

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
 Data File : BF130885.D
 Acq On : 31 Oct 2022 18:15
 Operator : CG\JU
 Sample : N5355-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 5518-1

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-BF102722.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	19	rVV	57882	66798	2.59%	0.451%
2	2.246	20	27	35	rVB	1233967	1549931	60.14%	10.467%
3	2.369	43	48	55	rBV	36882	46851	1.82%	0.316%
4	5.163	518	523	530	rVB	103961	119033	4.62%	0.804%
5	5.551	585	589	593	rBV	1186030	1094210	42.46%	7.390%
6	6.551	755	759	763	rBV	759169	697674	27.07%	4.712%
7	6.939	821	825	829	rBV	589772	470639	18.26%	3.178%
8	7.504	916	921	924	rBV	1555151	1535411	59.58%	10.369%
9	8.128	1023	1027	1040	rBV	143361	258180	10.02%	1.744%
10	8.228	1040	1044	1047	rVB	709290	574430	22.29%	3.879%
11	9.304	1222	1227	1230	rBV	2928282	2577228	100.00%	17.405%
12	9.986	1339	1343	1347	rVB	740736	588618	22.84%	3.975%
13	10.780	1474	1478	1481	rBV	1607306	1394249	54.10%	9.416%
14	11.480	1593	1597	1600	rBV	653202	517738	20.09%	3.497%
15	11.763	1639	1645	1656	rBV7	14023	36564	1.42%	0.247%
16	11.863	1658	1662	1666	rVB	48333	43313	1.68%	0.293%
17	11.998	1682	1685	1688	rBV	35573	32601	1.26%	0.220%
18	12.580	1776	1784	1794	rBV6	18460	47173	1.83%	0.319%
19	12.680	1796	1801	1810	rVV3	13779	29667	1.15%	0.200%
20	13.074	1863	1868	1871	rBV	2041427	1940581	75.30%	13.106%
21	14.021	2024	2029	2039	rBV2	83448	222905	8.65%	1.505%
