

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111722\
 Data File : BF131288.D
 Acq On : 17 Nov 2022 16:47
 Operator : CG\JU
 Sample : PB149128BL
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149128BL

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-BF111722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131288.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	31	40	46	rVB	60910	88720	2.68%	0.443%
2	4.593	422	426	431	rVB	148760	152307	4.60%	0.761%
3	5.204	524	530	541	rBV	630402	845370	25.54%	4.224%
4	5.587	589	595	598	rBV	2560703	2573676	77.75%	12.858%
5	6.581	758	764	767	rBV	2086651	2553018	77.13%	12.755%
6	6.969	826	830	833	rVB	639002	508424	15.36%	2.540%
7	7.534	920	926	929	rBV	1623765	1637361	49.46%	8.180%
8	8.257	1044	1049	1052	rBV	763829	671779	20.29%	3.356%
9	9.339	1227	1233	1236	rBV	3140234	3139412	94.84%	15.685%
10	10.022	1344	1349	1353	rBV	941994	803396	24.27%	4.014%
11	10.816	1479	1484	1487	rBV	2098940	1906687	57.60%	9.526%
12	11.522	1600	1604	1607	rBV	959388	836092	25.26%	4.177%
13	13.122	1871	1876	1879	rBV	3374996	3310223	100.00%	16.538%
14	14.174	2051	2055	2061	rBV	708453	583645	17.63%	2.916%
15	15.715	2311	2317	2322	rBV	320185	405666	12.25%	2.027%

