

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
 Data File : BM018411.D
 Acq On : 28 Dec 2018 00:04
 Operator : JU/SJ
 Sample : J6572-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 381204024-2

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	25	28	38	rVB2	142589	225811	2.08%	0.346%
2	5.357	415	420	426	rBV	384522	581038	5.35%	0.889%
3	6.399	593	597	603	rVB	215339	323172	2.97%	0.494%
4	6.934	683	688	697	rVB	305266	485659	4.47%	0.743%
5	7.781	826	832	839	rBV	1391430	2161809	19.90%	3.308%
6	8.940	1023	1029	1037	rBV	864323	1446090	13.31%	2.213%
7	10.575	1300	1307	1319	rVB	2056647	3556697	32.74%	5.442%
8	10.857	1349	1355	1360	rBV	378673	574622	5.29%	0.879%
9	11.986	1537	1547	1553	rVB4	138366	348806	3.21%	0.534%
10	13.045	1717	1727	1735	rBV	2888186	4267706	39.28%	6.530%
11	14.369	1947	1952	1956	rBV	89051	148905	1.37%	0.228%
12	14.427	1956	1962	1969	rVB2	3130780	4834463	44.50%	7.397%
13	15.051	2054	2068	2069	rBV	397785	1320339	12.15%	2.020%
14	15.792	2188	2194	2203	rVB6	88739	191967	1.77%	0.294%
15	15.916	2209	2215	2221	rBV	2021838	2875753	26.47%	4.400%
16	16.051	2233	2238	2245	rVB	244737	343176	3.16%	0.525%
