

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
 Data File : BM009905.D
 Acq On : 05 May 2017 16:47
 Operator : SJ/MA
 Sample : PB98666BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB98666BL

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:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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	4.304	201	207	218	rBV	969405	1387441	15.61%	3.231%
2	4.910	303	310	318	rBV	5453298	7450793	83.81%	17.350%
3	5.369	380	388	399	rBV	1413764	2118253	23.83%	4.933%
4	5.969	484	490	496	rVB	300799	444361	5.00%	1.035%
5	6.963	652	659	668	rBV	1462409	2281943	25.67%	5.314%
6	7.316	712	719	730	rVB	1323997	2121469	23.86%	4.940%
7	7.775	792	797	804	rVB	330390	518891	5.84%	1.208%
8	8.098	843	852	859	rBV	1374533	2228325	25.06%	5.189%
9	8.951	990	997	1006	rBV	1232873	2089212	23.50%	4.865%
10	10.575	1264	1273	1280	rBV	415080	685795	7.71%	1.597%
11	13.045	1686	1693	1701	rBV	2863086	4038171	45.42%	9.403%
12	14.433	1924	1929	1937	rVB3	609245	918820	10.33%	2.140%
13	15.933	2175	2184	2196	rBV	1860473	2594822	29.19%	6.042%
14	17.192	2392	2398	2404	rBV2	865889	1238189	13.93%	2.883%
15	18.062	2539	2546	2551	rBV3	88943	143786	1.62%	0.335%
16	19.345	2761	2764	2772	rBV5	71766	100267	1.13%	0.233%
17	19.815	2838	2844	2849	rBV	7561410	8890412	100.00%	20.702%
18	21.380	3105	3110	3115	rBV	1429874	1812808	20.39%	4.221%
