

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
 Data File : BM033557.D
 Acq On : 21 Dec 2021 16:46
 Operator : CG/JU
 Sample : PB141506BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB141506BL

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-BM122121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.407	194	199	209	rBV	49467	70425	3.58%	0.663%
2	5.013	297	302	311	rBV	301860	438900	22.29%	4.134%
3	5.478	374	381	396	rBV	830232	1204822	61.18%	11.349%
4	6.095	481	486	492	rBV	24576	34463	1.75%	0.325%
5	7.084	646	654	667	rBV	784134	1268382	64.41%	11.948%
6	7.913	788	795	802	rBV	140510	224956	11.42%	2.119%
7	9.084	983	994	1007	rBV	492532	844018	42.86%	7.950%
8	10.725	1265	1273	1287	rBV	159649	293685	14.91%	2.766%
9	13.183	1684	1691	1703	rBV	1108086	1639058	83.23%	15.440%
10	14.560	1918	1925	1932	rBV	241167	361339	18.35%	3.404%
11	16.048	2172	2178	2193	rBV	857117	1229575	62.44%	11.582%
12	17.307	2386	2392	2405	rVB	265480	395853	20.10%	3.729%
13	19.924	2832	2837	2845	rBV	1570056	1969297	100.00%	18.550%
14	21.483	3097	3102	3107	rBV	258317	345583	17.55%	3.255%
15	23.877	3504	3509	3521	rVB2	136842	295559	15.01%	2.784%

Sum of corrected areas: 10615915

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033557.D
Acq On : 21 Dec 2021 16:46
Operator : CG/JU
Sample : PB141506BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB141506BL

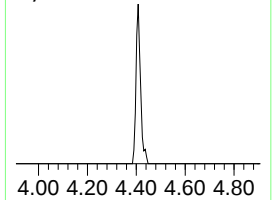
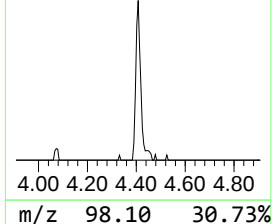
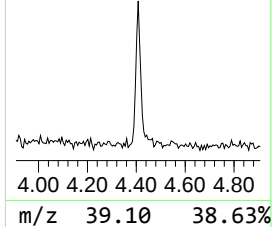
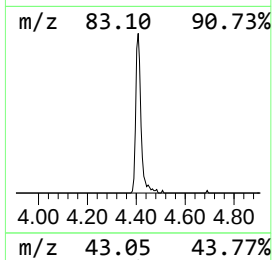
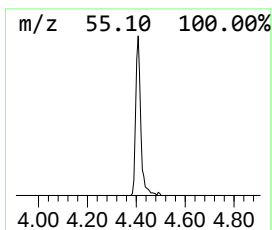
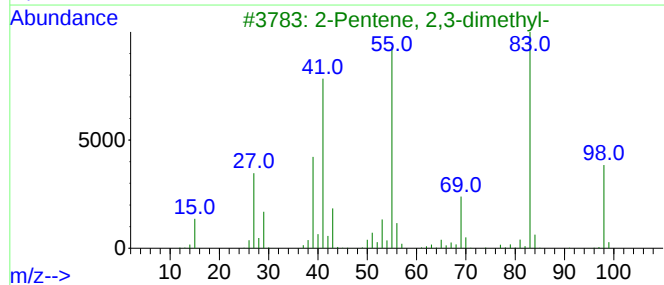
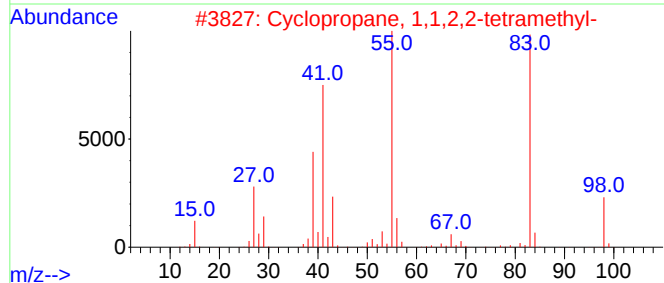
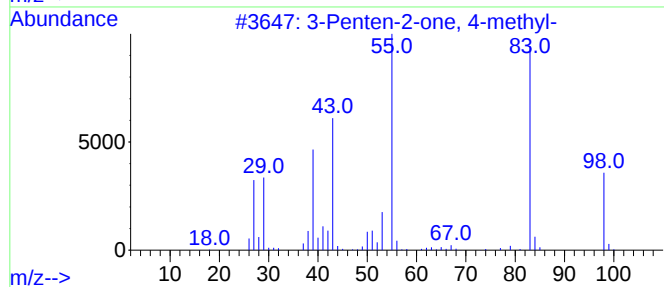
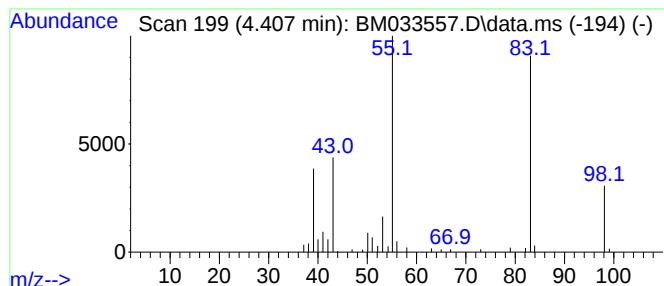
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.407	6.26 ng	70425	1,4-Dichlorobenzene-d4	7.913