17	16.127	2247	2251	2255	rVB4	112442	139236	1.28%	0.213%
18	16.333	2283	2286	2291	rVB3	95369	135421	1.25%	0.207%
19	16.939	2385	2389	2400	rVB10	50703	142945	1.32%	0.219%
20	17.174	2422	2429	2436	rVB	4210889	5921369	54.50%	9.060%
21	17.480	2474	2481	2488	rBV2	654333	1121595	10.32%	1.716%
22	18.068	2575	2581	2585	rBV	395779	612036	5.63%	0.936%
23	18.110	2585	2588	2591	rVV2	150876	218932	2.02%	0.335%
24	18.145	2591	2594	2601	rVB	74260	111349	1.02%	0.170%
25	19.351	2795	2799	2807	rBV2	518072	783135	7.21%	1.198%
26	19.692	2853	2857	2861	rBV	162647	232173	2.14%	0.355%
27	19.804	2871	2876	2883	rBV	8904171	10864511	100.00%	16.624%
28	21.362	3136	3141	3152	rVB	6196634	7921633	72.91%	12.121%
29	21.962	3240	3243	3248	rVB3	129242	178733	1.65%	0.273%
30	22.433	3320	3323	3328	rVB2	170512	207688	1.91%	0.318%
31	22.956	3408	3412	3419	rVB	314911	455451	4.19%	0.697%
32	23.539	3507	3511	3519	rVB	276637	456524	4.20%	0.699%
33	23.656	3523	3531	3542	rVB	4160898	7898094	72.70%	12.085%
34	24.215	3621	3626	3632	rVB2	247674	438678	4.04%	0.671%

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	24.697	3702	3708	3727	rVB6	383759	1065629	9.81%	1.631%
