

Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
 Data File : BM012604.D
 Acq On : 31 Oct 2017 11:56
 Operator : SJ/JU
 Sample : I5786-08DL 5X
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-7(0.5-1.5)_101017DL

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.693	99	103	109	rVB	43899	62343	1.26%	0.139%
2	4.081	165	169	178	rBV	111004	159526	3.21%	0.355%
3	5.387	387	391	395	rVB	59624	75940	1.53%	0.169%
4	5.516	407	413	424	rBV	226971	488340	9.84%	1.087%
5	5.881	470	475	484	rBV	133581	212206	4.28%	0.472%
6	6.146	512	520	524	rBV7	24352	55503	1.12%	0.124%
7	6.351	550	555	562	rBV7	22899	58035	1.17%	0.129%
8	6.851	629	640	647	rBV7	37312	111854	2.25%	0.249%
9	6.957	653	658	661	rBV2	51017	74373	1.50%	0.166%
10	7.028	661	670	677	rVV2	277789	615596	12.41%	1.370%
11	7.081	677	679	686	rVB	60439	87004	1.75%	0.194%
12	7.193	692	698	703	rBV	197143	310967	6.27%	0.692%
13	7.393	720	732	742	rVB	259641	483299	9.74%	1.076%
14	7.487	743	748	750	rBV2	117381	185730	3.74%	0.413%
15	7.787	790	799	801	rBV8	34253	88398	1.78%	0.197%
16	7.857	803	811	818	rVB	972386	1641769	33.09%	3.654%
17	7.975	827	831	838	rBV3	43263	87514	1.76%	0.195%
18	8.045	838	843	847	rVB5	50783	80798	1.63%	0.180%
19	8.410	899	905	910	rBV6	52725	116455	2.35%	0.259%
20	8.492	915	919	925	rBV4	42827	82499	1.66%	0.184%
21	8.563	926	931	938	rVB	238880	373466	7.53%	0.831%
