

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
 Data File : BF137747.D
 Acq On : 29 Apr 2024 10:44
 Operator : CG\JU
 Sample : PB160543BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB160543BL

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_F\Methods\8270-BF042324.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	9	13	22	rVB	768686	875587	8.62%	1.404%
2	4.740	447	451	455	rBV	873809	831539	8.19%	1.333%
3	5.334	544	552	555	rBV	4283624	6498796	64.00%	10.421%
4	5.698	609	614	617	rBV	5742654	5496694	54.13%	8.814%
5	6.087	676	680	683	rBV	405076	326585	3.22%	0.524%
6	6.675	774	780	782	rBV	4768675	5442337	53.60%	8.727%
7	7.063	842	846	849	rBV	2008143	1729614	17.03%	2.774%
8	7.622	935	941	944	rBV	4583481	5183225	51.05%	8.312%
9	8.345	1059	1064	1067	rBV	2489955	2348493	23.13%	3.766%
10	9.422	1241	1247	1250	rBV	9576705	9839995	96.91%	15.779%
11	10.104	1358	1363	1367	rBV	2878331	2734351	26.93%	4.385%
12	10.898	1492	1498	1501	rBV	4801225	4259843	41.95%	6.831%
13	11.604	1614	1618	1621	rBV	3188315	2755432	27.14%	4.419%
14	13.192	1883	1888	1891	rBV	9599218	10153977	100.00%	16.283%
15	14.251	2064	2068	2081	rBV	2539034	2160385	21.28%	3.464%
16	15.827	2330	2336	2346	rBV	1310468	1723172	16.97%	2.763%

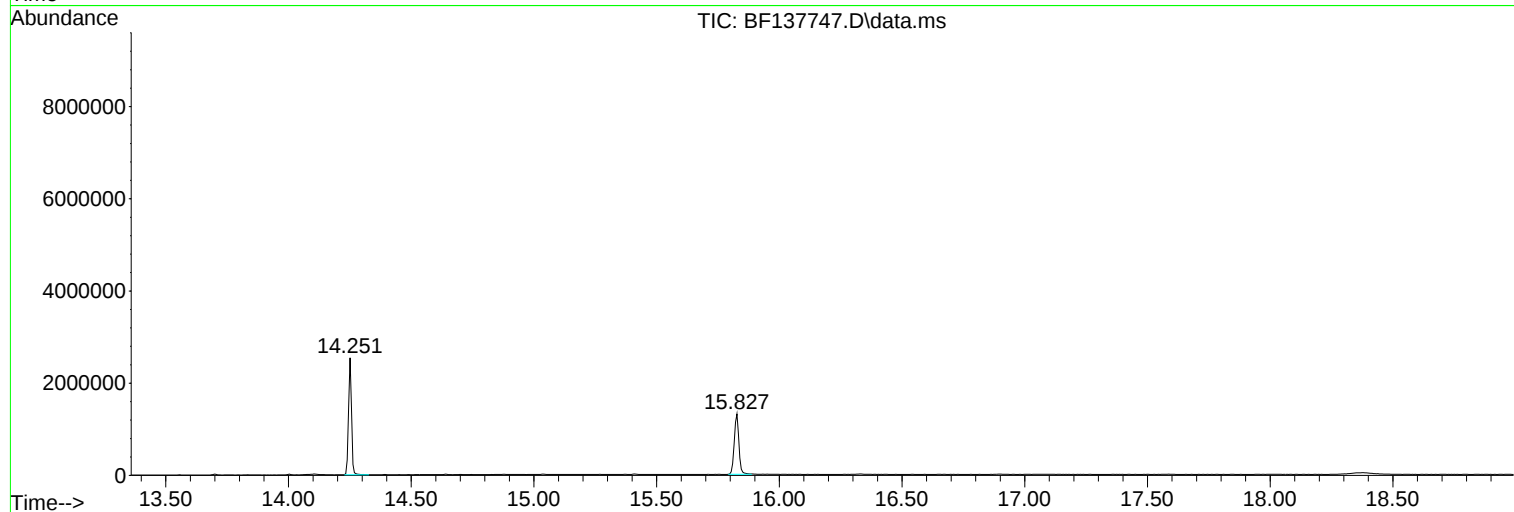
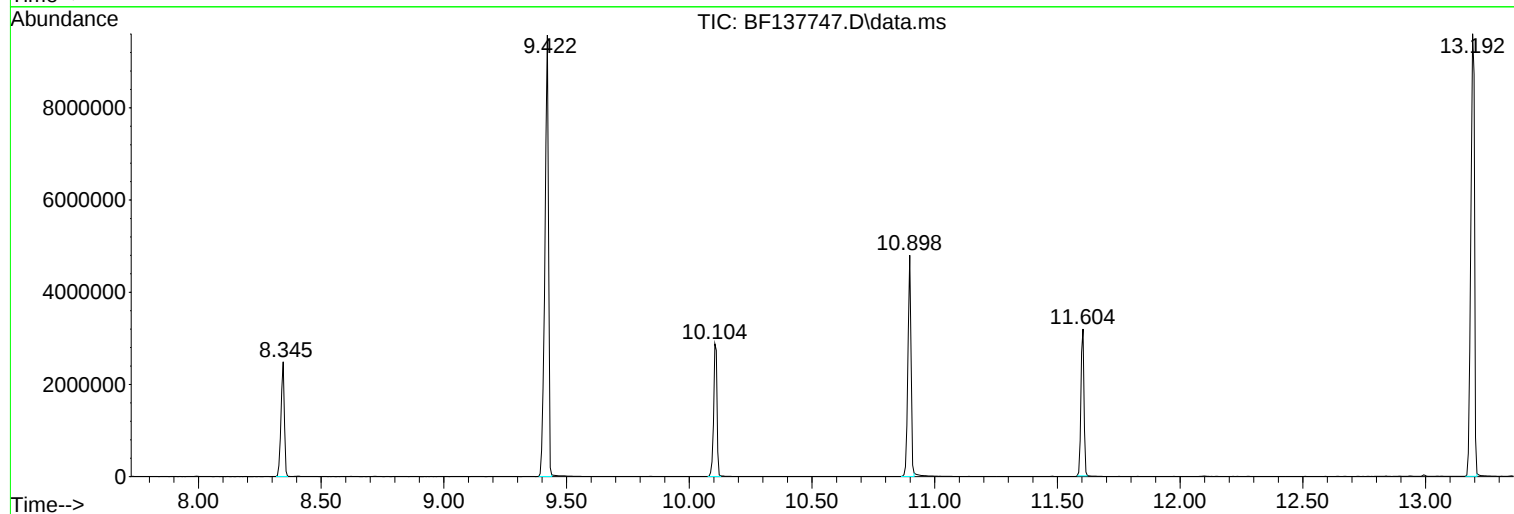
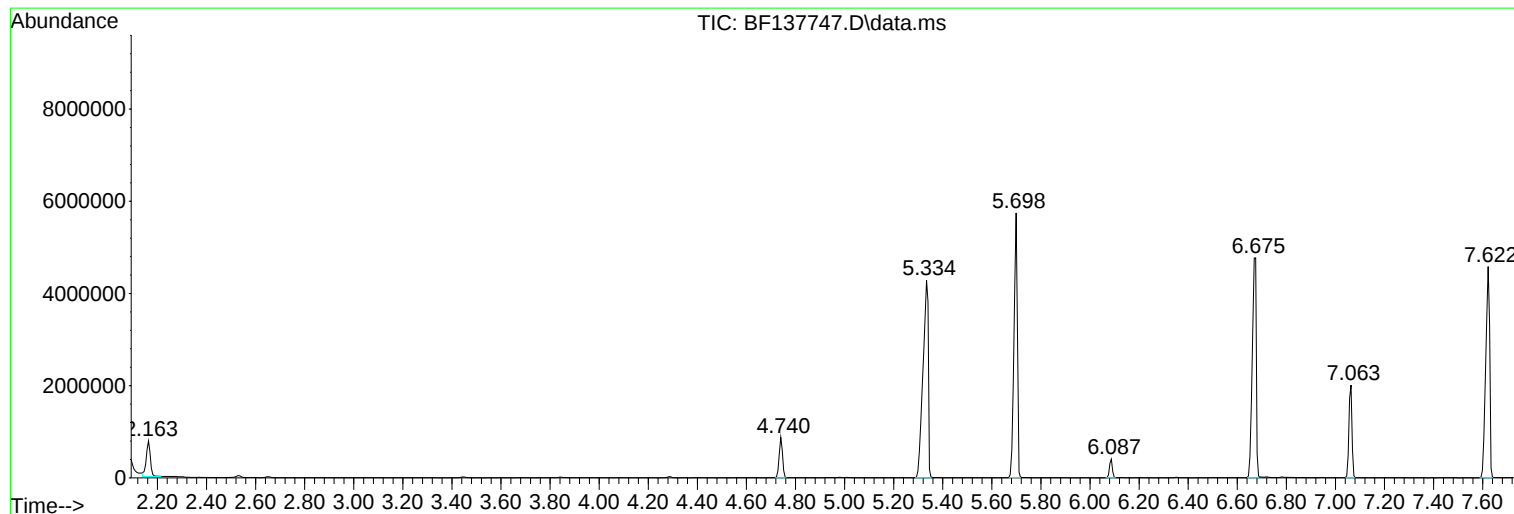
Sum of corrected areas: 62360025

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137747.D
Acq On : 29 Apr 2024 10:44
Operator : CG\JU
Sample : PB160543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB160543BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137747.D
Acq On : 29 Apr 2024 10:44
Operator : CG\JU
Sample : PB160543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB160543BL