22	14.127	2043	2047	2050	rVV	515381	429753	16.68%	2.902%
23	14.221	2058	2063	2067	rBV	106306	116723	4.53%	0.788%
24	14.992	2191	2194	2199	rVB	39937	38021	1.48%	0.257%
25	15.645	2300	2305	2310	rBV2	290392	378868	14.70%	2.559%

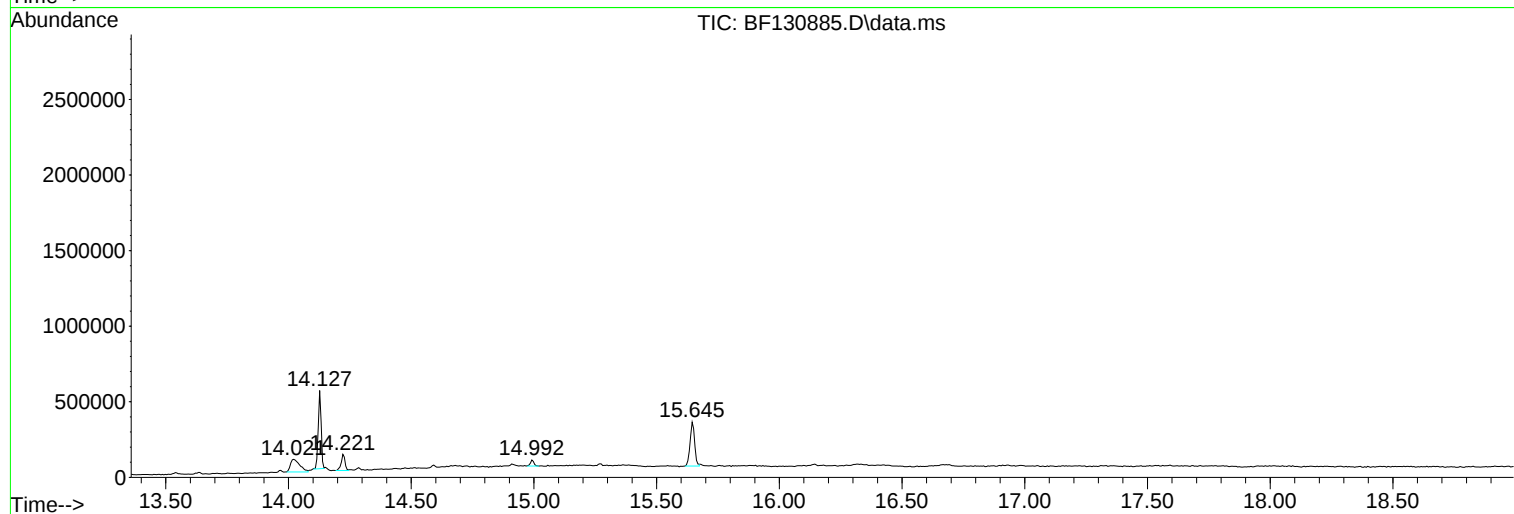
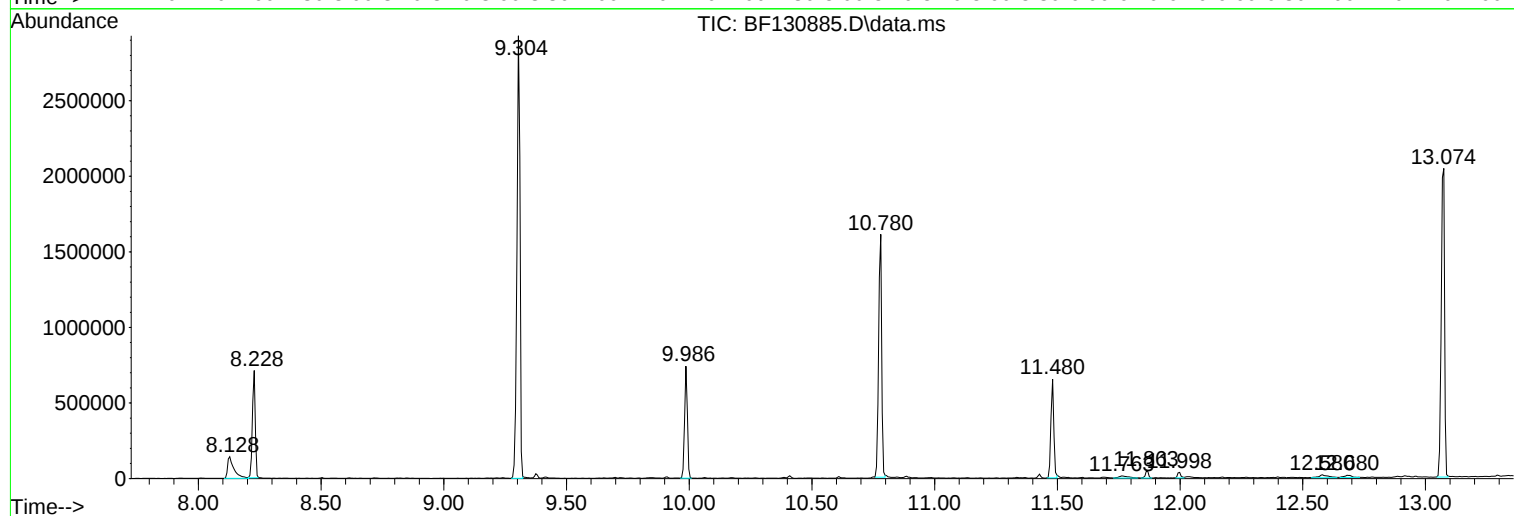
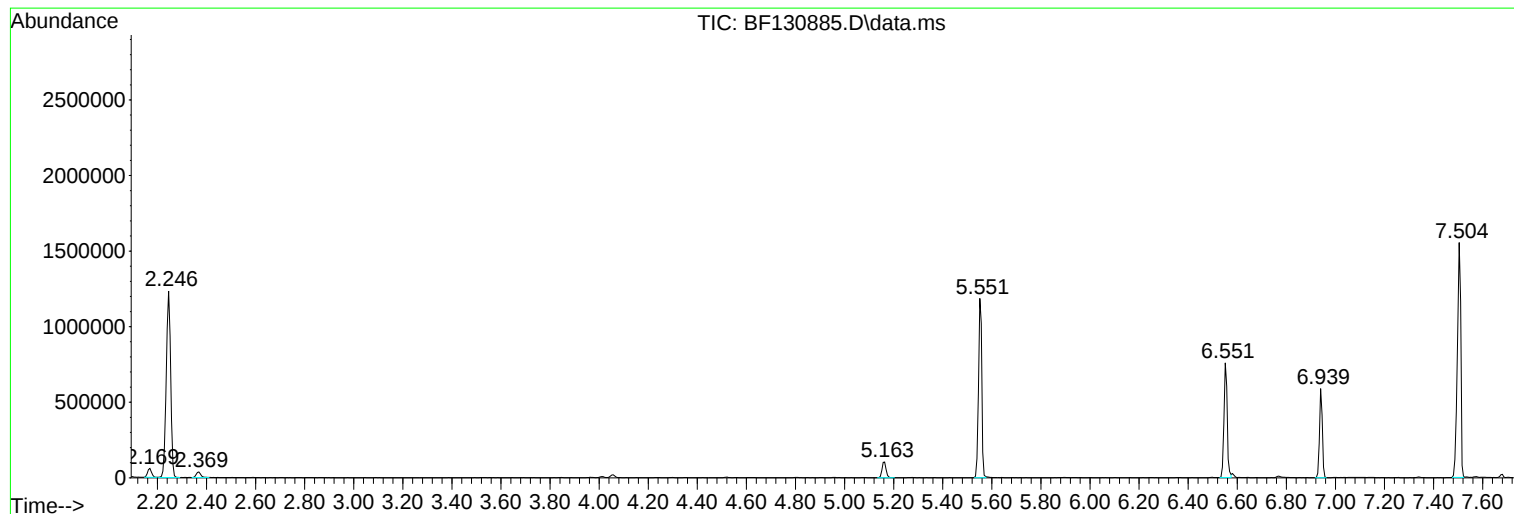
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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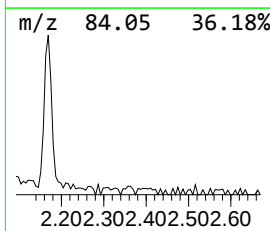
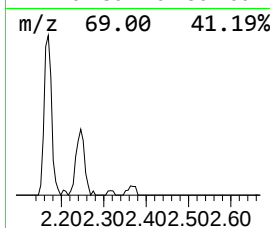
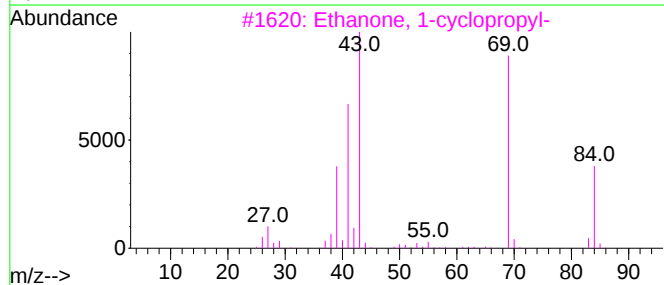
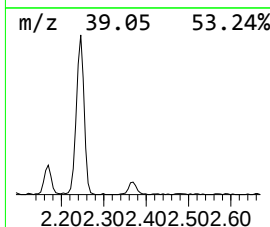
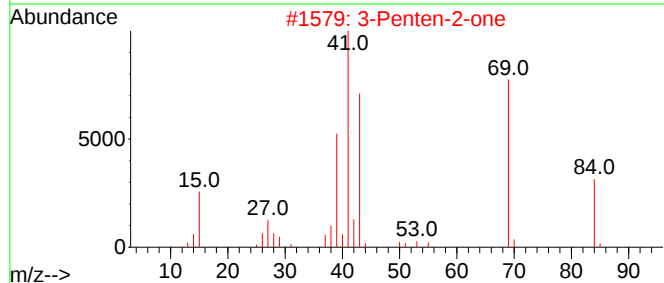
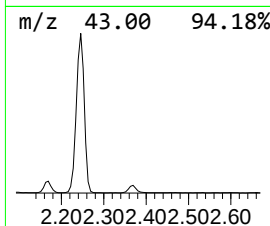
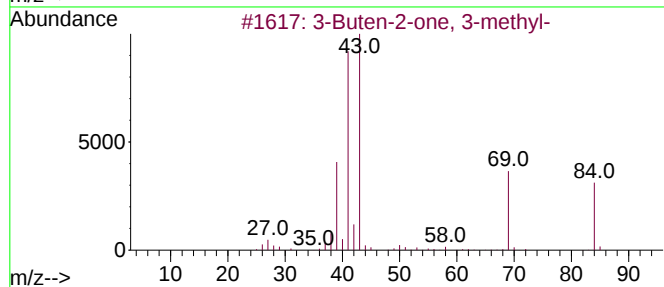