22	8.739	955	961	968	rVB	35123	91447	1.84%	0.204%
23	8.963	988	999	1002	rBV2	63141	148827	3.00%	0.331%
24	9.016	1002	1008	1013	rVV	220190	394600	7.95%	0.878%
25	9.081	1015	1019	1030	rVB	88747	172702	3.48%	0.384%
26	9.210	1037	1041	1049	rVB6	38370	78114	1.57%	0.174%
27	9.581	1100	1104	1109	rVB3	44414	73591	1.48%	0.164%
28	9.734	1124	1130	1137	rBV	179537	310405	6.26%	0.691%
29	9.834	1142	1147	1155	rBV8	35009	67372	1.36%	0.150%
30	9.975	1167	1171	1181	rBV6	45148	93635	1.89%	0.208%
31	10.275	1216	1222	1231	rVB	294345	499289	10.06%	1.111%
32	10.651	1276	1286	1293	rBV	1183433	2059159	41.50%	4.583%
33	10.786	1302	1309	1320	rVB	104260	217616	4.39%	0.484%
34	11.445	1415	1421	1431	rBV3	37671	83962	1.69%	0.187%

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 Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	11.969	1504	1510	1520	rVB2	35604	70195	1.41%	0.156%
36	13.898	1830	1838	1843	rBV	470937	686125	13.83%	1.527%
37	14.180	1880	1886	1896	rVB	510939	808286	16.29%	1.799%
38	14.492	1929	1939	1947	rBV2	1672226	2571070	51.81%	5.723%
39	14.698	1968	1974	1987	rBV	153658	285310	5.75%	0.635%
40	15.480	2101	2107	2113	rBV	698144	1027910	20.72%	2.288%
41	15.751	2141	2153	2159	rBV	30657	106028	2.14%	0.236%
42	15.845	2165	2169	2174	rVB	142119	193393	3.90%	0.430%
43	16.204	2226	2230	2232	rBV2	45797	61992	1.25%	0.138%
