485472	1023545	66.51%	6.770%
12	8.782	2178	2190	2203	rBV6	7477	19145	1.24%	0.127%
13	9.045	2249	2272	2284	rBV5	53894	125445	8.15%	0.830%
14	9.695	2464	2474	2483	rBV3	30912	59086	3.84%	0.391%
15	9.836	2502	2518	2540	rVB4	26211	63175	4.11%	0.418%
16	10.058	2570	2587	2599	rBV	808799	1509183	98.07%	9.981%
17	10.122	2599	2607	2623	rVB	206745	386706	25.13%	2.558%
18	10.254	2631	2648	2662	rVB	94243	166259	10.80%	1.100%
19	10.402	2683	2694	2704	rVB6	12357	24575	1.60%	0.163%
20	10.499	2708	2724	2727	rBV9	9215	15484	1.01%	0.102%
21	10.688	2775	2783	2794	rVB5	14371	25752	1.67%	0.170%
22	10.791	2807	2815	2824	rBV3	14712	26712	1.74%	0.177%
23	10.923	2847	2856	2863	rBV3	17492	27985	1.82%	0.185%
24	10.974	2866	2872	2884	rVB3	17386	29087	1.89%	0.192%
25	11.097	2901	2910	2917	rBV4	13242	22428	1.46%	0.148%
26	11.174	2924	2934	2949	rVB5	54593	108614	7.06%	0.718%
27	11.277	2955	2966	2976	rBV3	35823	58498	3.80%	0.387%
28	11.380	2984	2998	3020	rBV	776652	1408985	91.56%	9.319%
29	11.486	3020	3031	3047	rVB	60638	118684	7.71%	0.785%
30	11.598	3047	3066	3083	rBV3	319368	758622	49.30%	5.017%