36	24.974	3748	3755	3769	rBV4	838758	2763266	25.43%	4.228%

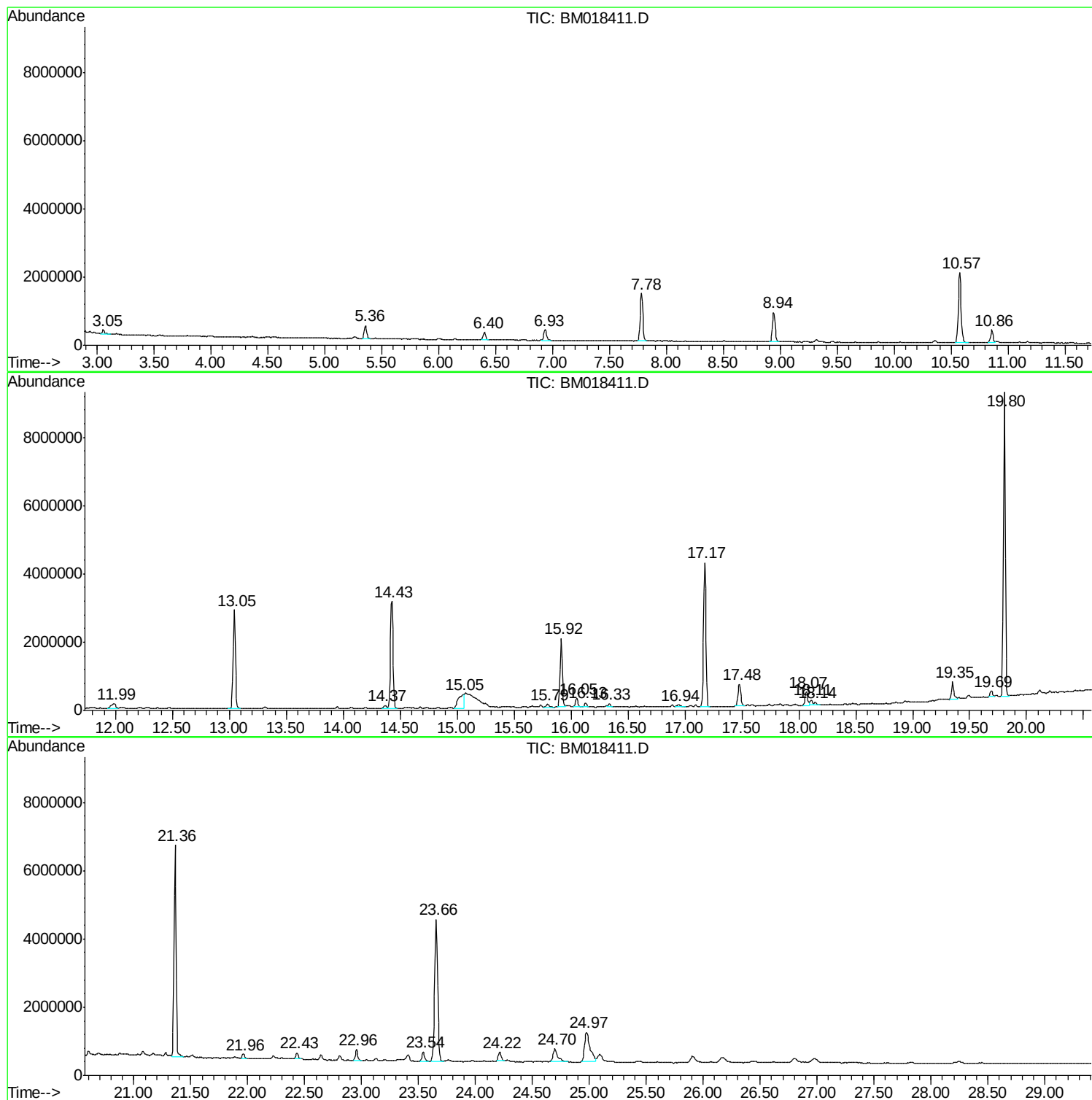
Sum of corrected areas: 65354411

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

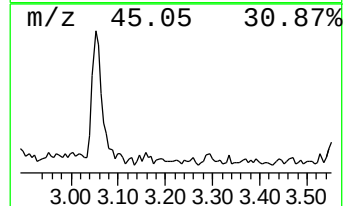
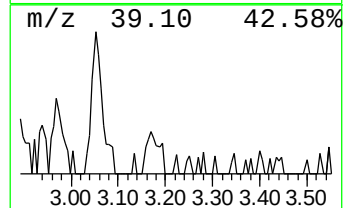
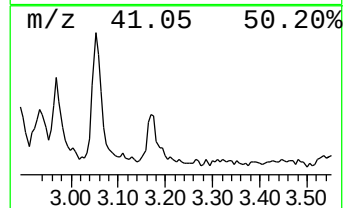
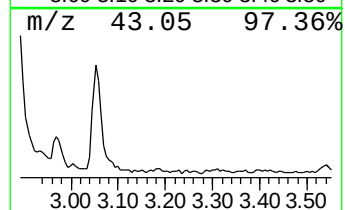
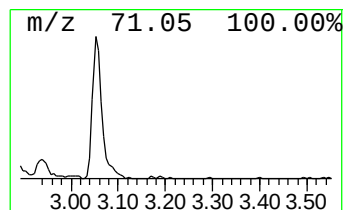
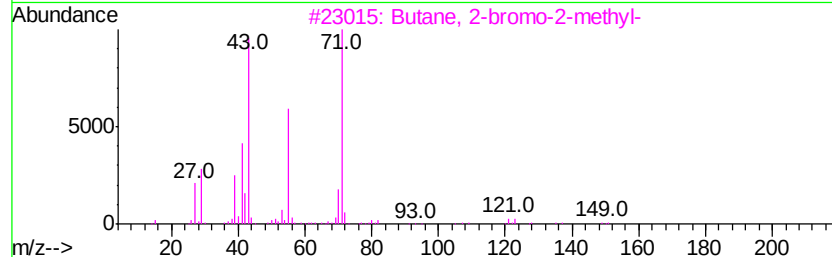
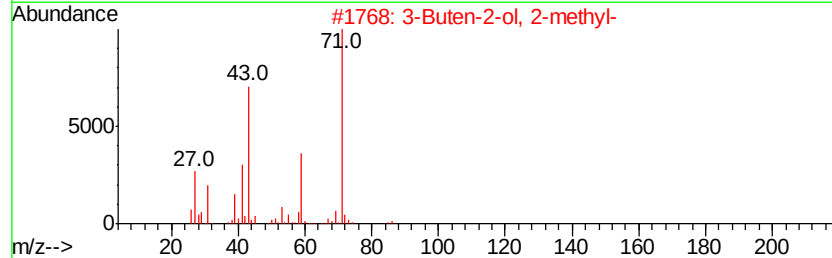
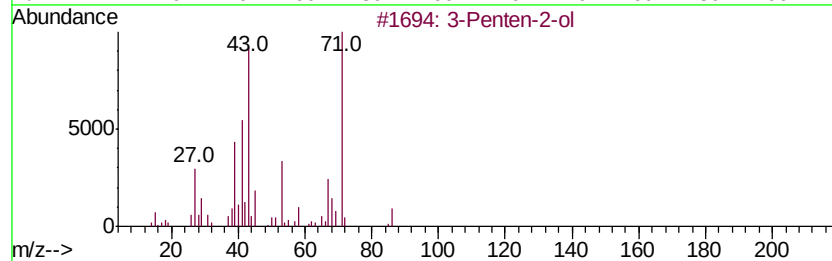
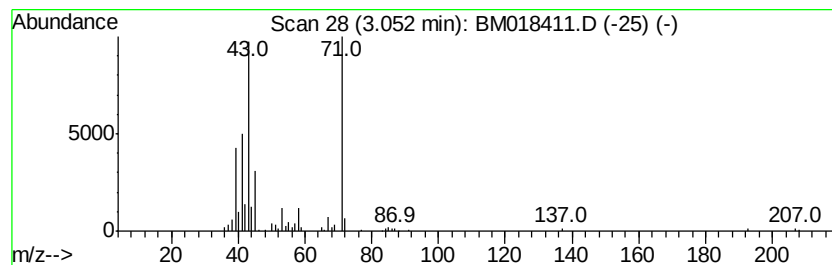
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	2.09 ng	225811	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-ol	86	C5H10O	001569-50-2	56
2		3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	47
3		Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	47
4		1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	45
5		Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

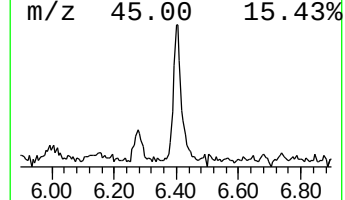
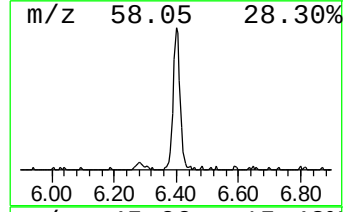
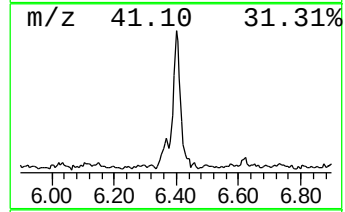
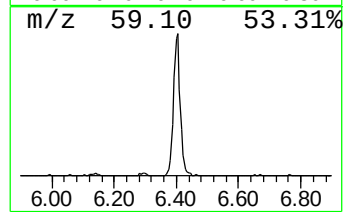