19	23.680	3495	3501	3508	rVB	970916	1880060	21.15%	4.378%

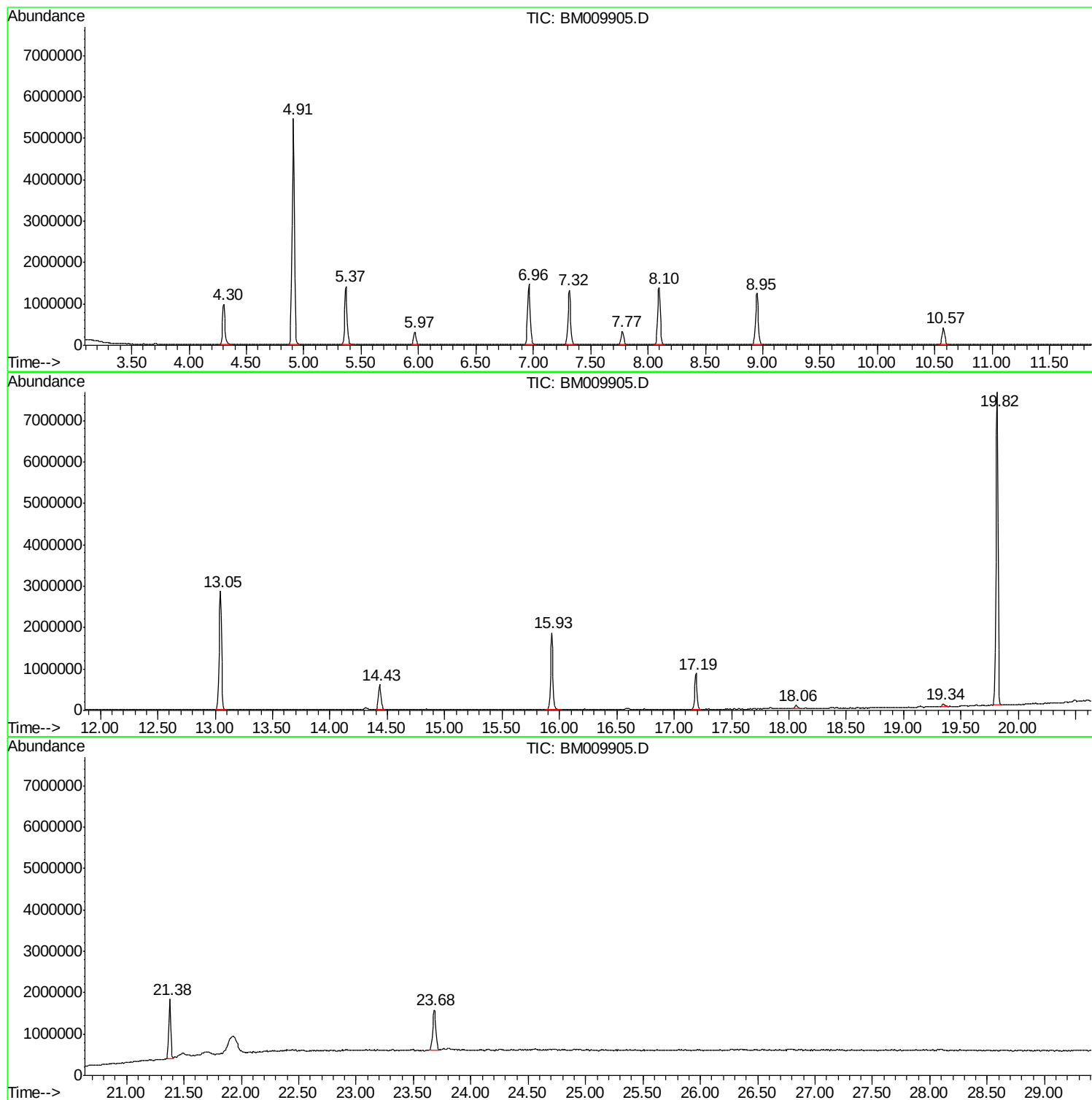
Sum of corrected areas: 42943818

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

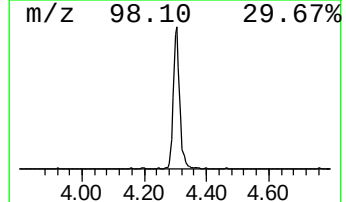
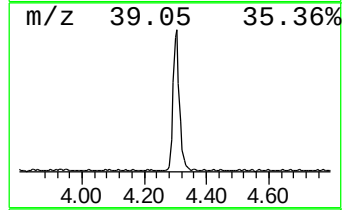
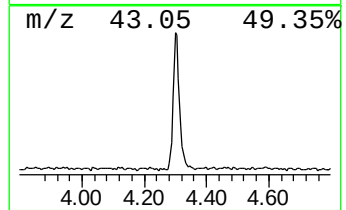
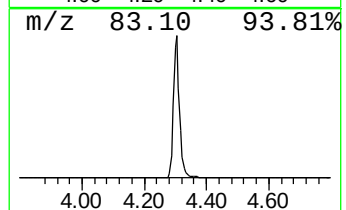
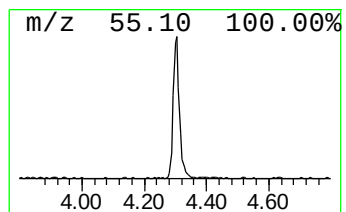
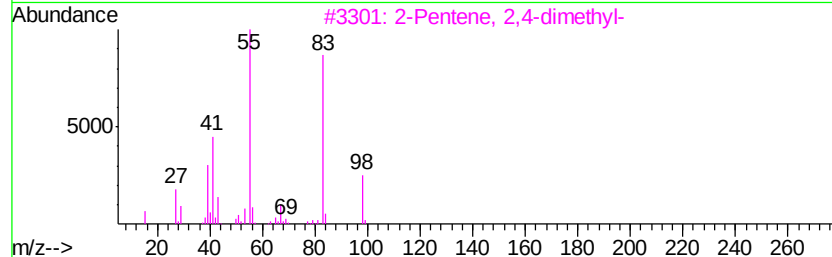
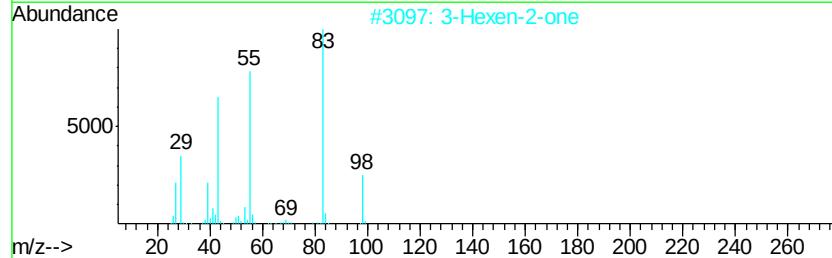
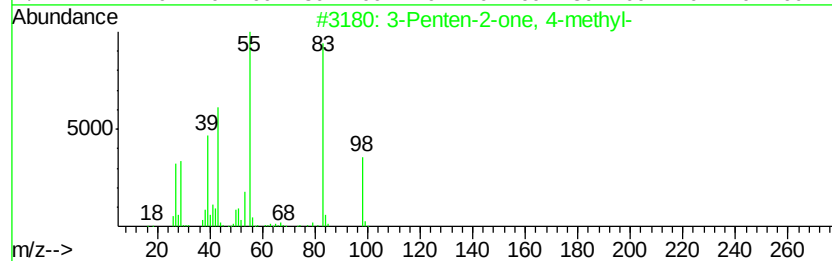
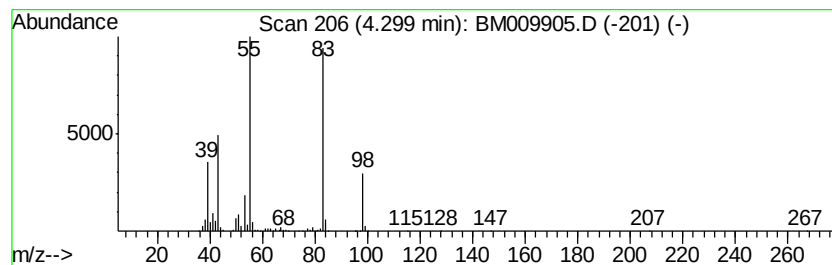
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	53.48 ng	1387440	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