31	11.923	3154	3167	3189	rVB	148339	313660	20.38%	2.074%
32	12.023	3192	3198	3206	rVB4	16665	22912	1.49%	0.152%
33	12.138	3229	3234	3247	rVB5	23573	37812	2.46%	0.250%
34	12.315	3283	3289	3292	rBV4	14067	16913	1.10%	0.112%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP-2

Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON
Sampling : 1
Start Thrs: 0.2
Stop Thrs : 0
Filtering: 5
Min Area: 3 % of largest Peak
Max Peaks: 100
Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Title : SW846 8260

35	12.379	3298	3309	3319	rBV	645093	1057865	68.74%	6.997%
36	12.630	3378	3387	3395	rBV	77715	139650	9.07%	0.924%
37	12.704	3402	3410	3421	rVB3	242874	386887	25.14%	2.559%
38	12.868	3456	3461	3476	rVB2	23923	43374	2.82%	0.287%
39	12.939	3477	3483	3491	rVV3	17952	22814	1.48%	0.151%
40	13.016	3497	3507	3517	rBV	158911	242479	15.76%	1.604%
41	13.068	3517	3523	3530	rVB6	17115	24805	1.61%	0.164%
42	13.215	3563	3569	3576	rVB5	22176	28456	1.85%	0.188%
43	13.318	3590	3601	3620	rVB2	822932	1538881	100.00%	10.178%