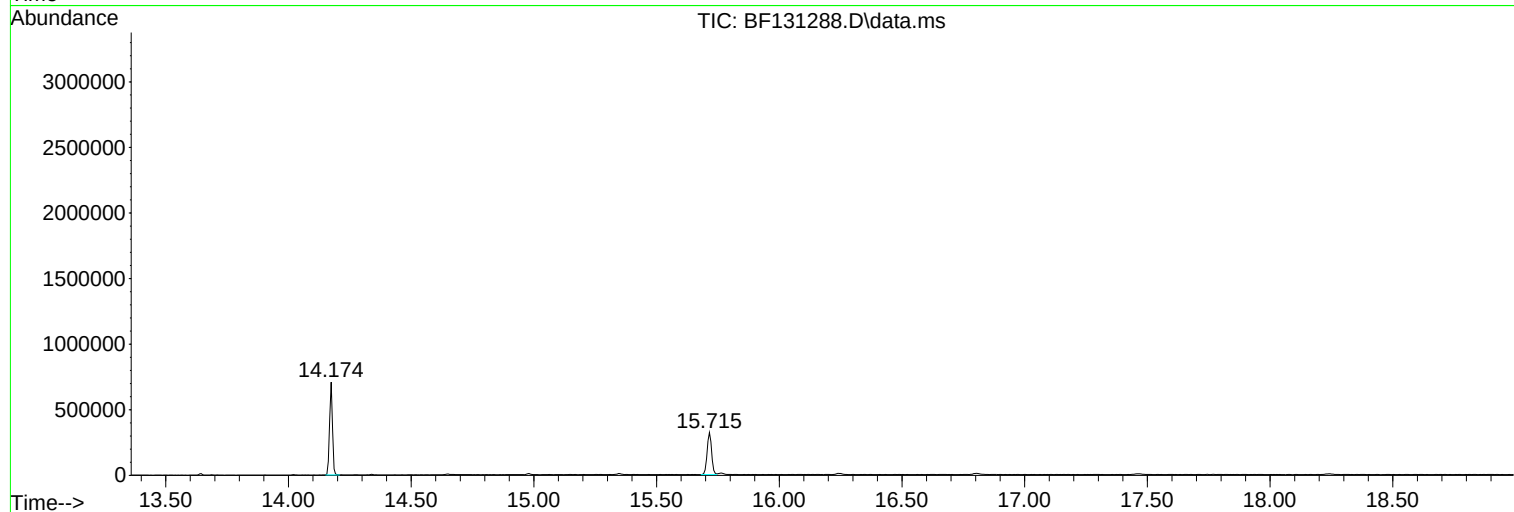
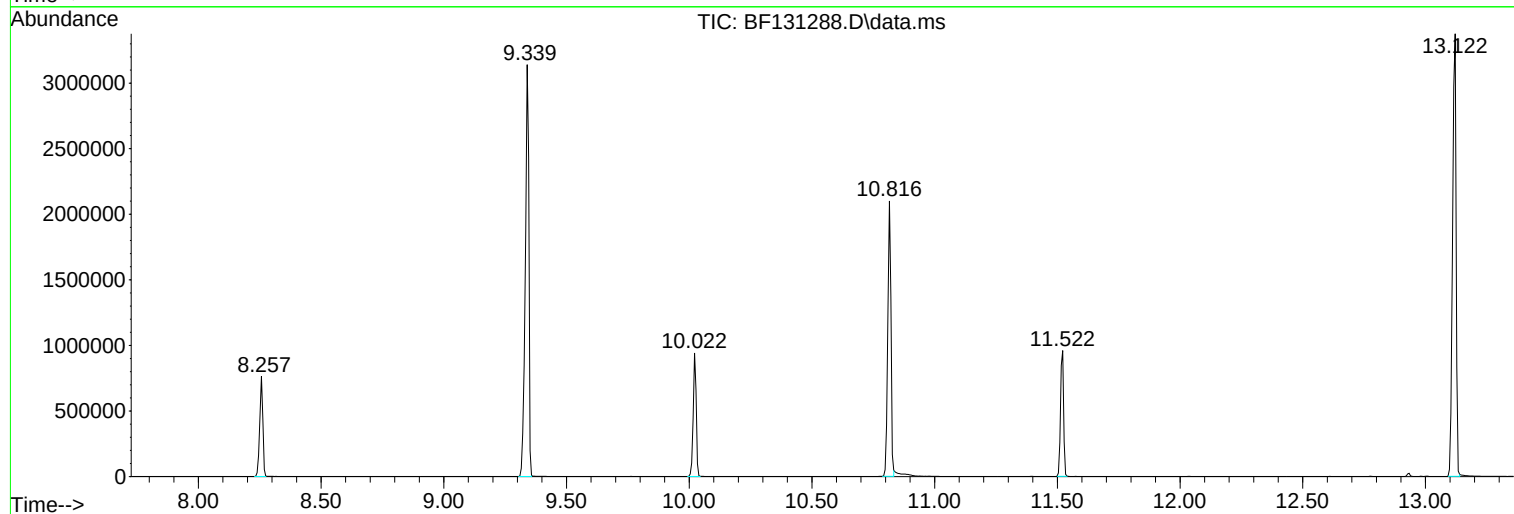
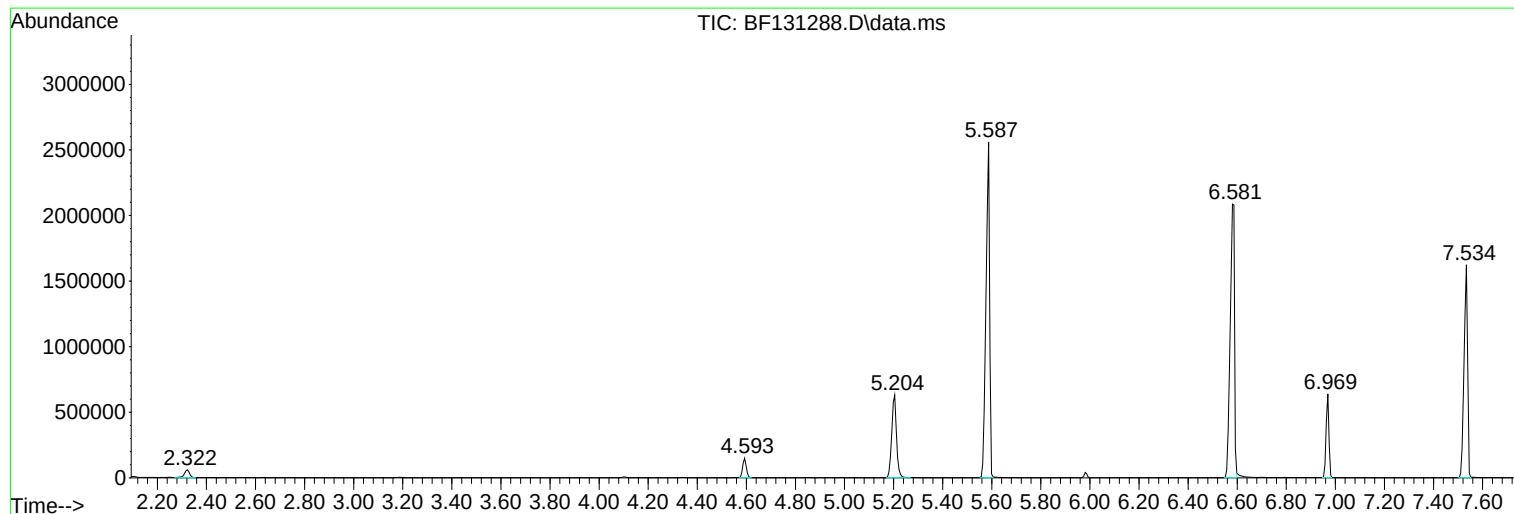
Sum of corrected areas: 20015776