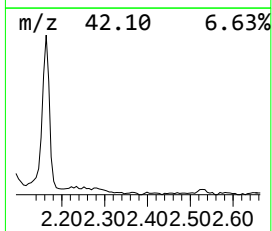
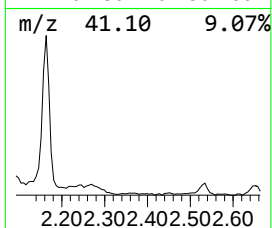
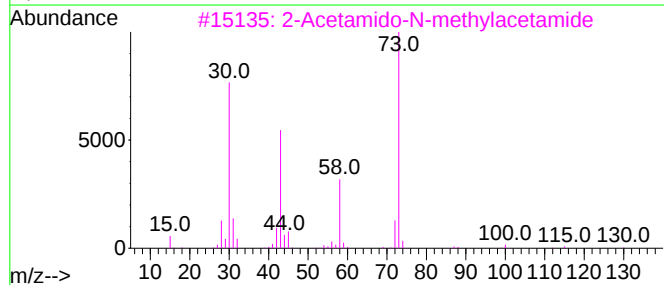
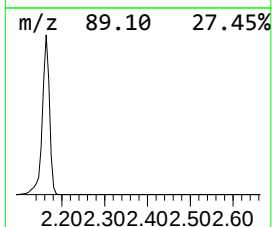
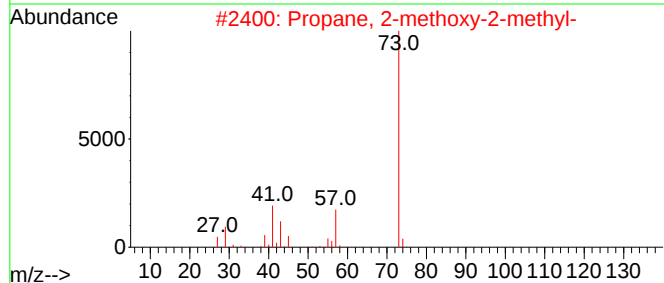
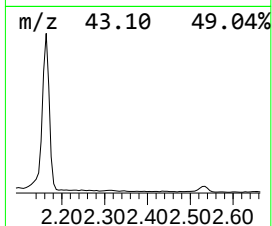
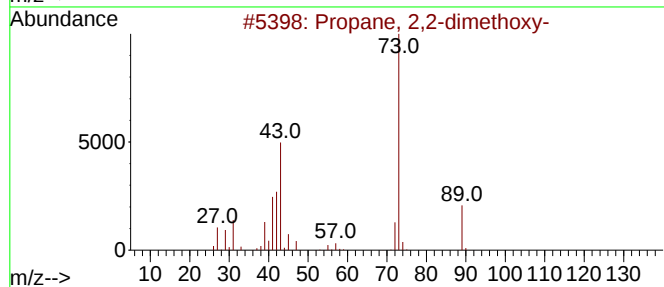
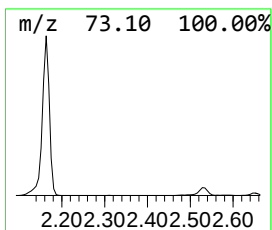
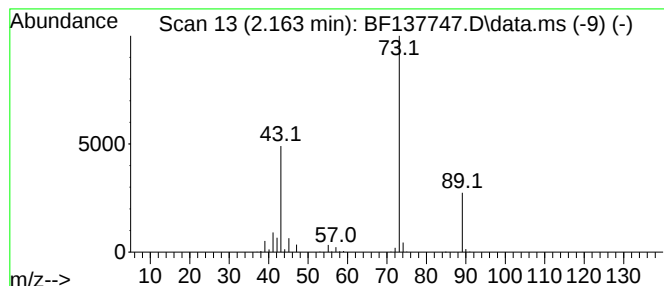
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	10.12 ng	875587	1,4-Dichlorobenzene-d4	7.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
4			1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	9
5			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137747.D
Acq On : 29 Apr 2024 10:44
Operator : CG\JU
Sample : PB160543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB160543BL

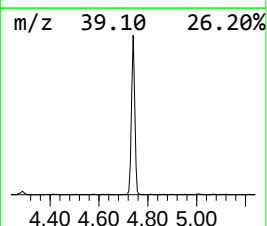