44	13.518	3659	3663	3669	rVB2	20242	21871	1.42%	0.145%
45	13.560	3670	3676	3686	rBV4	26753	39273	2.55%	0.260%
46	13.650	3695	3704	3711	rBV	105593	158210	10.28%	1.046%
47	13.698	3712	3719	3731	rVB2	71601	115976	7.54%	0.767%
48	13.862	3765	3770	3779	rVB3	30014	41882	2.72%	0.277%
49	13.971	3797	3804	3812	rBV7	28979	44589	2.90%	0.295%
50	14.141	3849	3857	3861	rBV6	38427	66523	4.32%	0.440%
51	14.273	3892	3898	3904	rBV5	26415	34510	2.24%	0.228%
52	14.498	3962	3968	3976	rVB2	60174	86745	5.64%	0.574%
53	14.559	3977	3987	3998	rBV4	67537	154123	10.02%	1.019%
54	15.103	4144	4156	4179	rBV	645595	1162130	75.52%	7.686%
55	15.302	4213	4218	4229	rVB4	40155	59078	3.84%	0.391%
56	15.865	4384	4393	4404	rVB4	30546	65545	4.26%	0.434%
57	16.125	4462	4474	4489	rBV	281764	562196	36.53%	3.718%
58	16.312	4519	4532	4556	rVB	247608	560016	36.39%	3.704%

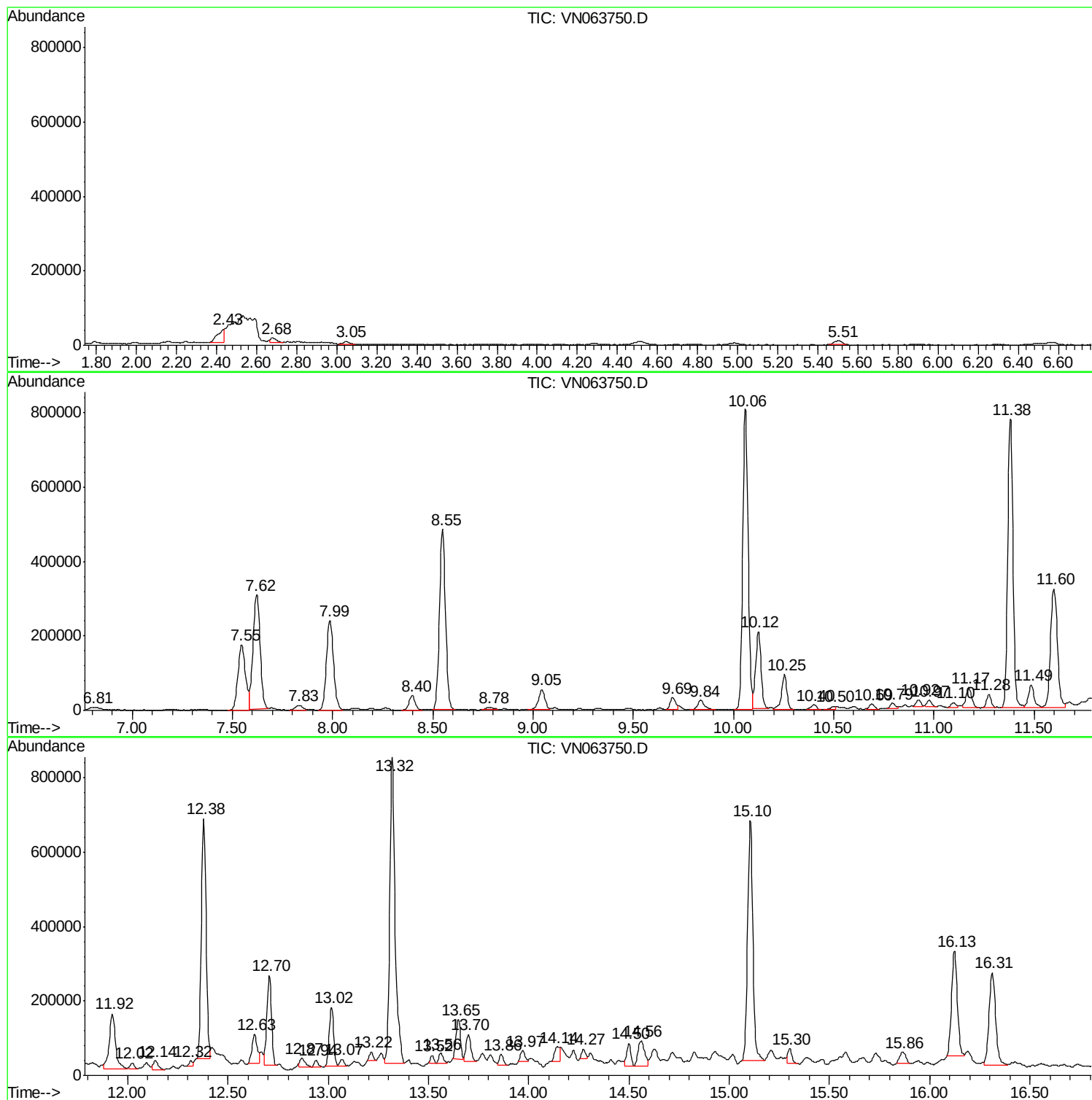
Sum of corrected areas: 15119863

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
DRUM-COMP-2

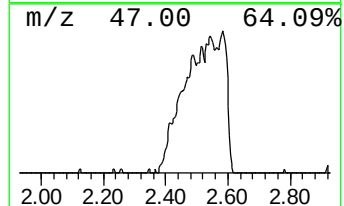
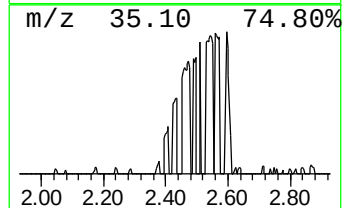