44	17.045	2370	2373	2380	rVB5	38192	63530	1.28%	0.141%
45	17.233	2399	2405	2410	rBV2	2092586	3004563	60.55%	6.688%
46	17.274	2410	2412	2416	rVV	61618	73339	1.48%	0.163%
47	17.333	2416	2422	2432	rVB2	734614	1111238	22.39%	2.473%
48	17.857	2508	2511	2517	rVB	49347	58822	1.19%	0.131%
49	18.127	2551	2557	2564	rBV	1998365	2850167	57.44%	6.344%
50	18.198	2564	2569	2574	rVB	3325175	4130215	83.24%	9.193%
51	18.909	2687	2690	2694	rVB	137420	179161	3.61%	0.399%
52	19.286	2749	2754	2767	rBV	2287487	4962092	100.00%	11.045%
53	19.403	2770	2774	2782	rVV	917753	1331513	26.83%	2.964%
54	19.621	2806	2811	2821	rBV2	994598	1556415	31.37%	3.464%
55	20.539	2964	2967	2971	rVB	594709	674269	13.59%	1.501%
56	21.315	3096	3099	3104	rBV	1500499	1559221	31.42%	3.471%
57	21.403	3110	3114	3119	rBV	3014879	3864761	77.89%	8.602%
58	23.709	3502	3506	3513	rVB2	2203959	3955587	79.72%	8.804%

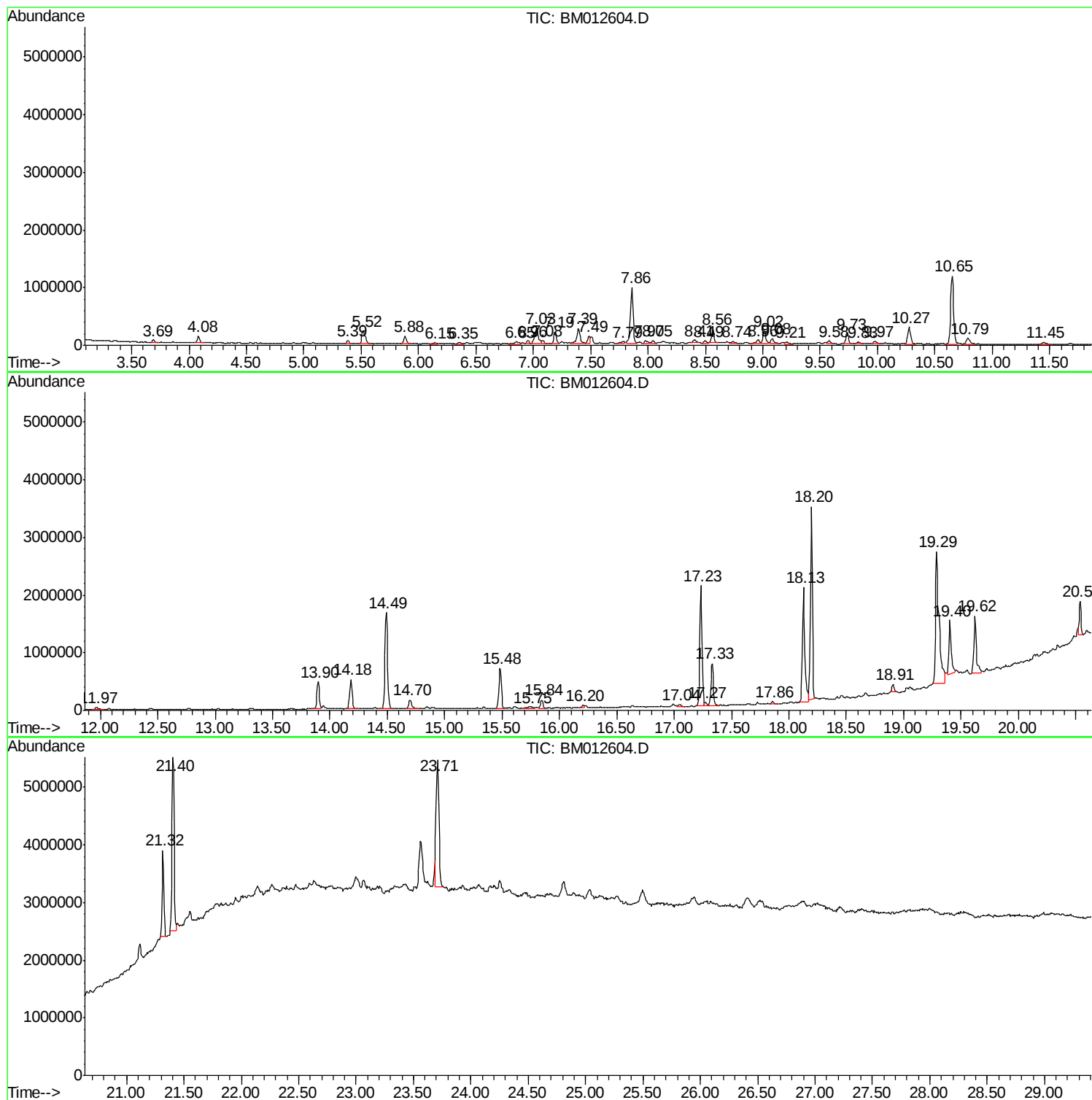
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TIC Library : C:\DATABASE\NIST11.L
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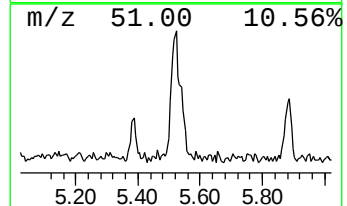
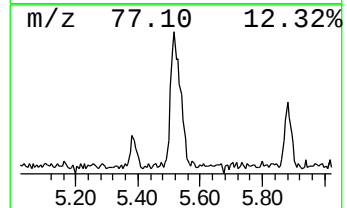
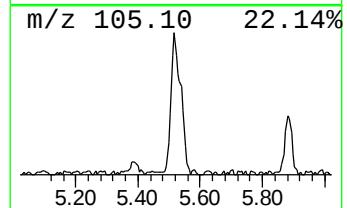
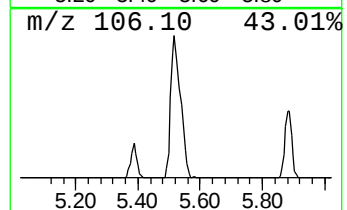
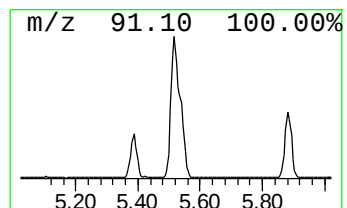
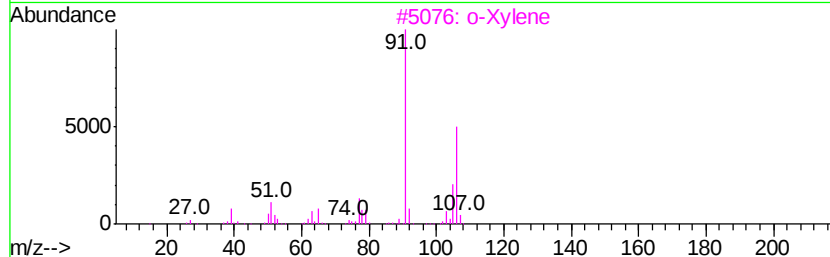
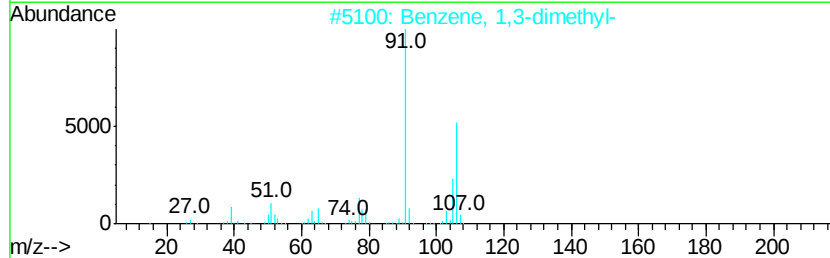