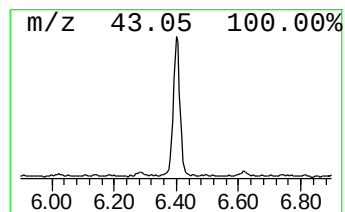
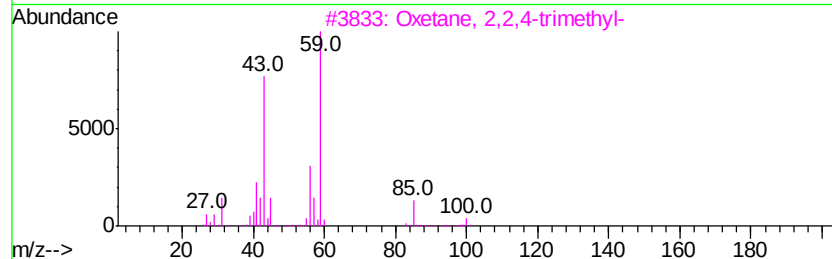
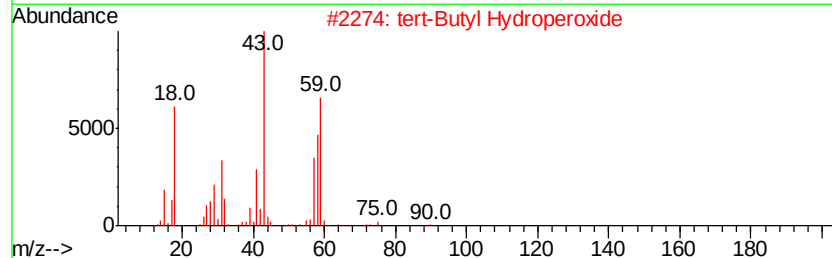
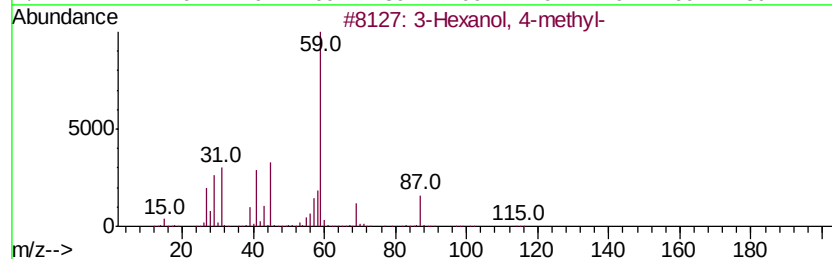
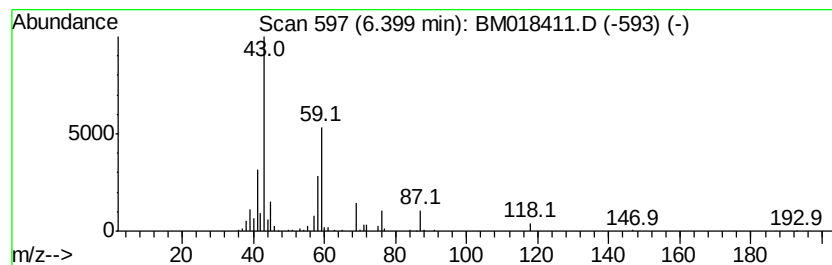
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.40 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	2.99 ng	323172	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Hexanol, 4-methyl-	116	C7H16O	000615-29-2	47
2	tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	38	
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	37	
4	2-Ethoxyethyl acetate	132	C6H12O3	000111-15-9	28	
5	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	25	



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

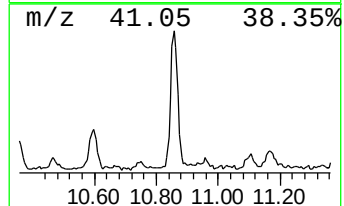
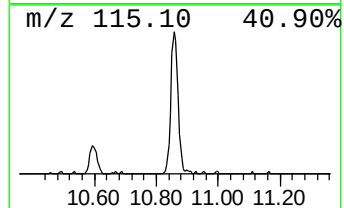
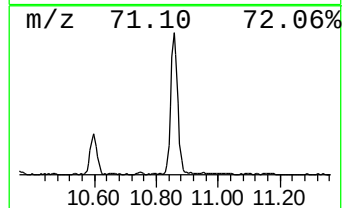
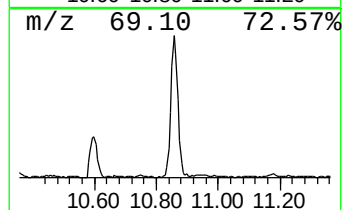
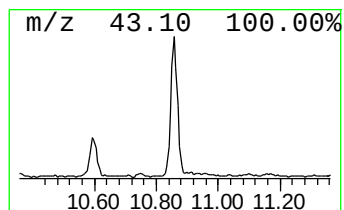
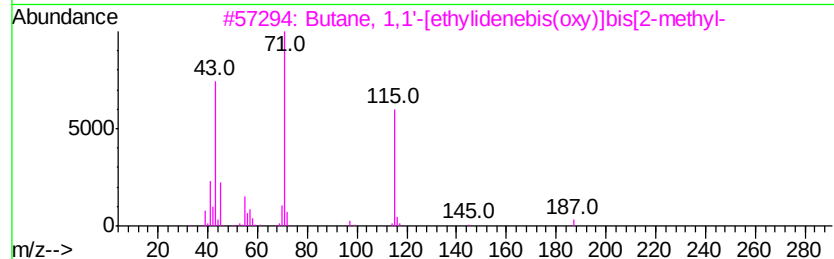
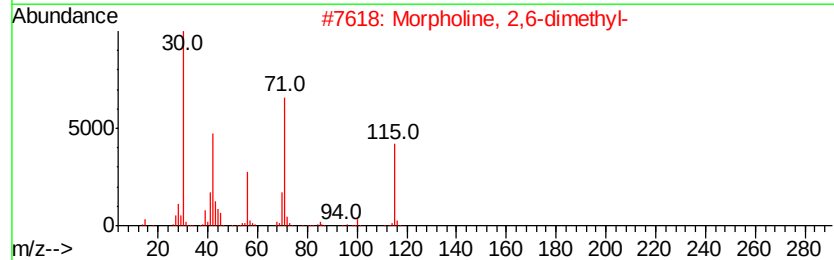
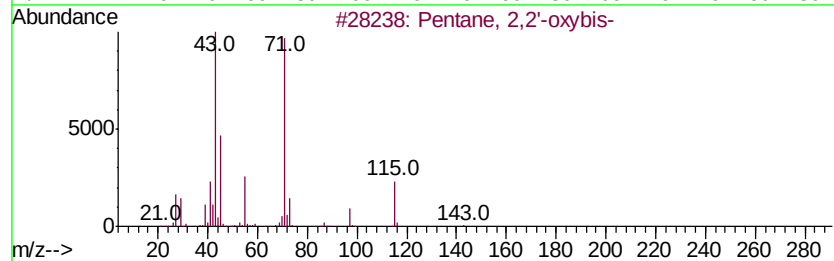
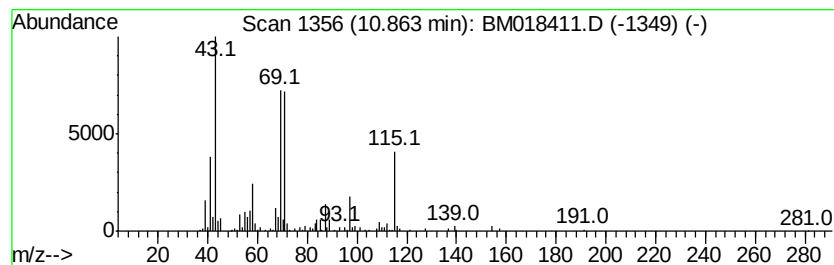
Instrument :
BNA_M
ClientSampleId :