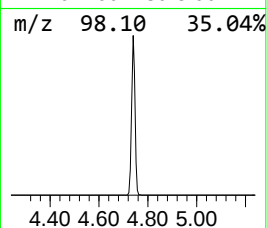
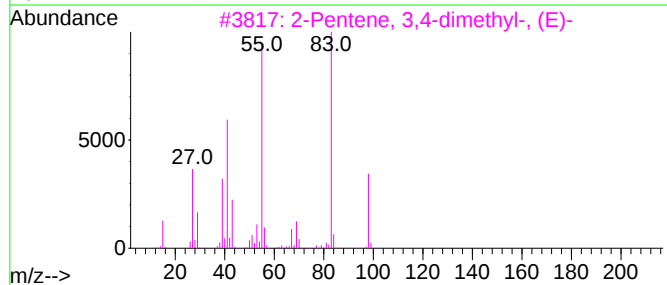
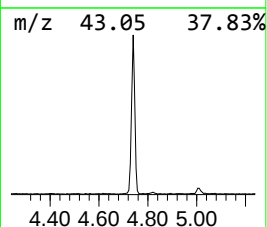
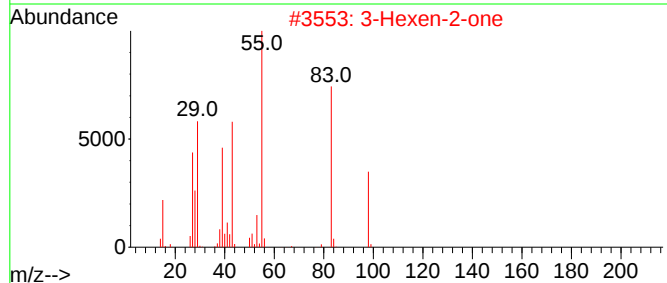
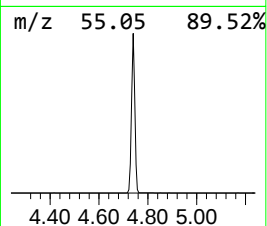
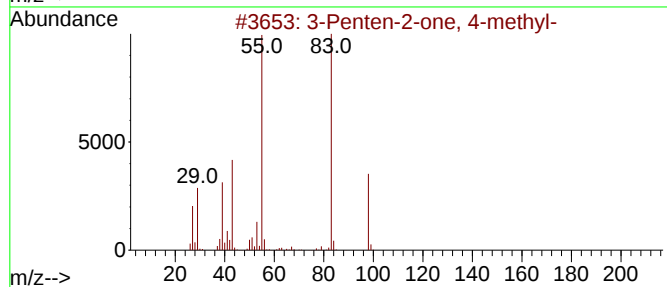
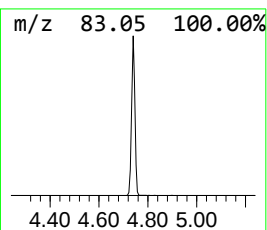
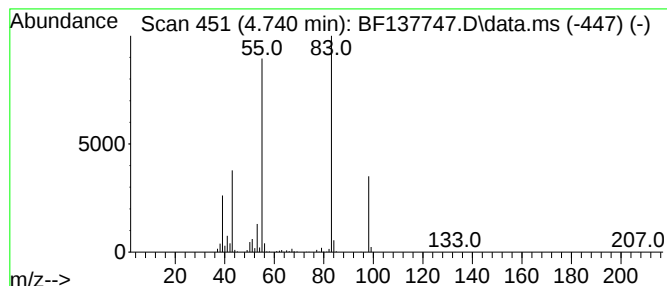
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.740	9.62 ng	831539	1,4-Dichlorobenzene-d4	7.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137747.D
Acq On : 29 Apr 2024 10:44
Operator : CG\JU
Sample : PB160543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB160543BL

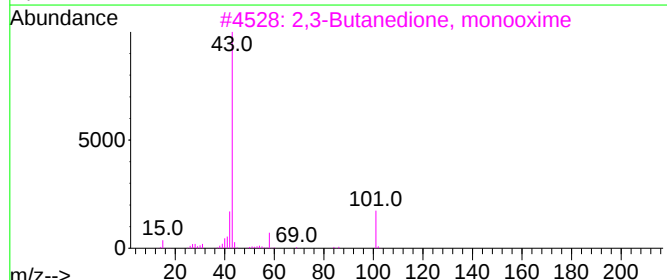
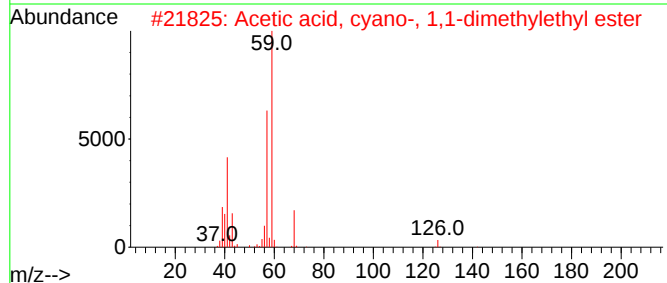
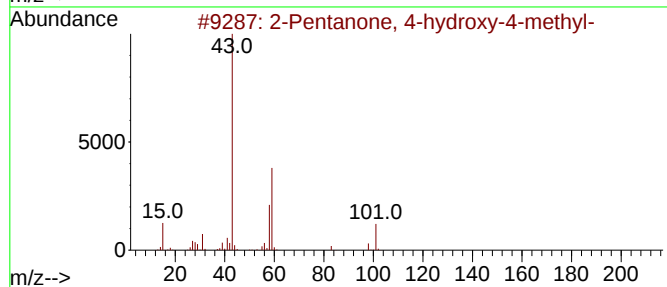
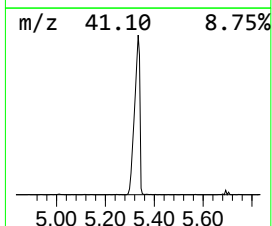
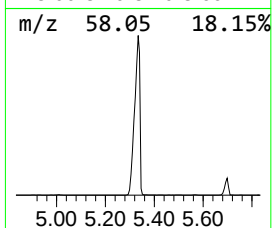
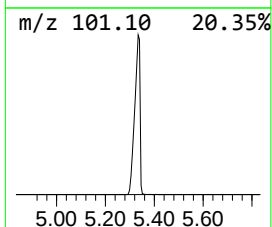