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111722\
Data File : BF131288.D
Acq On : 17 Nov 2022 16:47
Operator : CG\JU
Sample : PB149128BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149128BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.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\BF111722\
Data File : BF131288.D
Acq On : 17 Nov 2022 16:47
Operator : CG\JU
Sample : PB149128BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149128BL

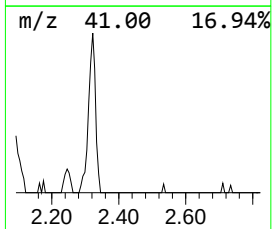
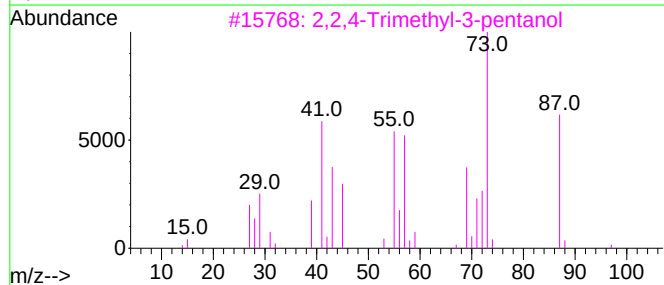
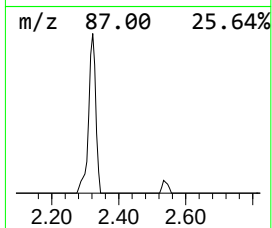
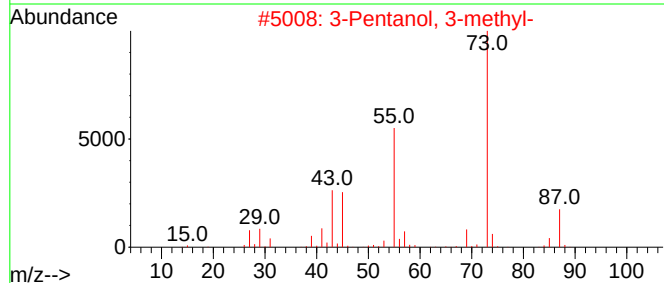
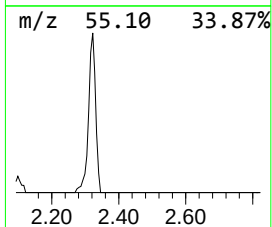
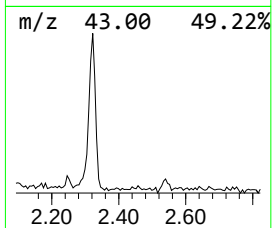
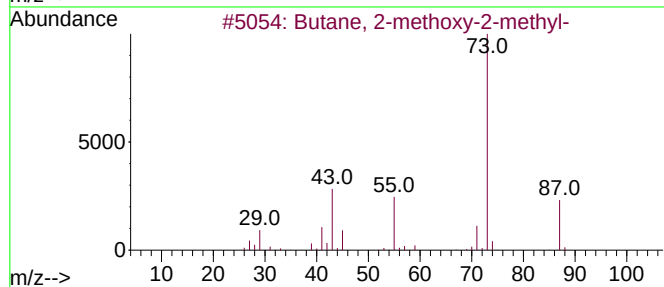
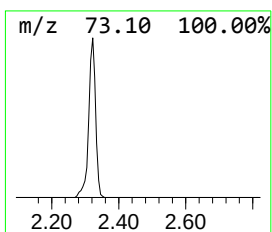
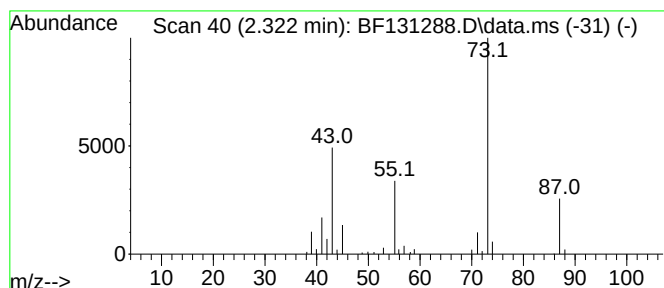
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	3.49 ng	88720	1,4-Dichlorobenzene-d4	6.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	45
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111722\
Data File : BF131288.D
Acq On : 17 Nov 2022 16:47
Operator : CG\JU
Sample : PB149128BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149128BL