381204024-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.86 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.86	3.23 ng	574622	Naphthalene-d8	10.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	47
2	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	38
3	Butane, 1,1'-[ethylidenebis(oxy)]-	202	C12H26O2	013535-43-8	37
4	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	35
5	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

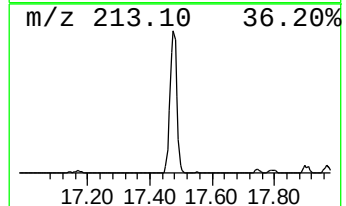
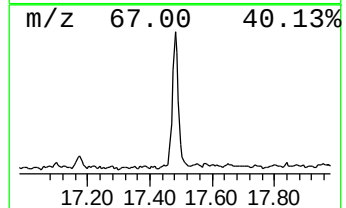
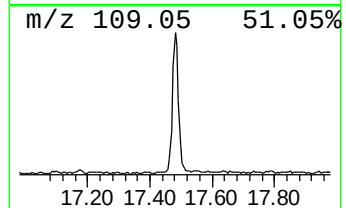
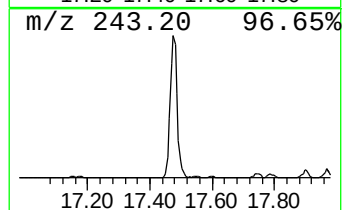
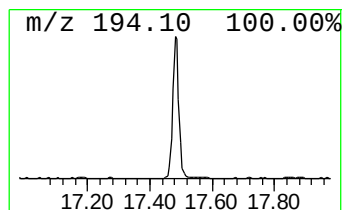
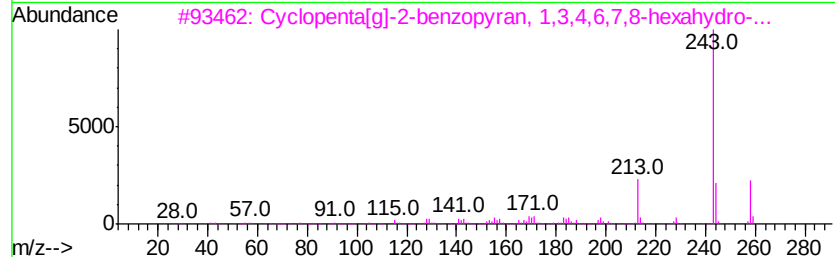
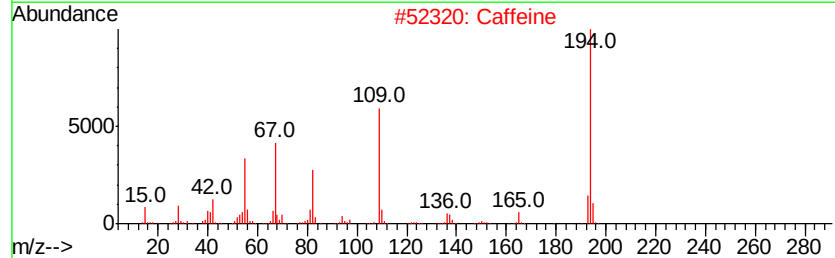
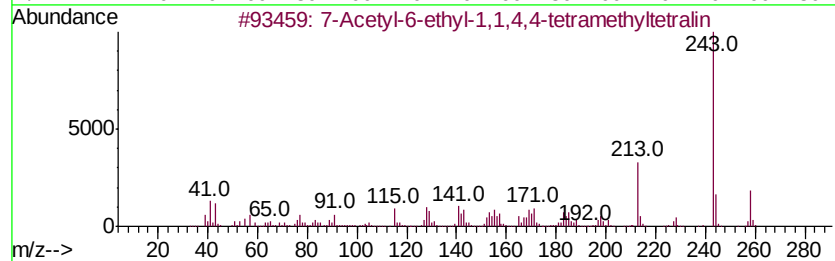
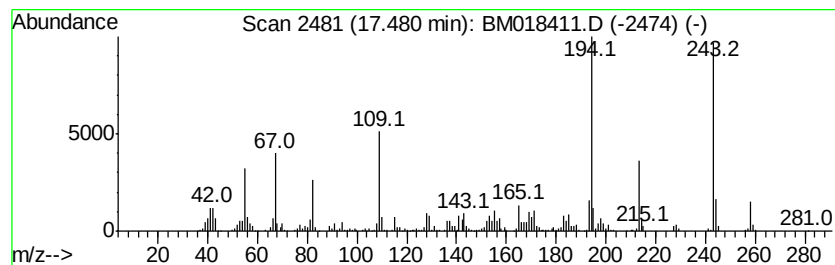
Instrument :
BNA_M
ClientSampleId :
381204024-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 7-Acetyl-6-ethyl-1,1,4,4-te... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.48	3.79 ng	1121600	Phenanthrene-d10	17.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Acetyl-6-ethyl-1,1,4,4-tetrame...	258	C18H26O	000088-29-9	95