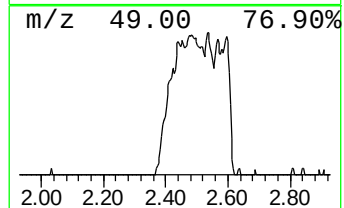
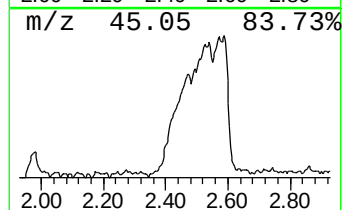
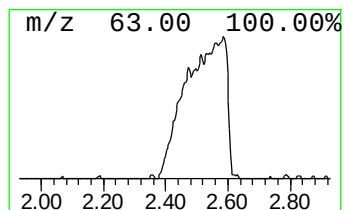
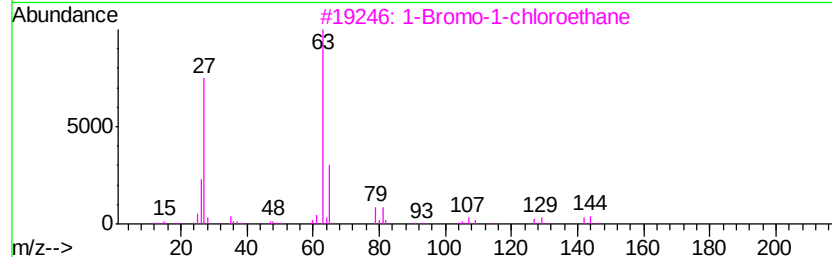
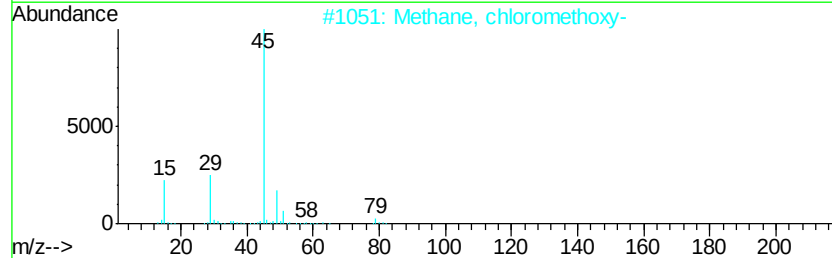
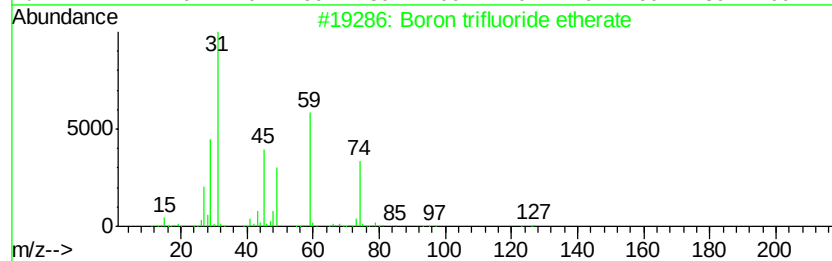
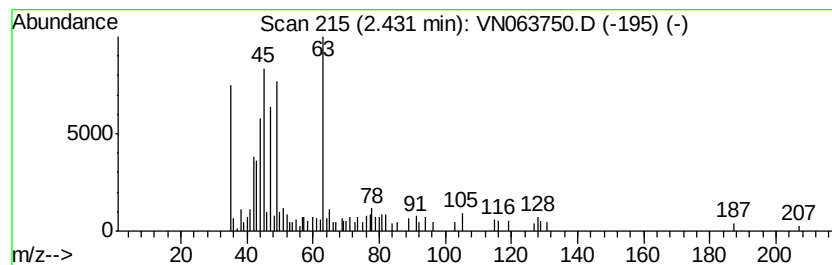
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.43 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	5.40 ug/l	81566	Pentafluorobenzene	7.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Boron trifluoride etherate	142	C4H10BF3O	000109-63-7	12
2		Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
3		1-Bromo-1-chloroethane	142	C2H4BrCl	000593-96-4	9
4		Bis(.beta.-chloroethyl) sulfoxide	174	C4H8Cl2OS	005819-08-9	9
5		Carbonochloridic acid, 4-nitroph...	201	C7H4ClNO4	007693-46-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

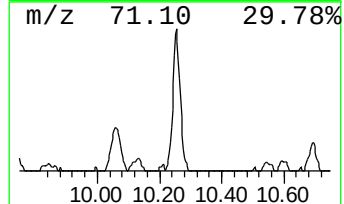
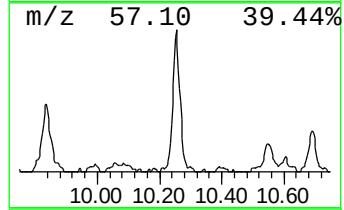
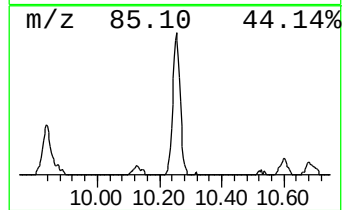
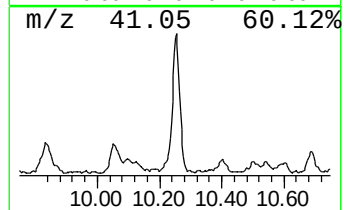
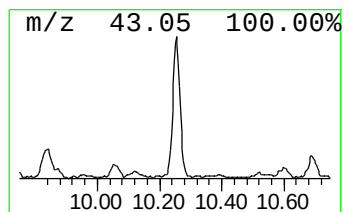
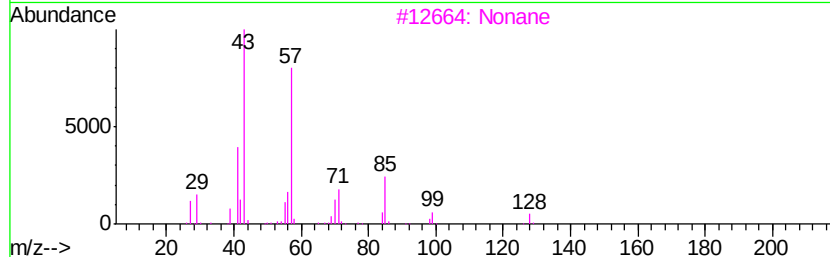