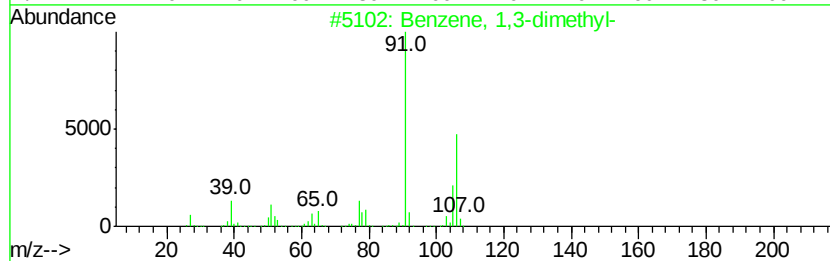
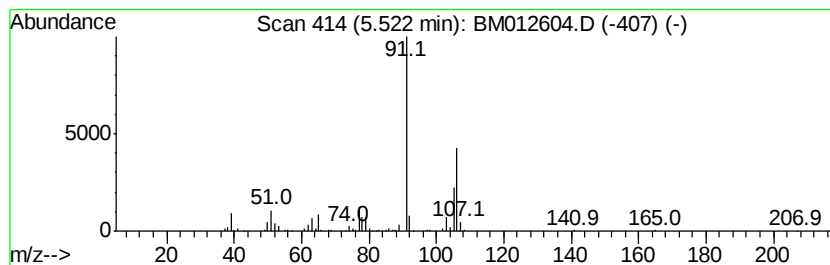
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	5.95 ng/ul	488340	1,4-Dichlorobenzene-d4	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2		Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
3		o-Xylene	106	C8H10	000095-47-6	97
4		p-Xylene	106	C8H10	000106-42-3	95
5		p-Xylene	106	C8H10	000106-42-3	95



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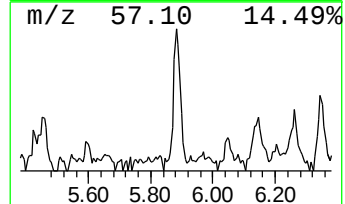
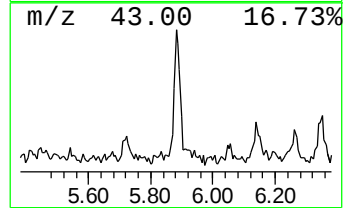
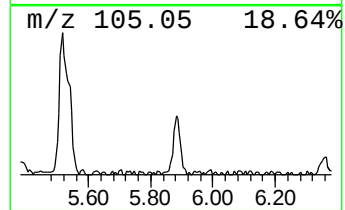
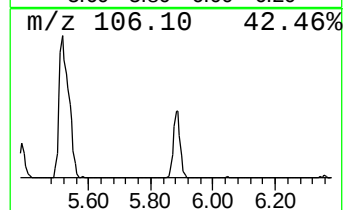
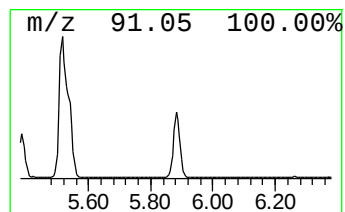
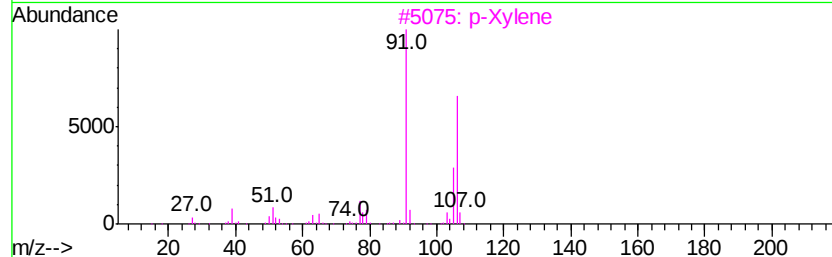
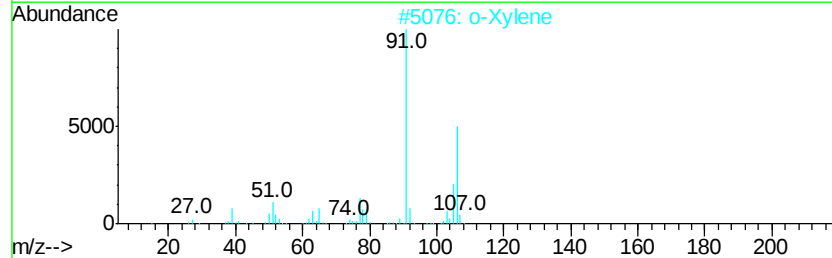
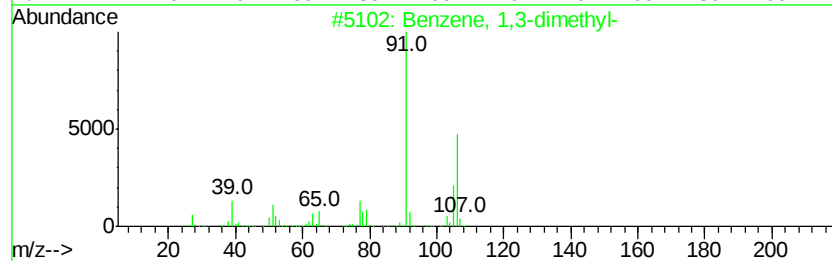
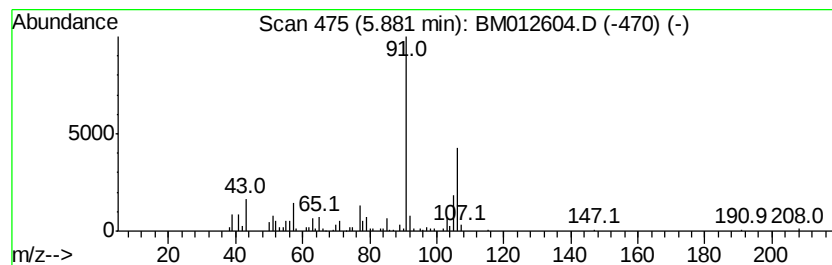
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.88	2.59 ng/ul	212206	1,4-Dichlorobenzene-d4	7.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	95
2			o-Xylene	106	C8H10	000095-47-6	94
3			p-Xylene	106	C8H10	000106-42-3	94
4			p-Xylene	106	C8H10	000106-42-3	93
5			o-Xylene	106	C8H10	000095-47-6	93



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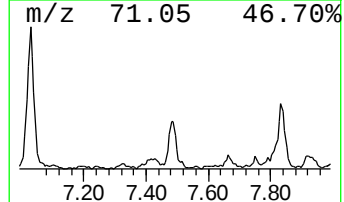
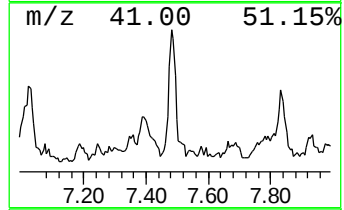
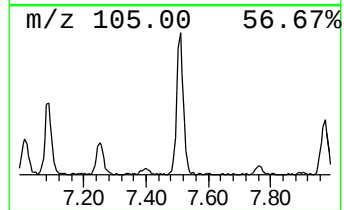