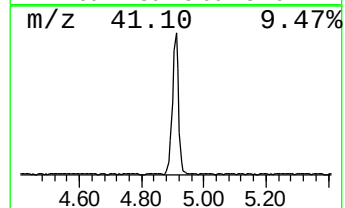
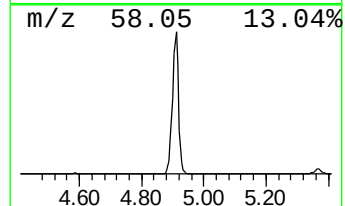
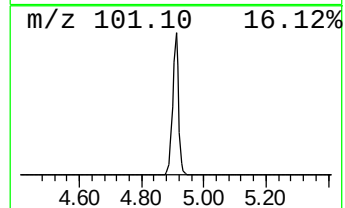
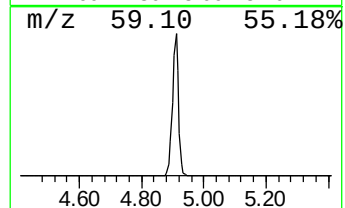
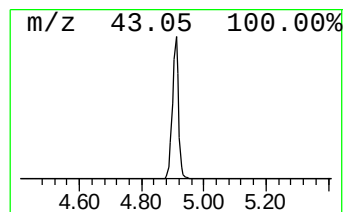
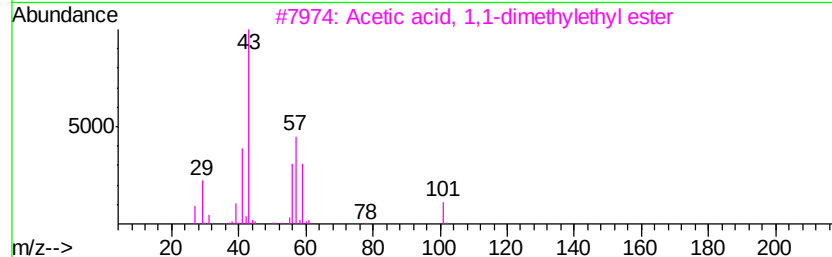
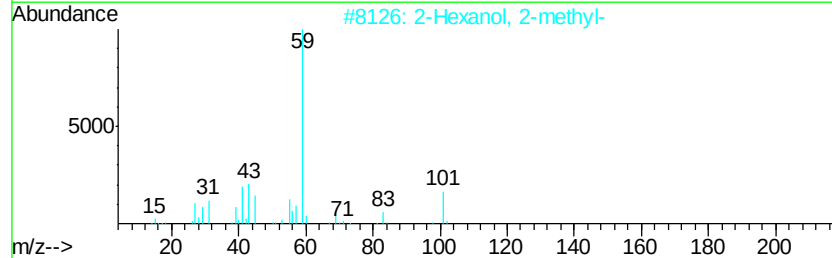
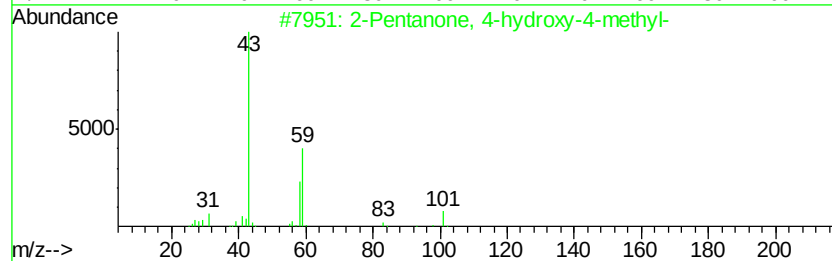
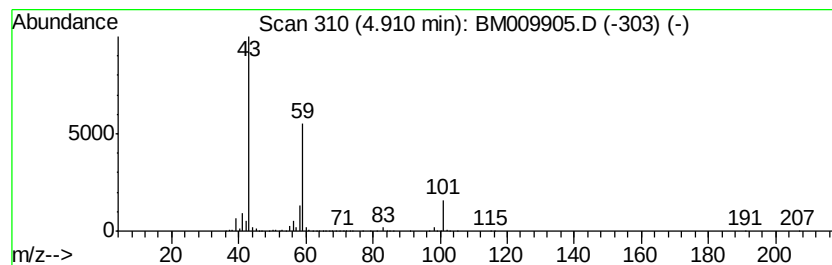
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	287.18 ng	7450790	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

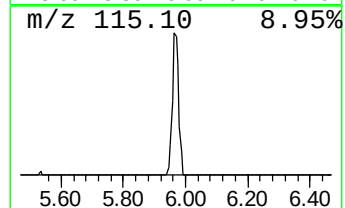
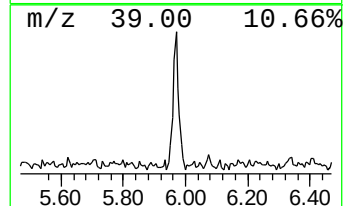
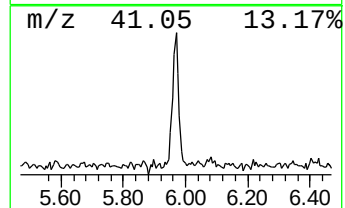