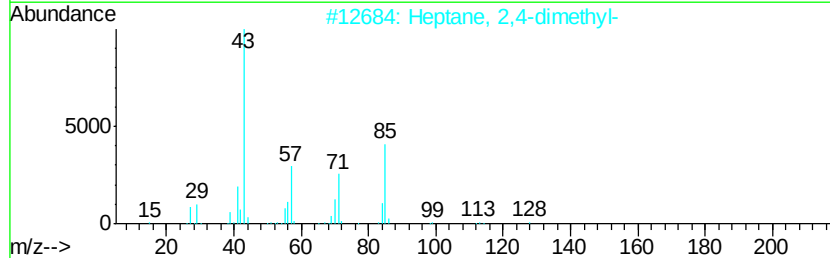
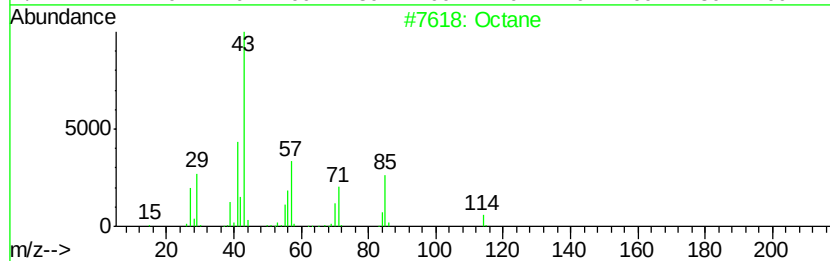
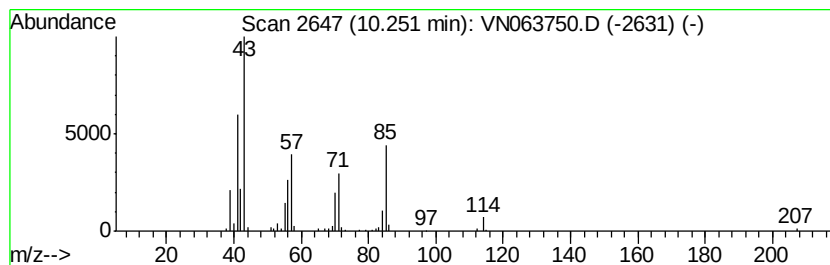
Instrument :
MSVOA_N
ClientSampled :
DRUM-COMP-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	5.90 ug/l	166259	Chlorobenzene-d5	11.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octane		114 C8H18	000111-65-9 91
2	Heptane, 2,4-dimethyl-		128 C9H20	002213-23-2 64
3	Nonane		128 C9H20	000111-84-2 59
4	Undecane, 2,4-dimethyl-		184 C13H28	017312-80-0 53
5	Hexane, 1,1'-oxybis-		186 C12H26O	000112-58-3 50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52a/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

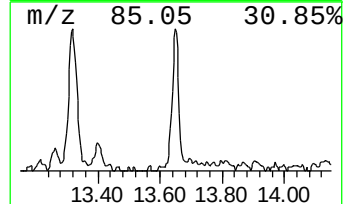
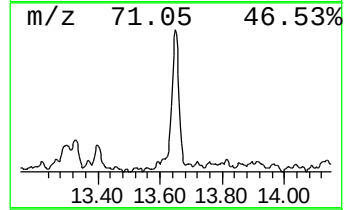
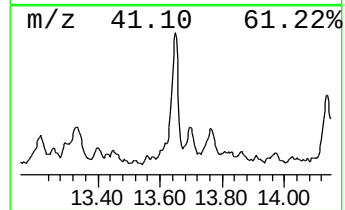
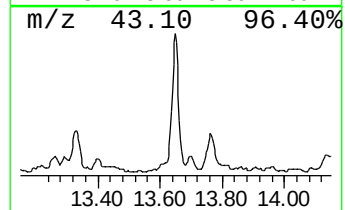
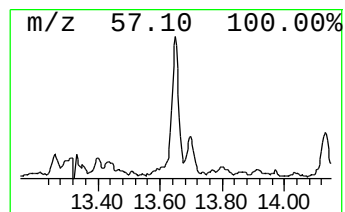
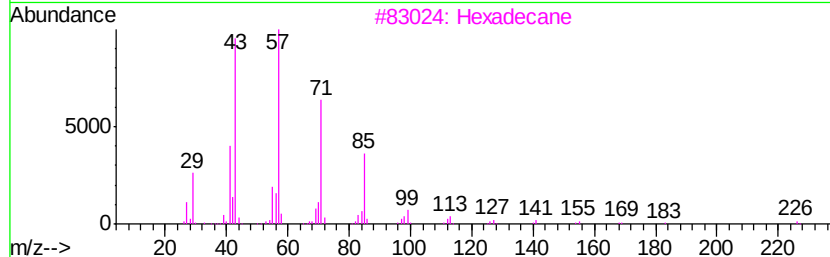
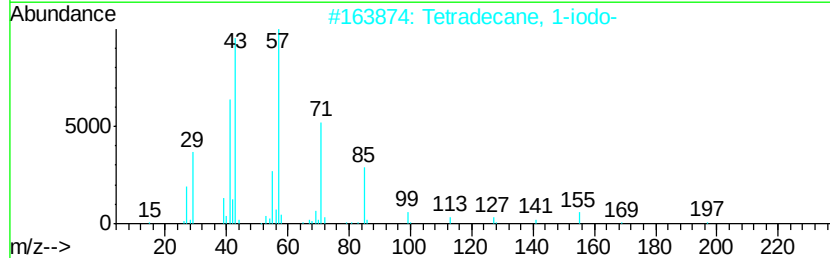
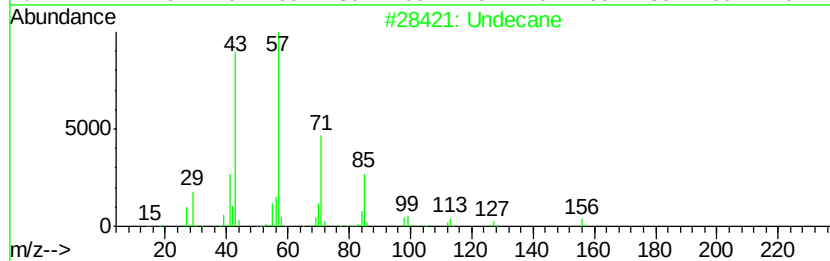
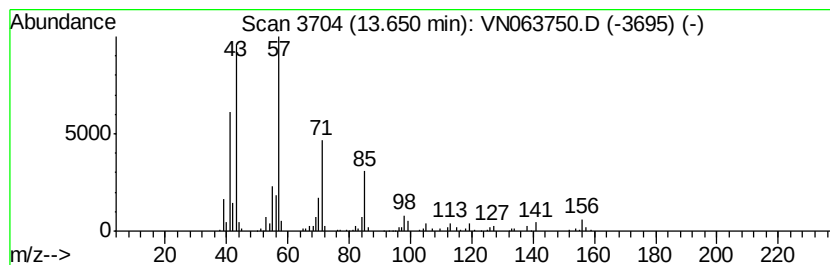
Instrument :
MSVOA_N
ClientSampled :