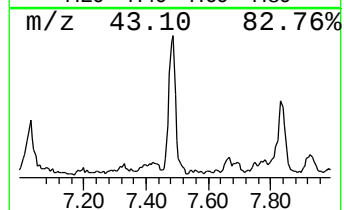
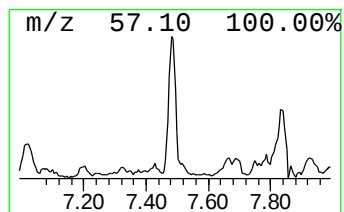
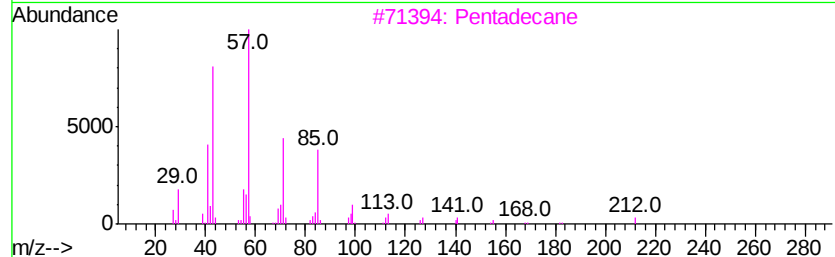
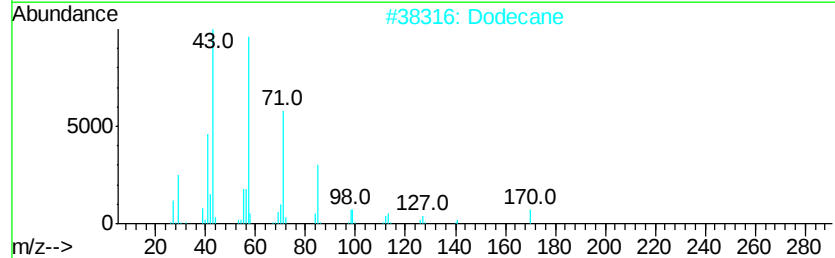
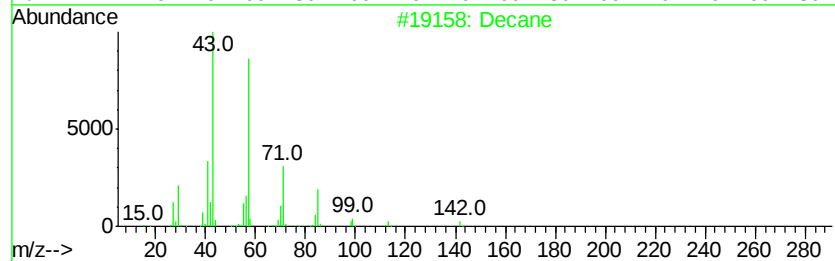
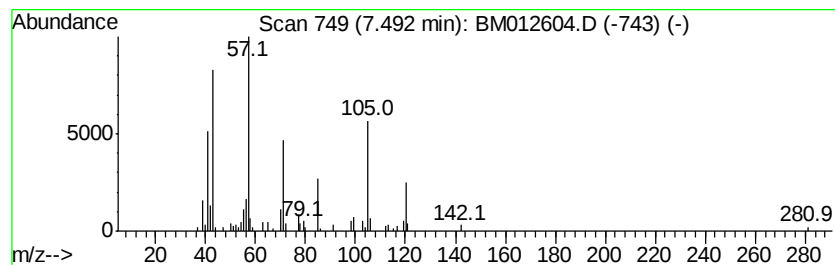
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.49	2.26 ng/ul	185730	1,4-Dichlorobenzene-d4	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane	142	C10H22	000124-18-5	81
2		Dodecane	170	C12H26	000112-40-3	64
3		Pentadecane	212	C15H32	000629-62-9	64
4		Heptadecane	240	C17H36	000629-78-7	64
5		3,5-Dimethyldodecane	198	C14H30	107770-99-0	64



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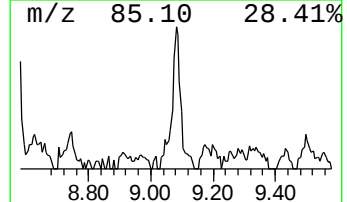
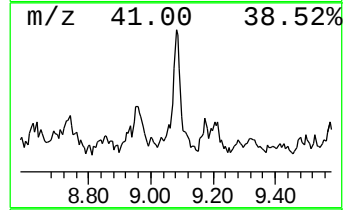
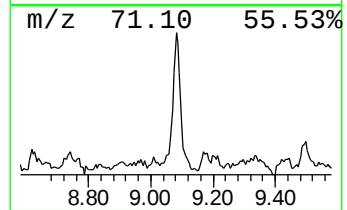
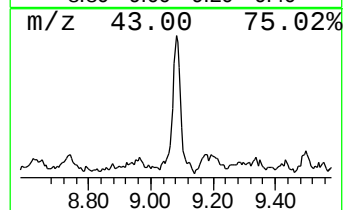
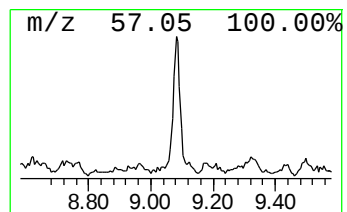
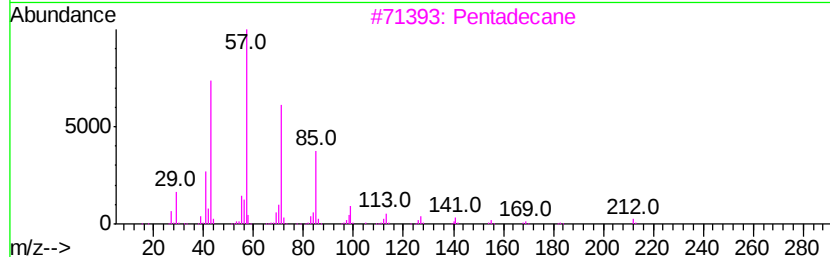
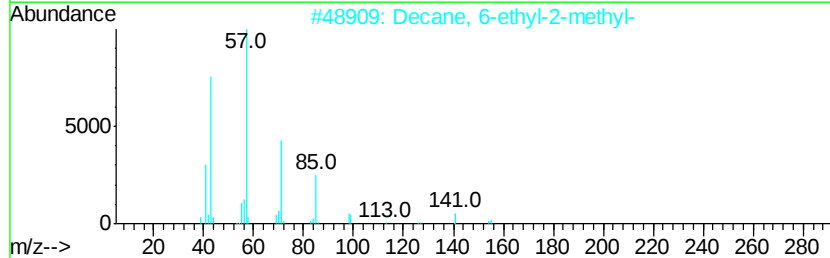
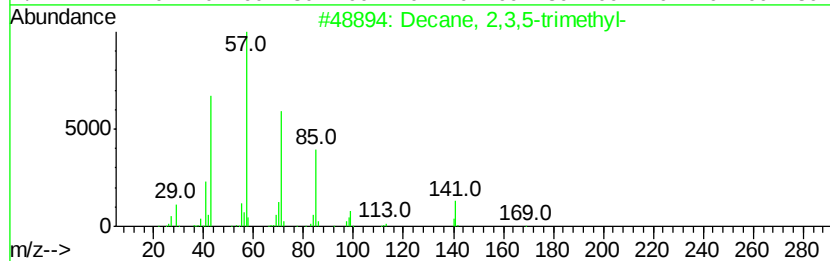
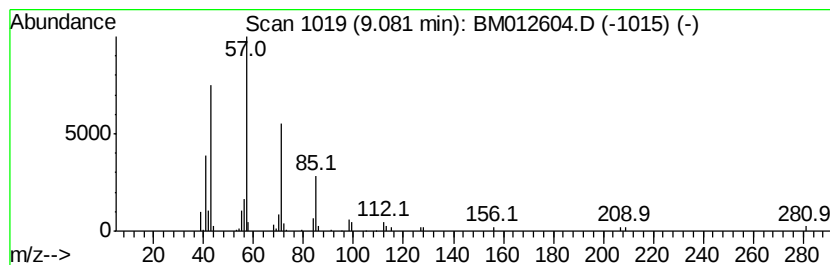
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.08	2.10 ng/ul	172702	1,4-Dichlorobenzene-d4	7.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
2			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72
3			Pentadecane	212	C15H32	000629-62-9	72
4			Tetradecane	198	C14H30	000629-59-4	72