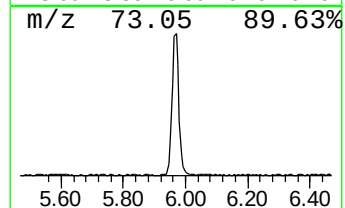
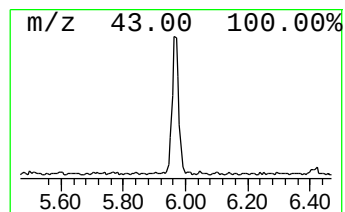
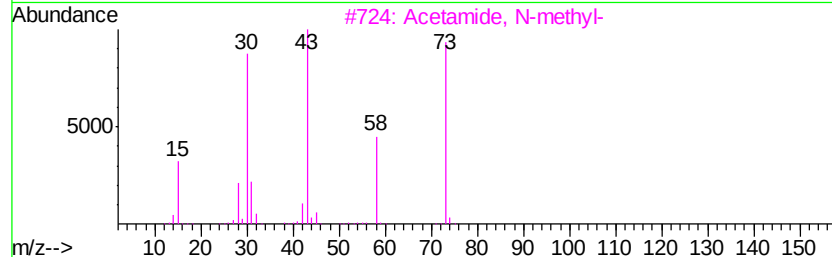
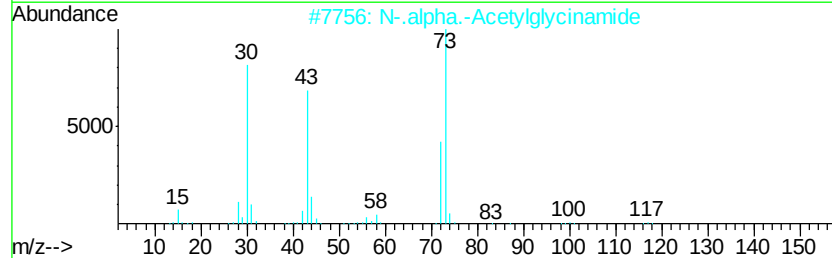
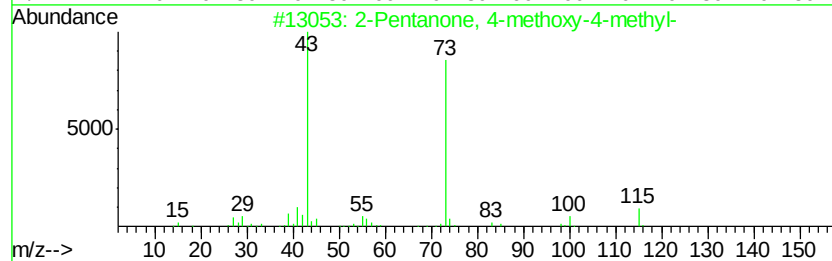
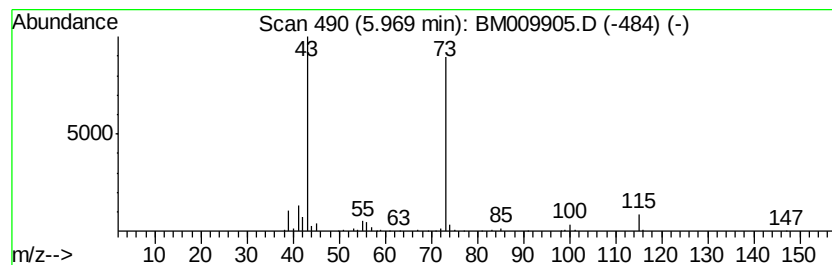
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	17.13 ng	444361	1,4-Dichlorobenzene-d4	7.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	47
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

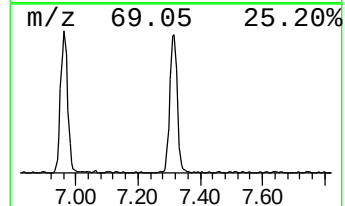
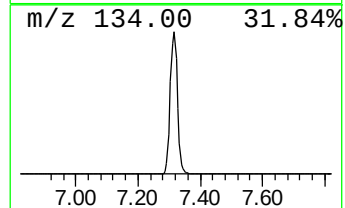
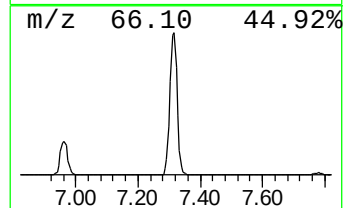
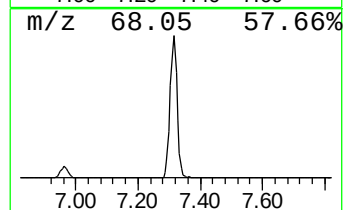
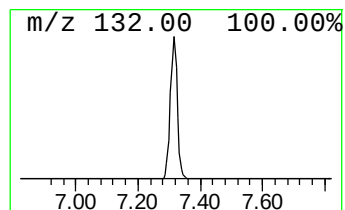
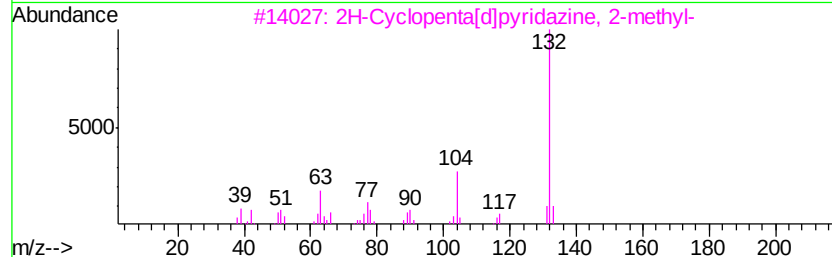