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2		Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	64
3		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	64
4		3-Hexen-2-one	98	C6H10O	000763-93-9	62
5		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033557.D
Acq On : 21 Dec 2021 16:46
Operator : CG/JU
Sample : PB141506BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

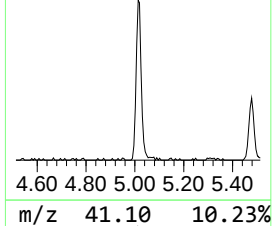
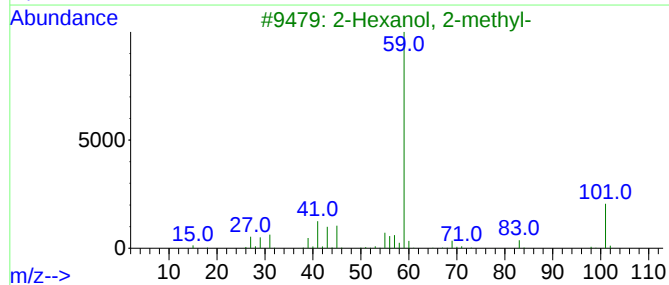
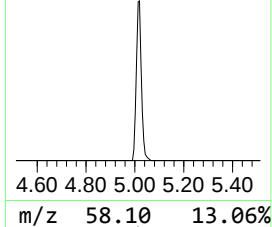
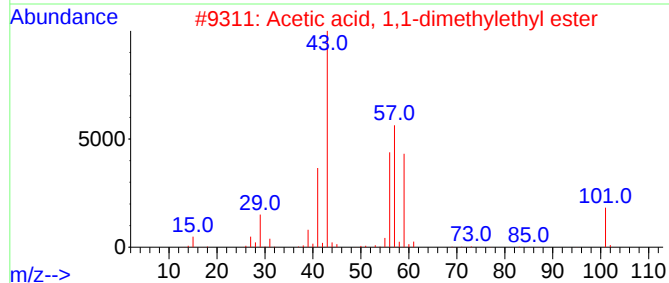
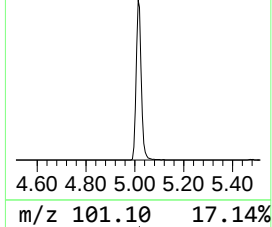
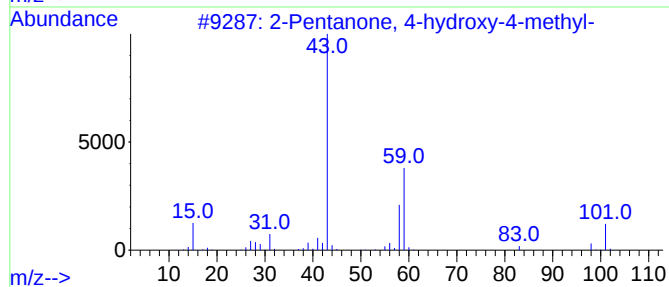
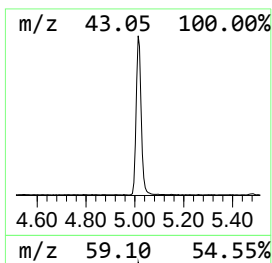
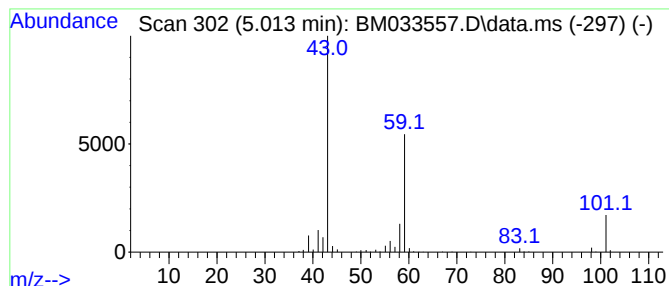
Instrument :
BNA_M
ClientSampleId :
PB141506BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
5.013	39.02 ng	438900	1,4-Dichlorobenzene-d4			7.913
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
4	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	23
5	1-Butene, 4-ethoxy-		100	C6H12O	044611-46-3	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033557.D
Acq On : 21 Dec 2021 16:46
Operator : CG/JU
Sample : PB141506BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB141506BL