5			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64



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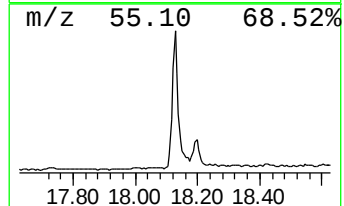
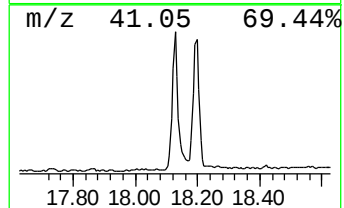
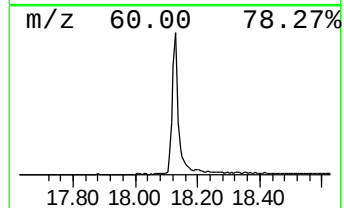
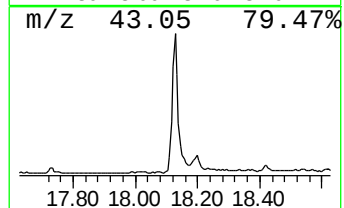
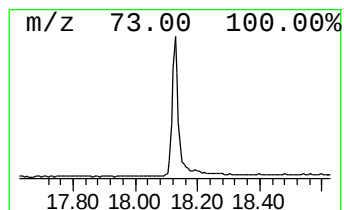
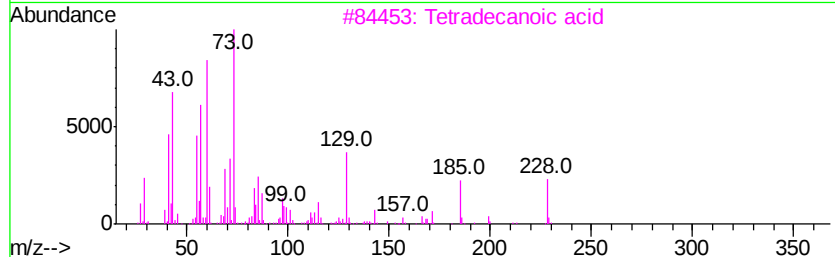
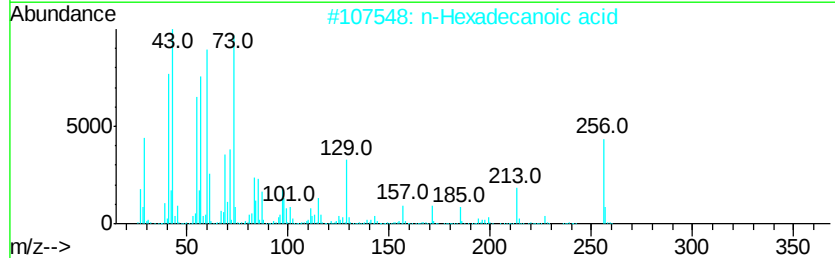
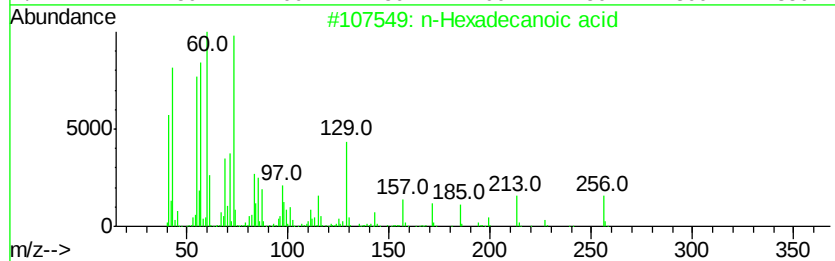
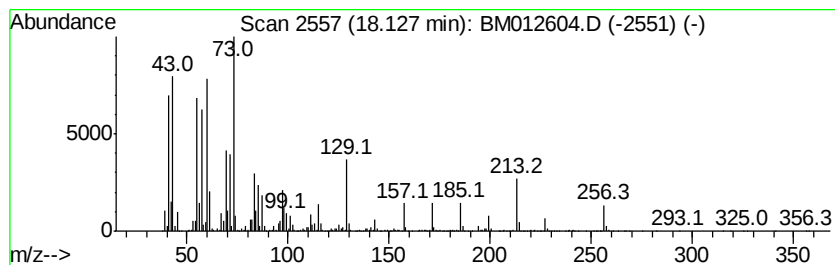
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	18.97 ng/ul	2850170	Phenanthrene-d10	17.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	95
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	89



Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012604.D
Acq On : 31 Oct 2017 11:56
Operator : SJ/JU
Sample : I5786-08DL 5X
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-7(0.5-1.5)_101017DL

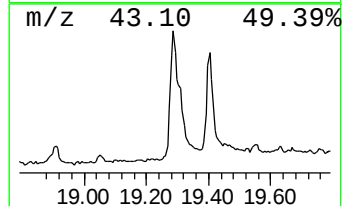
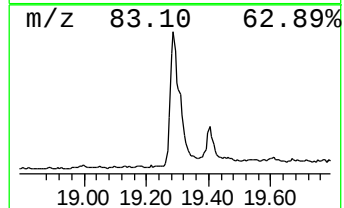
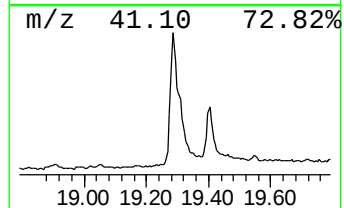
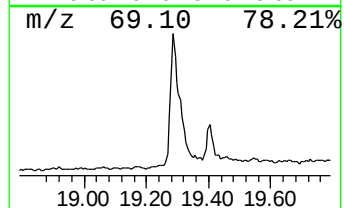
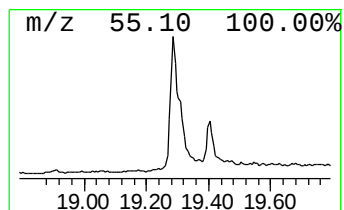
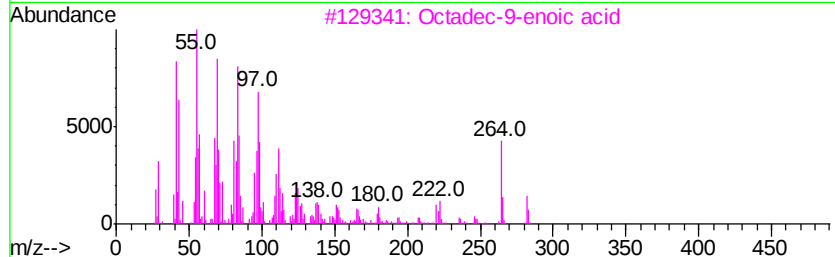
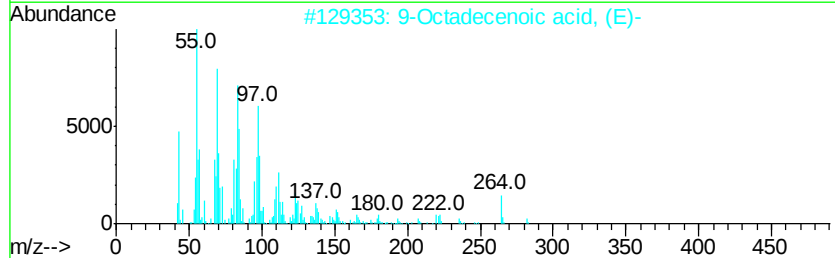
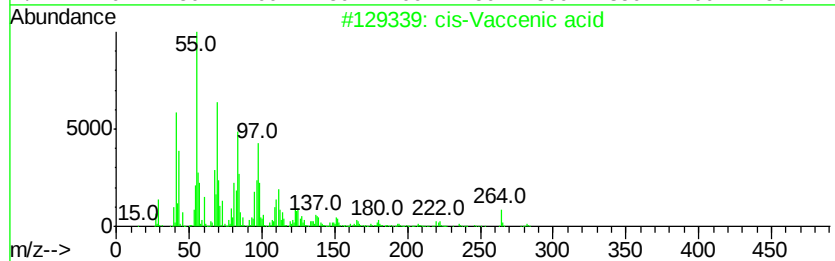
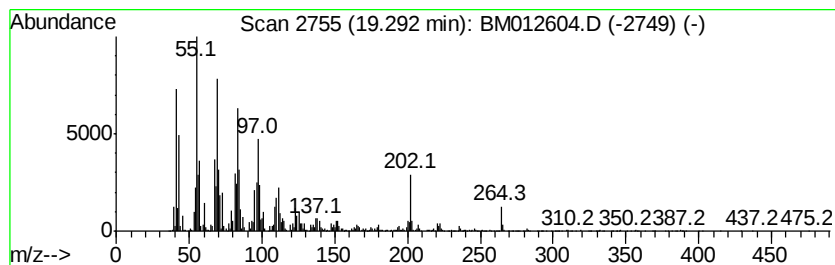