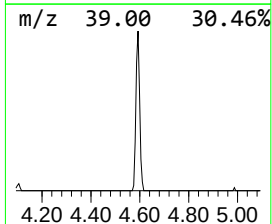
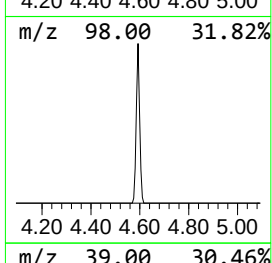
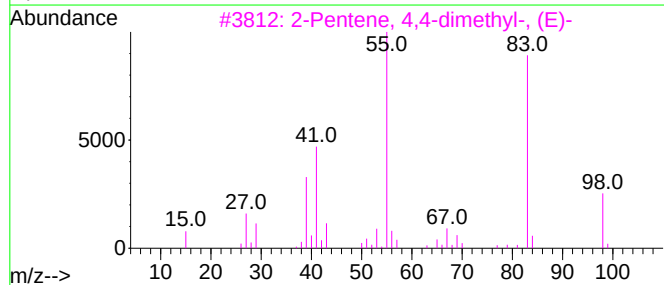
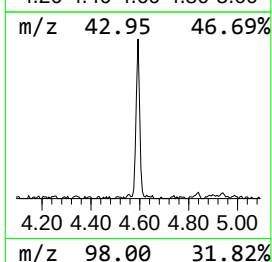
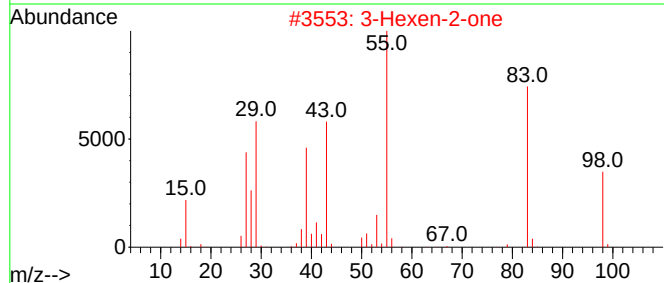
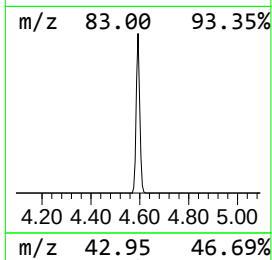
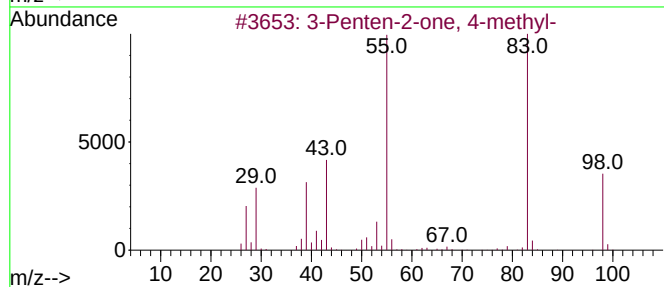
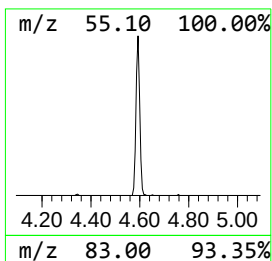
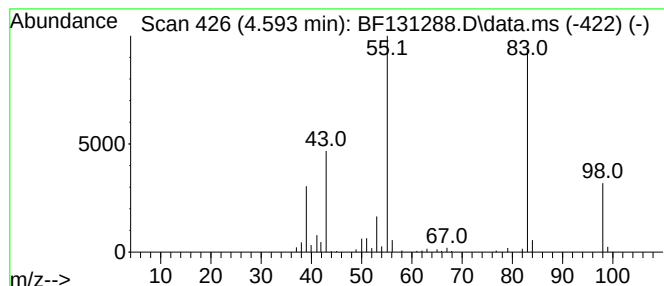
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.593	5.99 ng	152307	1,4-Dichlorobenzene-d4	6.969