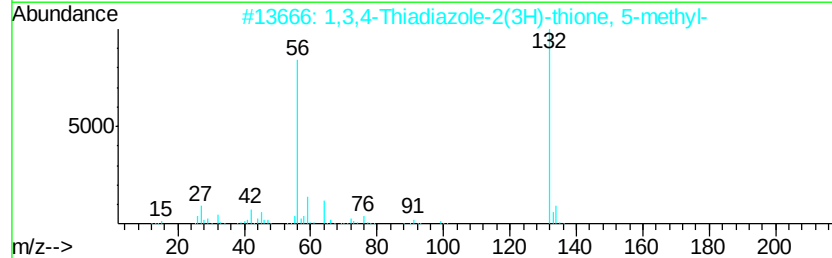
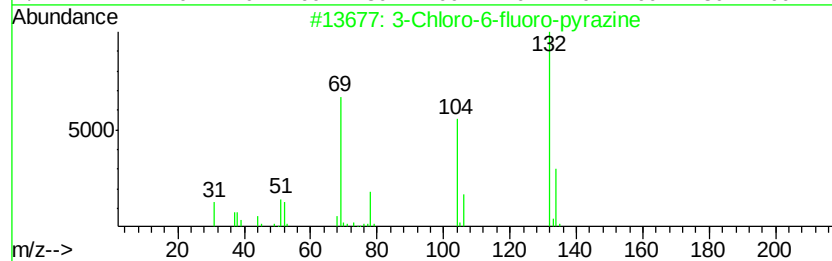
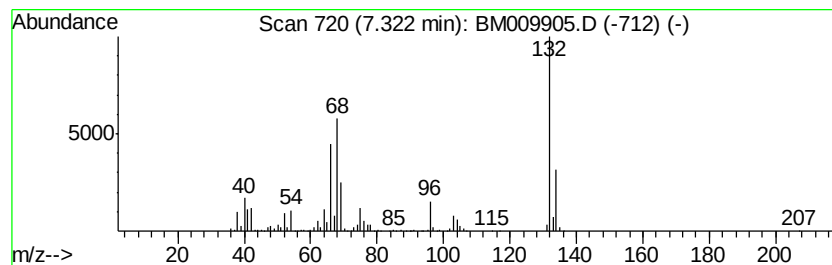
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.32 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	81.77 ng	2121470	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

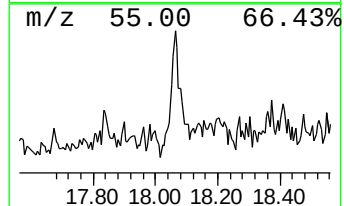
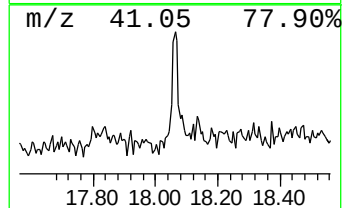
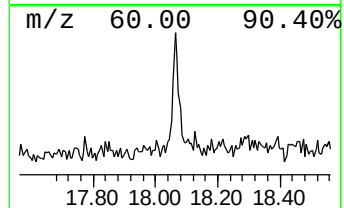
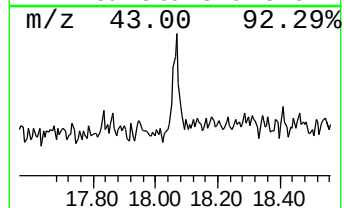
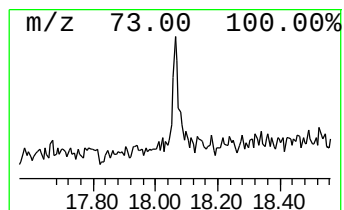
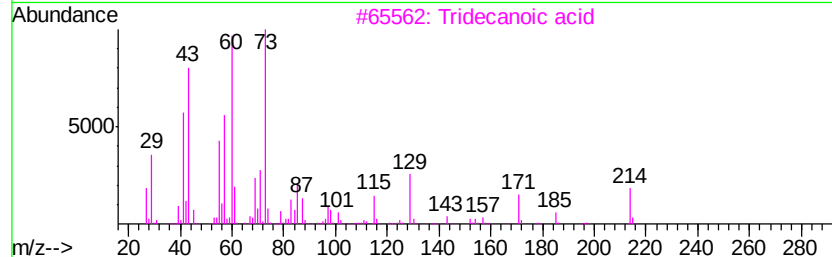
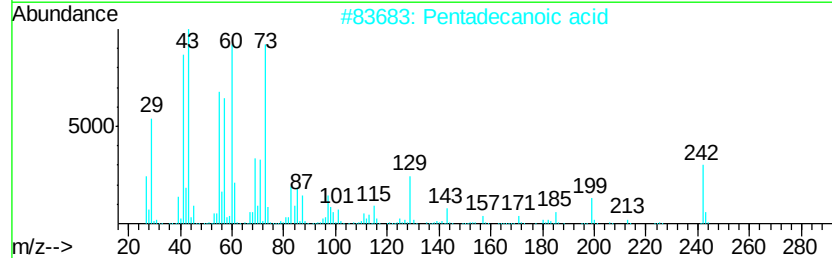
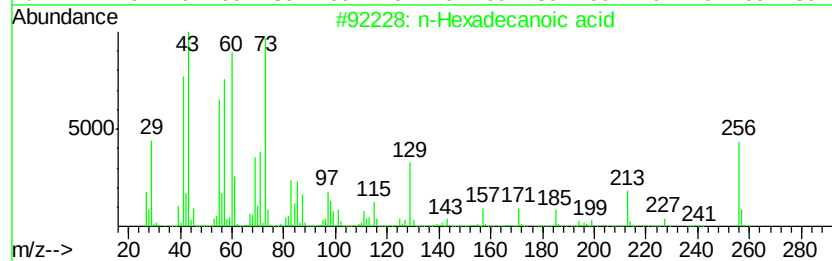
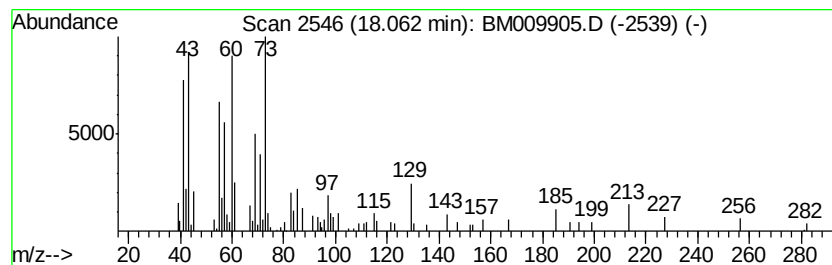
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	2.32 ng	143786	Phenanthrene-d10	17.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009905.D
Acq On : 05 May 2017 16:47
Operator : SJ/MA
Sample : PB98666BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB98666BL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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-one, 4...	4.30	53.5	ng	1387440	1	7.77	518891	20.0
2-Pentanone, 4-hy...	4.91	287.2	ng	7450790	1	7.77	518891	20.0
2-Pentanone, 4-me...	5.97	17.1	ng	444361	1	7.77	518891	20.0
unknown7.32	7.32	81.8	ng	2121470	1	7.77	518891	20.0
n-Hexadecanoic acid	18.06	2.3	ng	143786	4	17.19	1238190	20.0