2	Caffeine	194	C8H10N4O2	000058-08-2	95
3	Cyclopenta[<i>a</i>]-2-benzopyran, 1,3,...	258	C18H26O	001222-05-5	95
4	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	50
5	Galaxolide 2	258	C18H26O	1000285-26-7	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

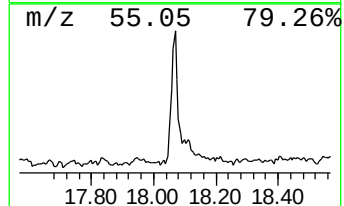
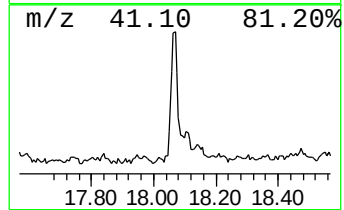
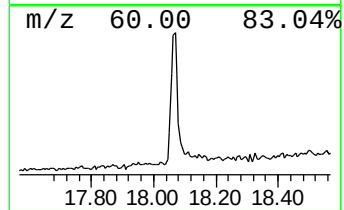
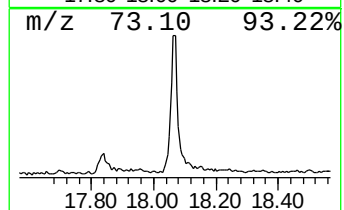
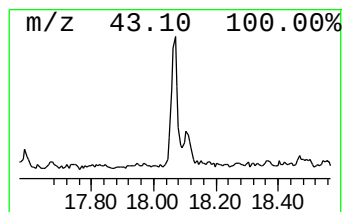
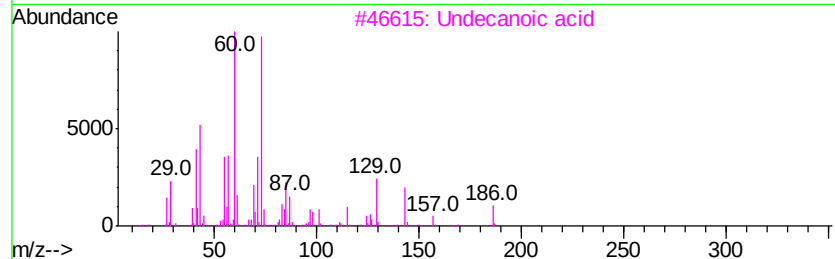
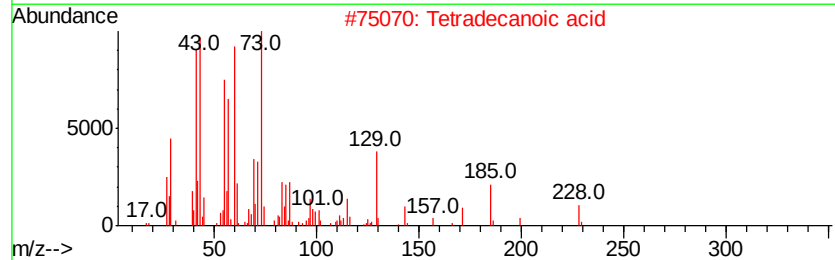
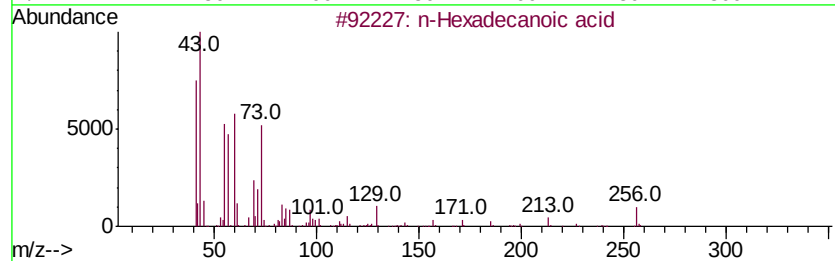
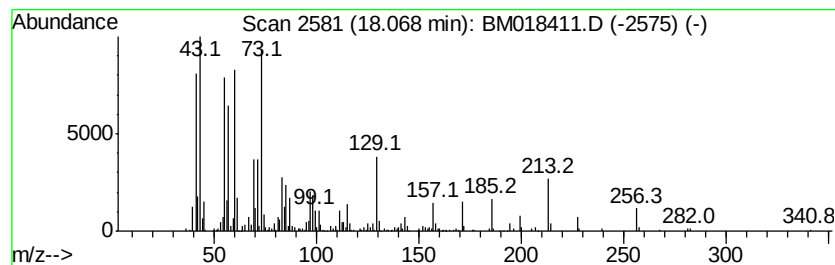
Instrument :
BNA_M
ClientSampleId :
381204024-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	2.07 ng	612036	Phenanthrene-d10	17.17
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Hexadecanoic acid	256 C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228 C14H28O2	000544-63-8	89
3	Undecanoic acid	186 C11H22O2	000112-37-8	70
4	Pentadecanoic acid	242 C15H30O2	001002-84-2	64
5	n-Decanoic acid	172 C10H20O2	000334-48-5	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

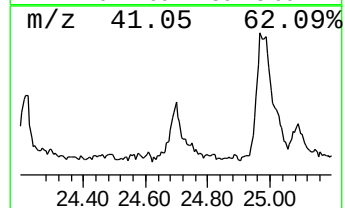