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 cis-Vaccenic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.29	33.03 ng/ul	4962090	Phenanthrene-d10	17.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
3		Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	99
4		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97
5		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	96



Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012604.D
Acq On : 31 Oct 2017 11:56
Operator : SJ/JU
Sample : I5786-08DL 5X
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-7(0.5-1.5)_101017DL

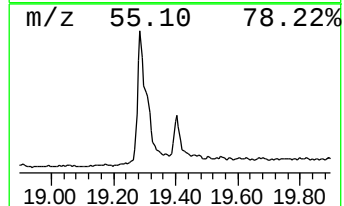
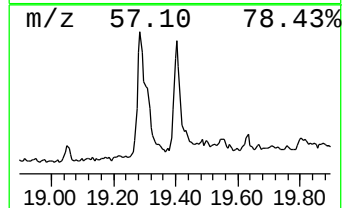
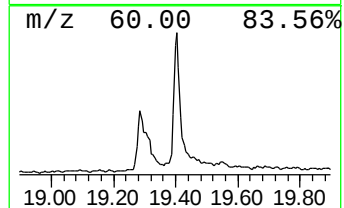
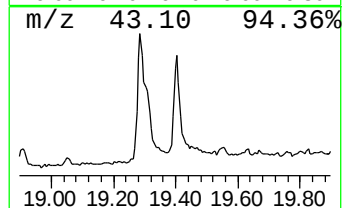
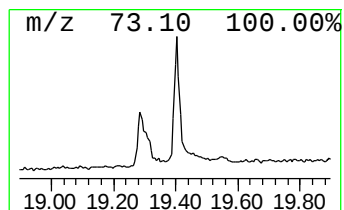
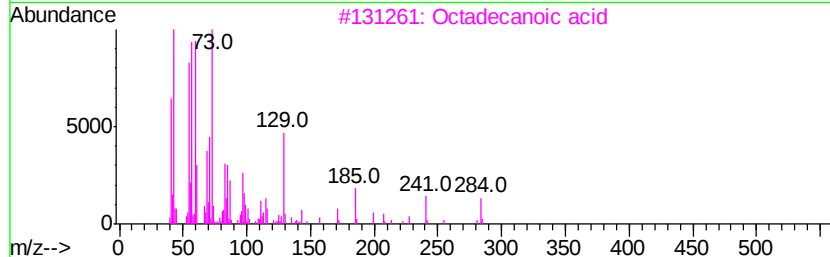
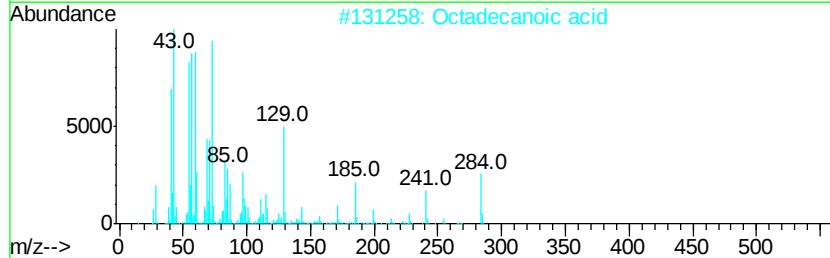
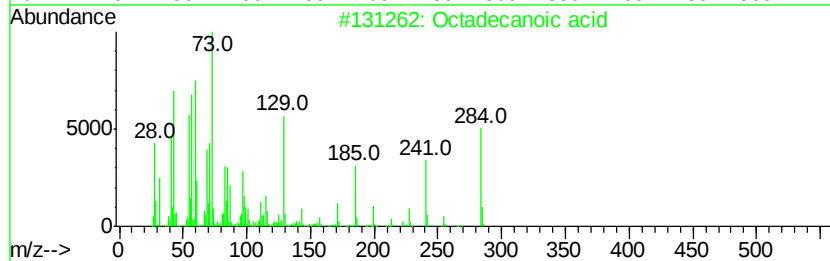
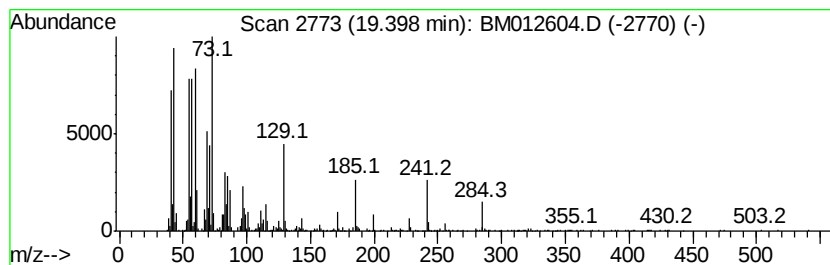
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.40	6.89 ng/ul	1331510	Chrysene-d12	21.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	99
3		Octadecanoic acid	284	C18H36O2	000057-11-4	95
4		Octadecanoic acid	284	C18H36O2	000057-11-4	93
5		Tetracosanoic acid	368	C24H48O2	000557-59-5	93



Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012604.D
Acq On : 31 Oct 2017 11:56
Operator : SJ/JU
Sample : I5786-08DL 5X