DRUM-COMP-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	5.14 ug/l	158210	1,4-Dichlorobenzene-d4	13.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane		156 C11H24	001120-21-4 94
2	Tetradecane, 1-iodo-		324 C14H29I	019218-94-1 72
3	Hexadecane		226 C16H34	000544-76-3 72
4	Tridecane		184 C13H28	000629-50-5 72
5	3-Ethyl-3-methylheptane		142 C10H22	017302-01-1 53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52a/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
DRUM-COMP-2

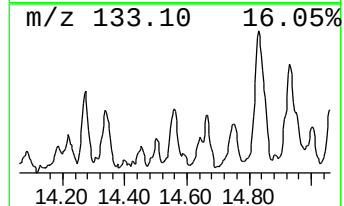
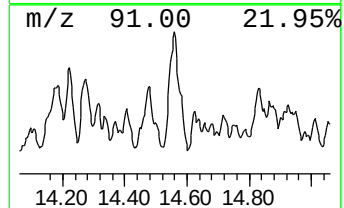
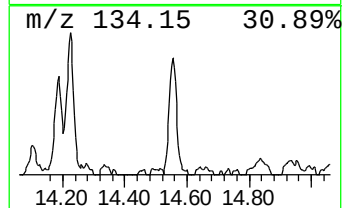
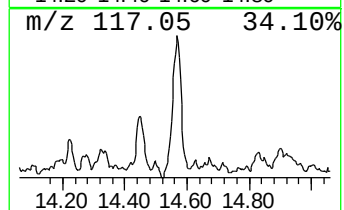
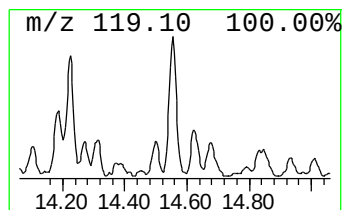
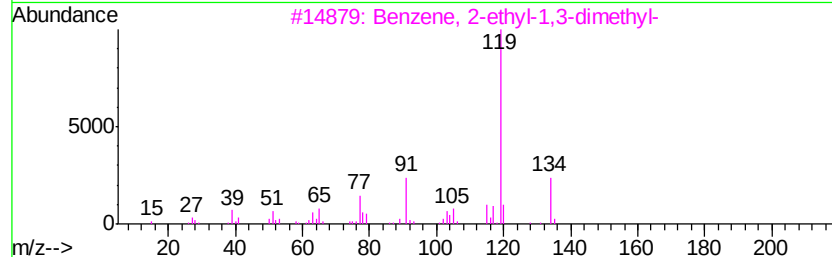
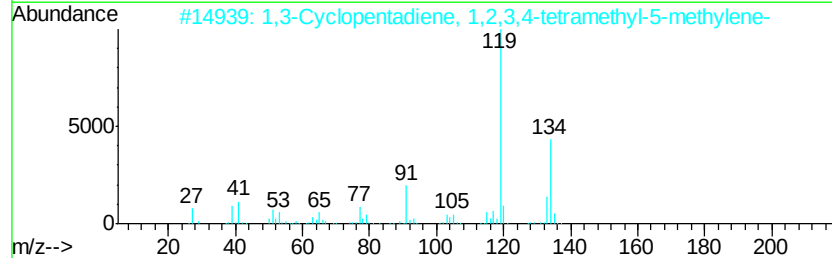
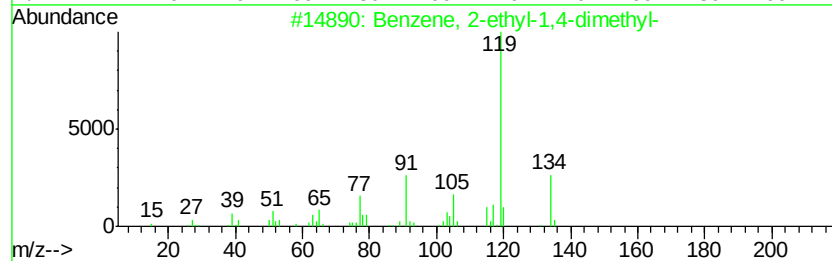
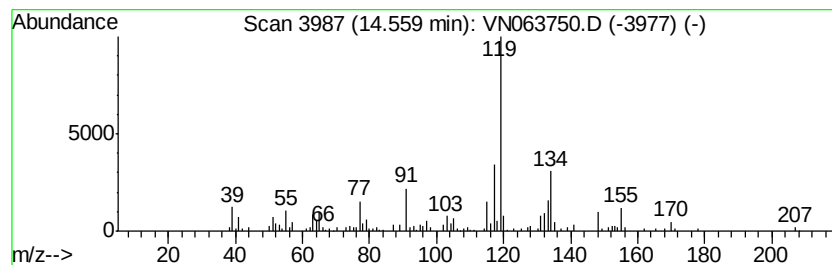
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	5.01 ug/l	154123	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	64
2		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	64