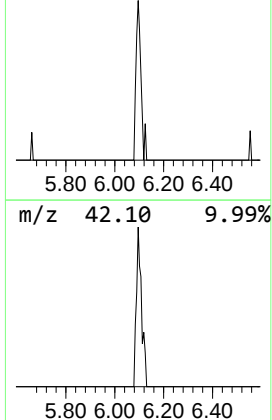
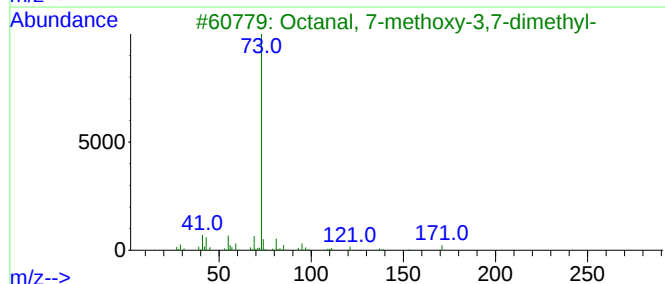
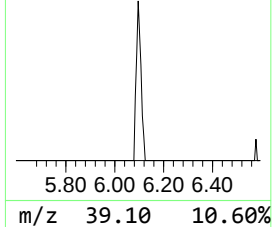
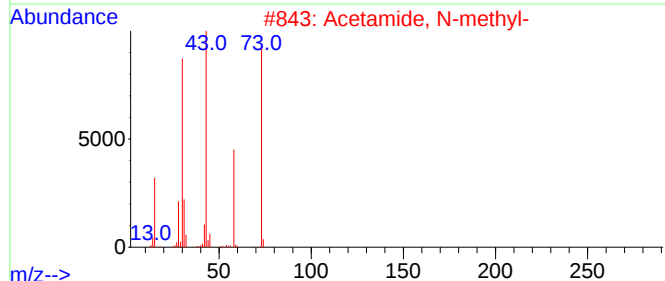
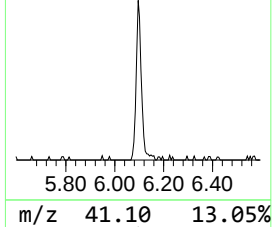
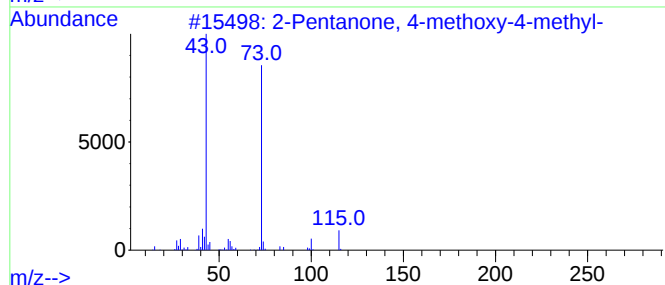
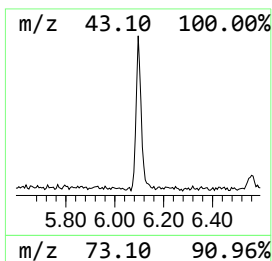
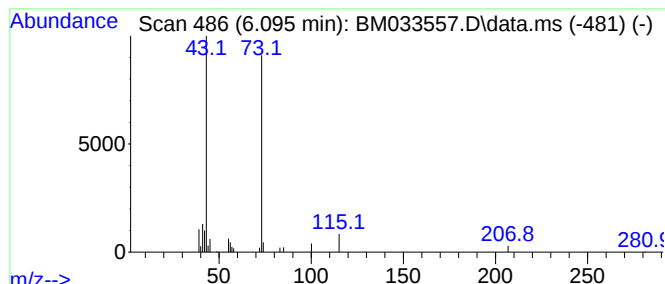
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.095	3.06 ng	34463	1,4-Dichlorobenzene-d4	7.913

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	53
3		Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	17
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033557.D
Acq On : 21 Dec 2021 16:46
Operator : CG/JU
Sample : PB141506BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB141506BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.407	6.3	ng	70425	1	7.913	224956	20.0
2-Pentanone, 4-...	5.013	39.0	ng	438900	1	7.913	224956	20.0
2-Pentanone, 4-...	6.095	3.1	ng	34463	1	7.913	224956	20.0