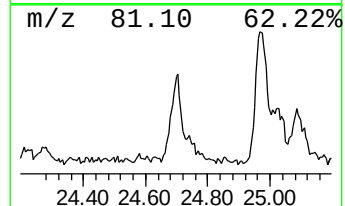
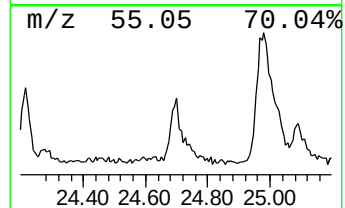
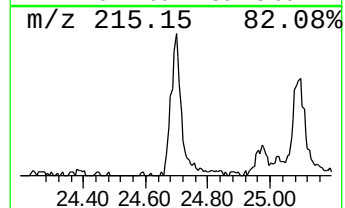
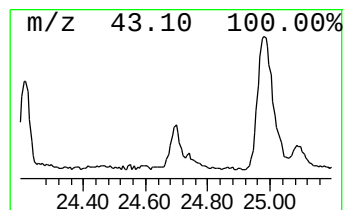
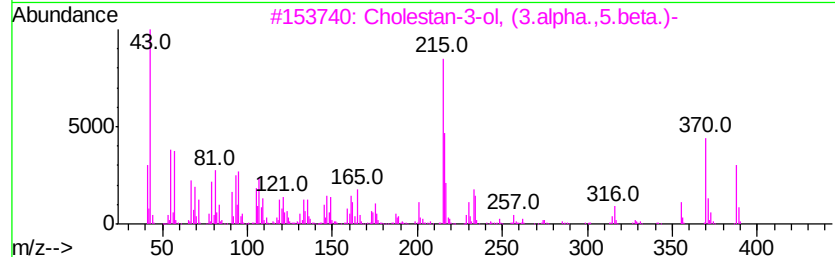
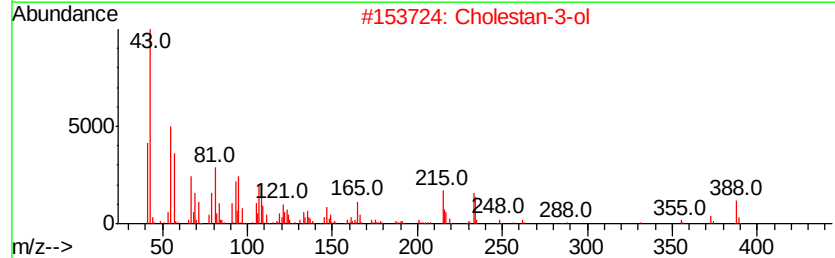
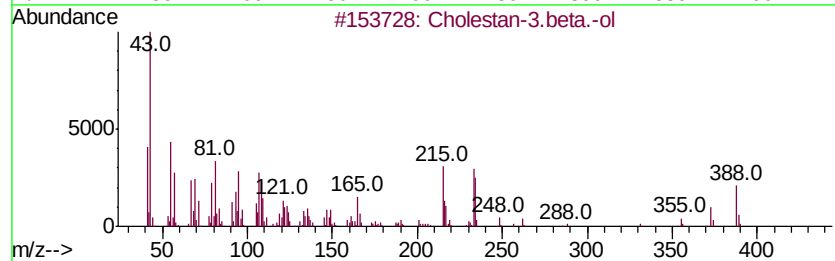
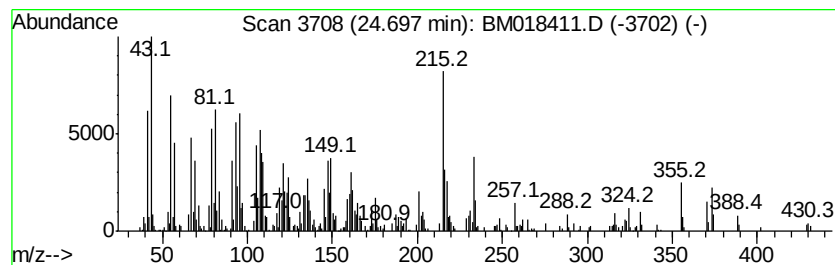
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cholestan-3.beta.-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.70	2.70 ng	1065630	Perylene-d12	23.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholestan-3.beta.-ol	388	C27H48O	017608-41-2	89
2		Cholestan-3-ol	388	C27H48O	027409-41-2	78
3		Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	64
4		Cholest-2-ene	370	C27H46	015910-23-3	58
5		Cholestanol	388	C27H48O	000080-97-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

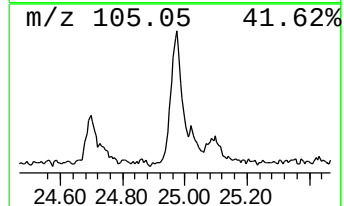
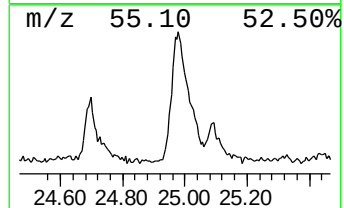
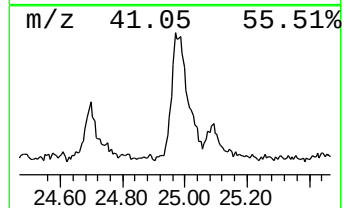
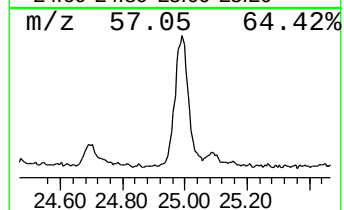
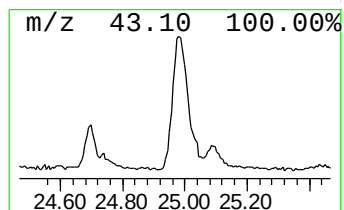
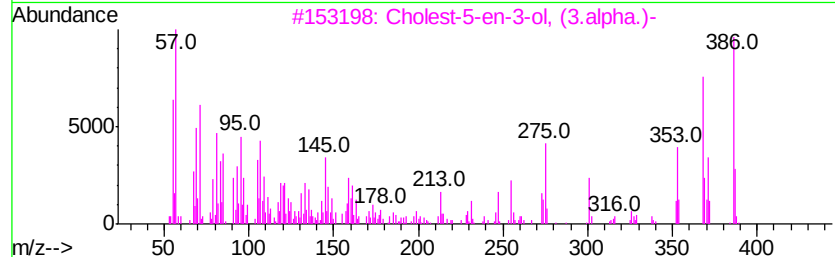
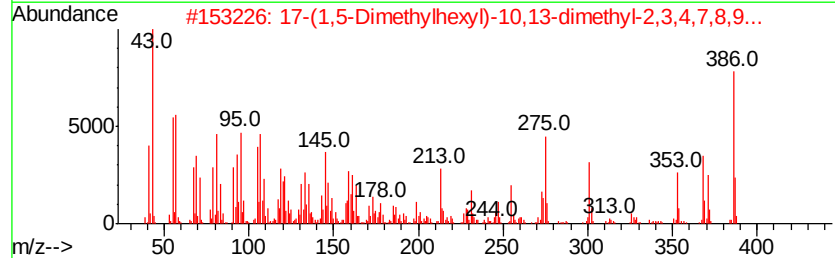