3		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	64
4		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64
5		o-Cymene	134	C10H14	000527-84-4	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP-2

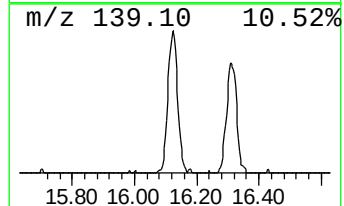
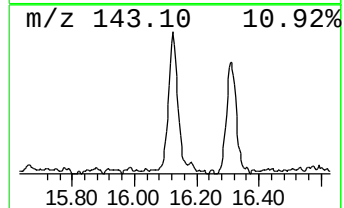
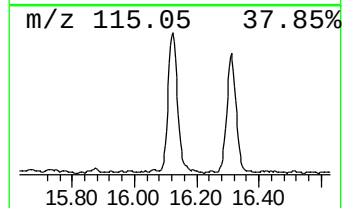
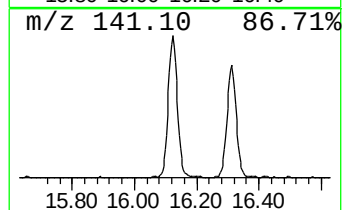
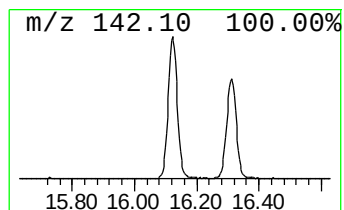
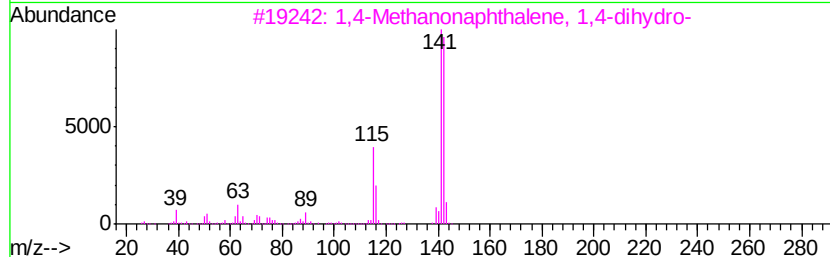
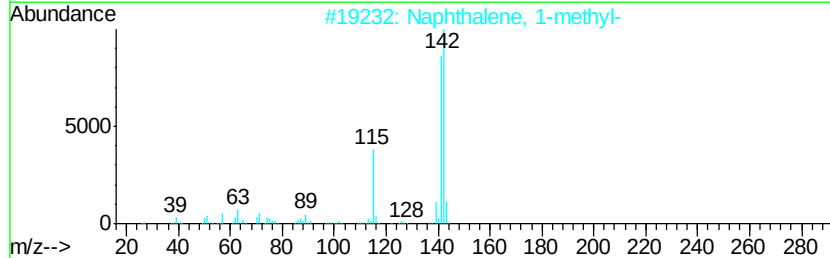
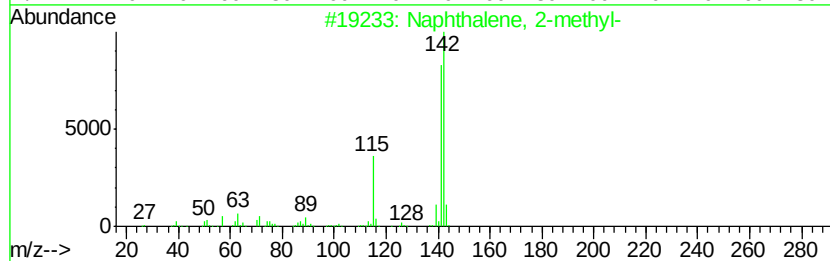
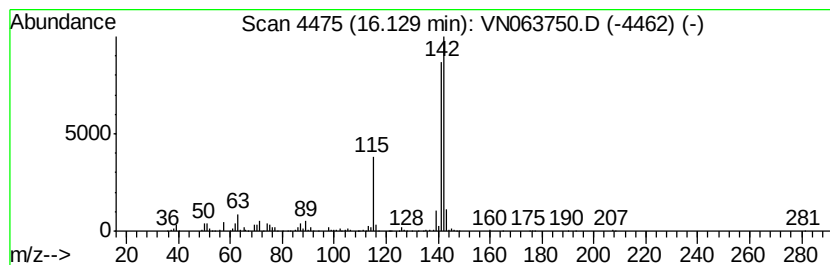
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	18.27 ug/l	562196	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5		Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

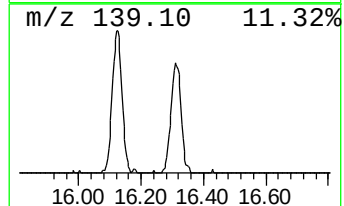
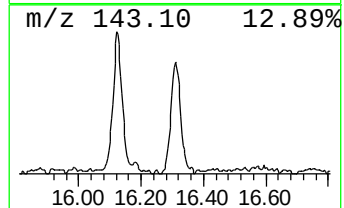
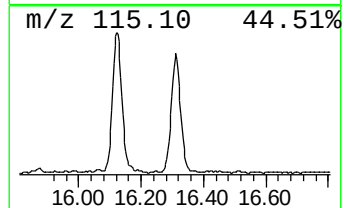
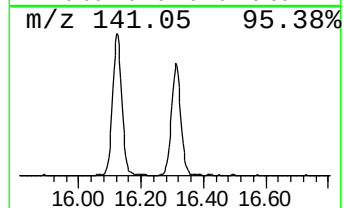
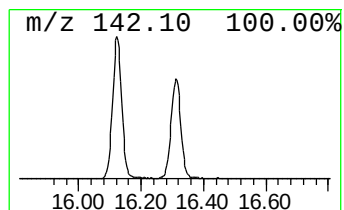
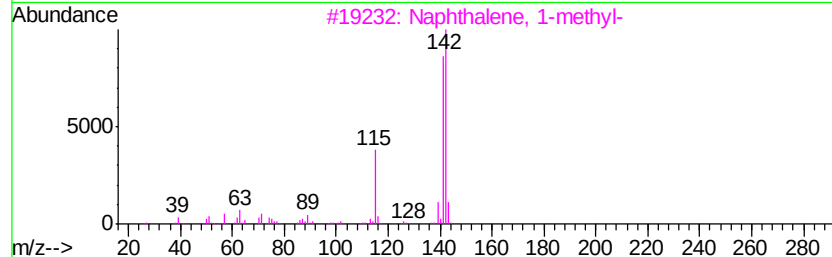
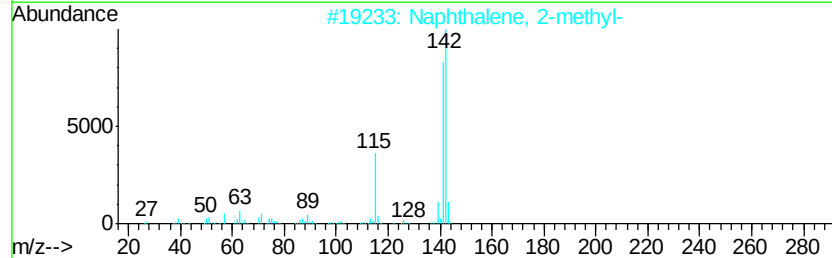