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-7(0.5-1.5)_101017DL

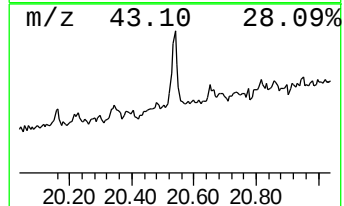
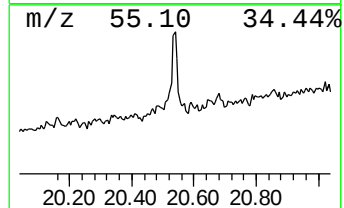
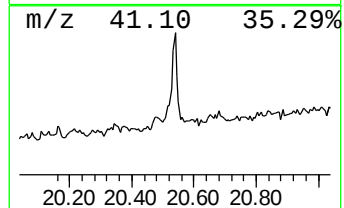
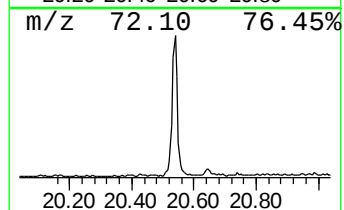
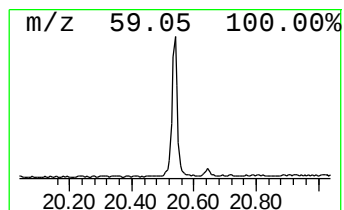
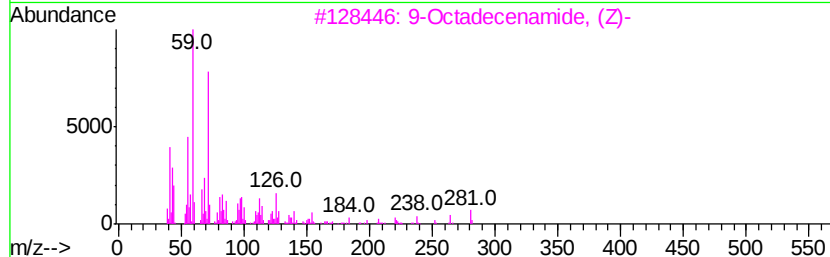
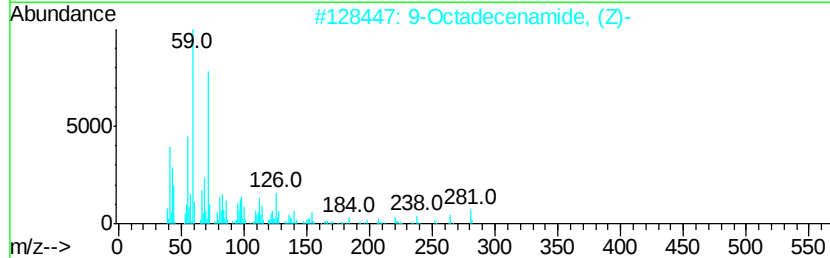
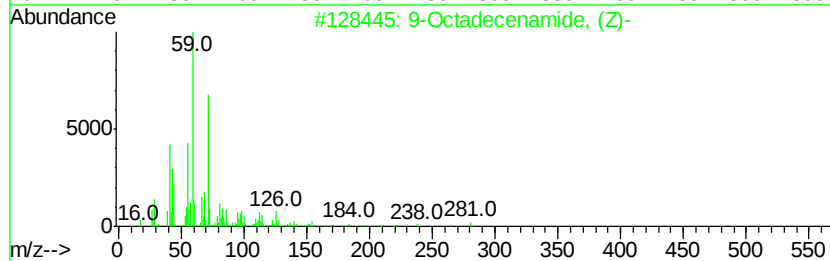
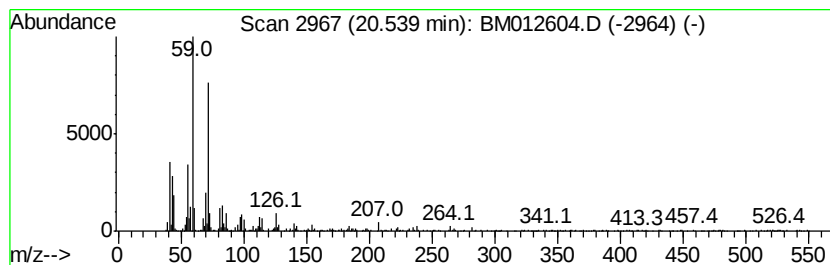
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.54	3.49 ng/ul	674269	Chrysene-d12	21.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
4		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM103017\
 Data File : BM012604.D
 Acq On : 31 Oct 2017 11:56
 Operator : SJ/JU
 Sample : I5786-08DL 5X
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
 Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,3-dime...	5.52	6.0	ng/ul	488340	1	7.86	1641770	20.0
(DEL) Alkane: Str...	5.88	2.6	ng/ul	212206	1	7.86	1641770	20.0
(DEL) Alkane: Str...	7.49	2.3	ng/ul	185730	1	7.86	1641770	20.0
(DEL) Alkane: Str...	9.08	2.1	ng/ul	172702	1	7.86	1641770	20.0
n-Hexadecanoic acid	18.13	19.0	ng/ul	2850170	4	17.23	3004560	20.0
cis-Vaccenic acid	19.29	33.0	ng/ul	4962090	4	17.23	3004560	20.0
Octadecanoic acid	19.40	6.9	ng/ul	1331510	5	21.40	3864760	20.0
9-Octadecenamide, ...	20.54	3.5	ng/ul	674269	5	21.40	3864760	20.0