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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111722\
Data File : BF131288.D
Acq On : 17 Nov 2022 16:47
Operator : CG\JU
Sample : PB149128BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149128BL

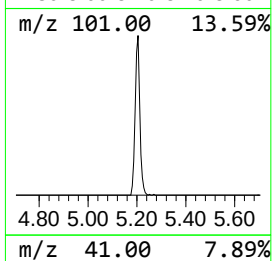
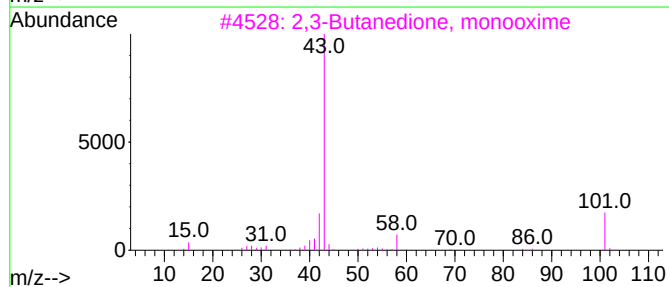
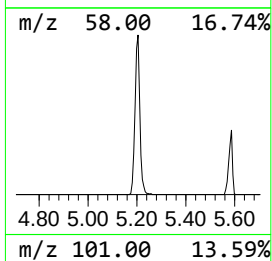
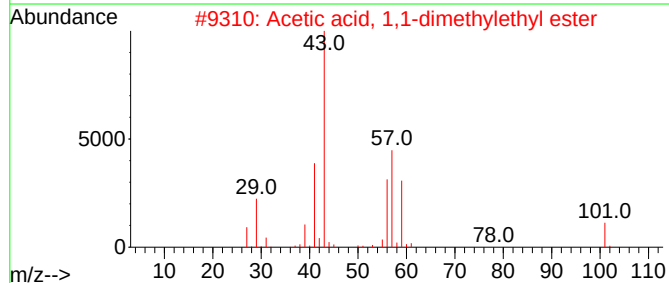
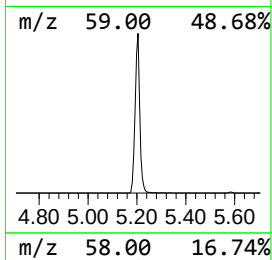
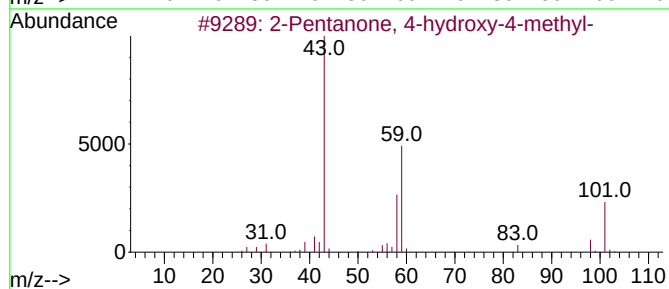
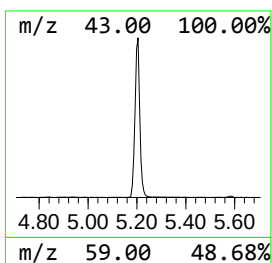
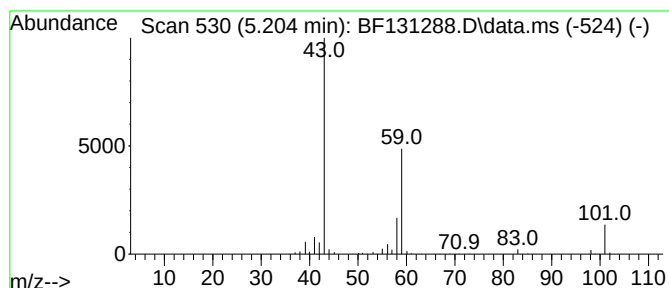
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.204	33.25 ng	845370	1,4-Dichlorobenzene-d4	6.969

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	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Acetone	58	C3H6O	000067-64-1	12
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111722\
Data File : BF131288.D
Acq On : 17 Nov 2022 16:47
Operator : CG\JU
Sample : PB149128BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149128BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.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
Butane, 2-metho...	2.322	3.5	ng	88720	1	6.969	508424	20.0
3-Penten-2-one,...	4.593	6.0	ng	152307	1	6.969	508424	20.0
2-Pentanone, 4-...	5.204	33.3	ng	845370	1	6.969	508424	20.0