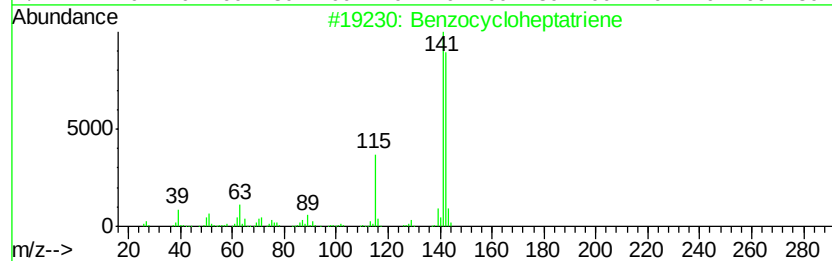
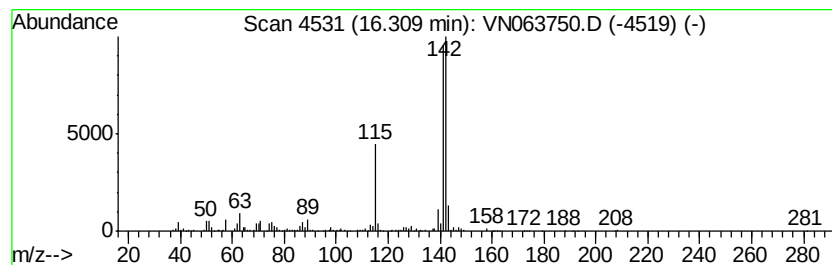
Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	18.20 ug/l	560016	1,4-Dichlorobenzene-d4	13.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzocycloheptatriene	142 C11H10	000264-09-5 96
2		Naphthalene, 2-methyl-	142 C11H10	000091-57-6 96
3		Naphthalene, 1-methyl-	142 C11H10	000090-12-0 96
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142 C11H10	002443-46-1 91
5		1,4-Methanonaphthalene, 1,4-dihy...	142 C11H10	004453-90-1 91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN093020\
Data File : VN063750.D
Acq On : 30 Sep 2020 15:32
Operator : JC/MD
Sample : L4129-17
Misc : 9.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.43	2.43	5.4	ug/l	81566	1	7.62	754606	50.0
Octane	10.25	5.9	ug/l	166259	3	11.38	1408990	50.0
Undecane	13.65	5.1	ug/l	158210	4	13.32	1538880	50.0
Benzene, 2-ethyl-...	14.56	5.0	ug/l	154123	4	13.32	1538880	50.0
Naphthalene, 1-me...	16.13	18.3	ug/l	562196	4	13.32	1538880	50.0
Benzocycloheptatr...	16.31	18.2	ug/l	560016	4	13.32	1538880	50.0