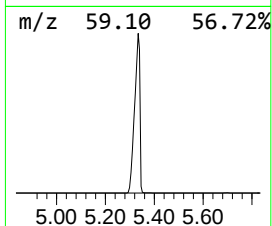
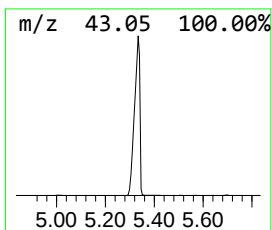
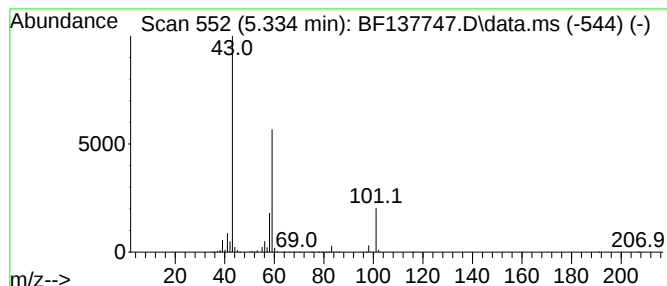
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.334	75.15 ng	6498800	1,4-Dichlorobenzene-d4	7.063

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137747.D
Acq On : 29 Apr 2024 10:44
Operator : CG\JU
Sample : PB160543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

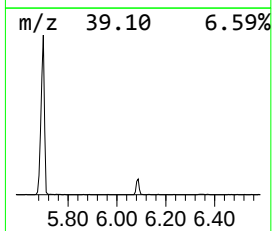
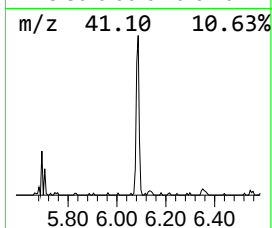
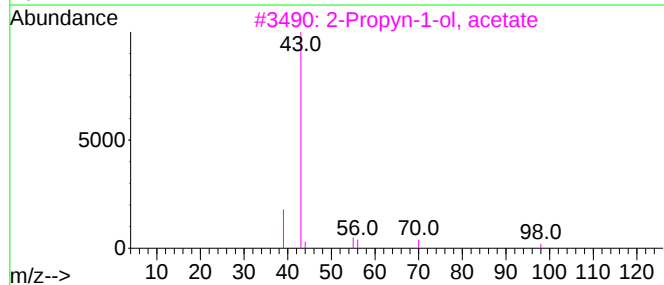
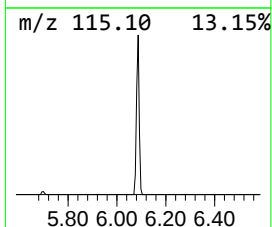
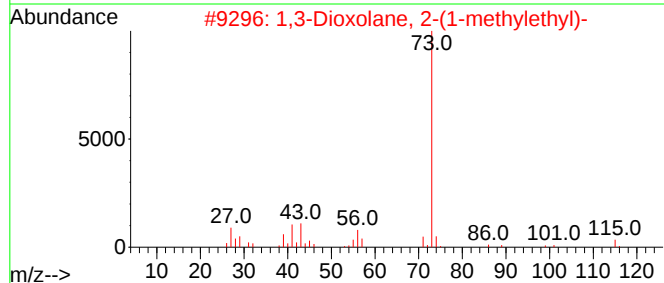
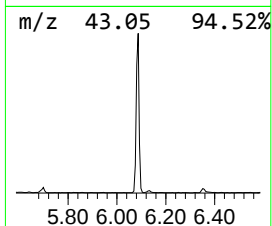
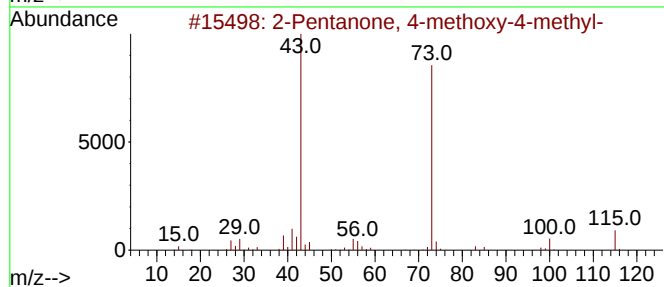
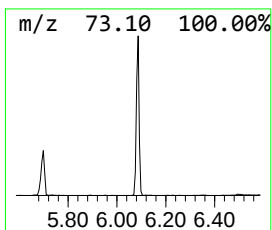
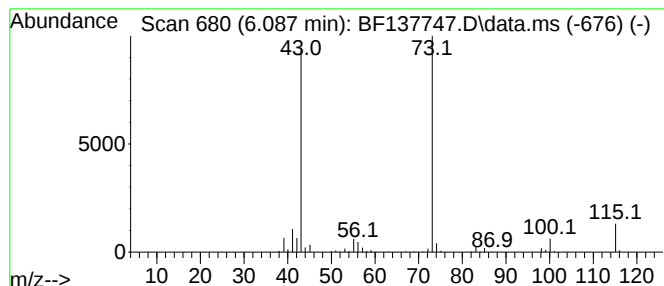
Instrument :
BNA_F
ClientSampleId :
PB160543BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
6.087	3.78 ng	326585	1,4-Dichlorobenzene-d4			7.063
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	83
2	1,3-Dioxolane, 2-(1-methylethyl)-		116	C6H12O2	000822-83-3	10
3	2-Propyn-1-ol, acetate		98	C5H6O2	000627-09-8	9
4	4-Penten-2-one, 4-methyl-		98	C6H10O	003744-02-3	9
5	Acetamide, N-butyl-		115	C6H13NO	001119-49-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137747.D
Acq On : 29 Apr 2024 10:44
Operator : CG\JU
Sample : PB160543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB160543BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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
Propane, 2,2-di...	2.163	10.1	ng	875587	1	7.063	1729610	20.0
3-Penten-2-one,...	4.740	9.6	ng	831539	1	7.063	1729610	20.0
2-Pentanone, 4-...	5.334	75.2	ng	6498800	1	7.063	1729610	20.0
2-Pentanone, 4-...	6.087	3.8	ng	326585	1	7.063	1729610	20.0