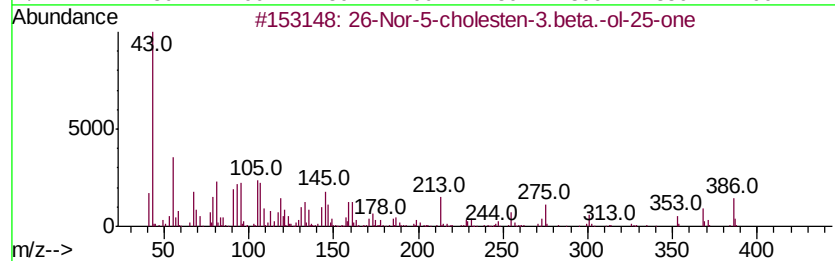
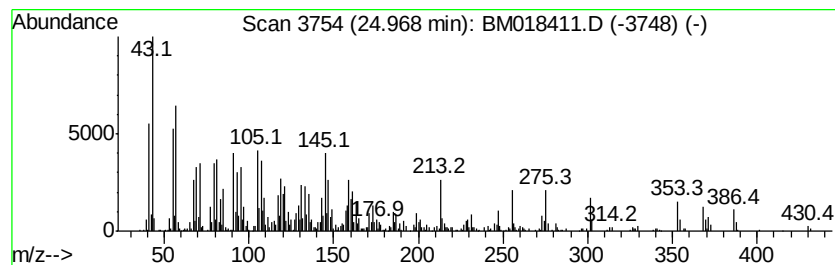
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 26-Nor-5-cholesten-3.beta.-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.97	7.00 ng	2763270	Perylene-d12	23.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	96
2		17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	90
3		Cholest-5-en-3-ol, (3.alpha.)-	386	C27H46O	000474-77-1	66
4		Cholesterol	386	C27H46O	000057-88-5	58
5		Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM122718\
Data File : BM018411.D
Acq On : 28 Dec 2018 00:04
Operator : JU/SJ
Sample : J6572-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
381204024-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-ol	3.05	2.1 ng		225811	1	7.78	2161810	20.0
unknown6.40	6.40	3.0 ng		323172	1	7.78	2161810	20.0
unknown10.86	10.86	3.2 ng		574622	2	10.57	3556700	20.0
7-Acetyl-6-ethyl-...	17.48	3.8 ng		1121600	4	17.17	5921370	20.0
n-Hexadecanoic acid	18.07	2.1 ng		612036	4	17.17	5921370	20.0
Cholestan-3.beta.-ol	24.70	2.7 ng		1065630	6	23.66	7898090	20.0
26-Nor-5-choleste...	24.97	7.0 ng		2763270	6	23.66	7898090	20.0