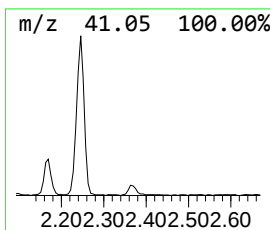
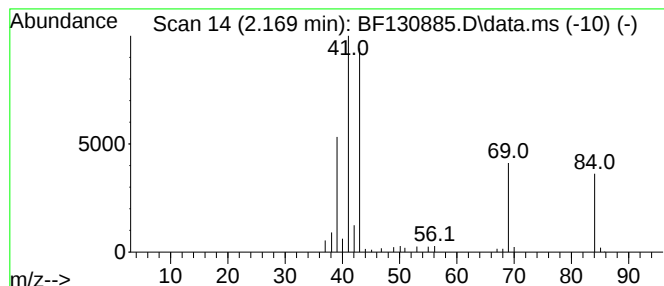
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Buten-2-one, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	2.84 ng	66798	1,4-Dichlorobenzene-d4	6.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2		3-Penten-2-one	84	C5H8O	000625-33-2	86
3		Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	58
4		Methacrolein	70	C4H6O	000078-85-3	47
5		Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	28



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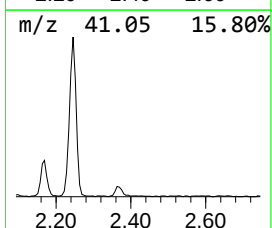
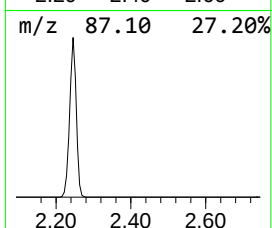
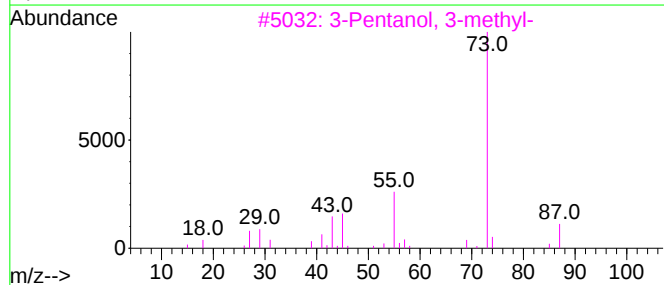
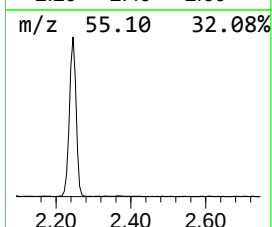
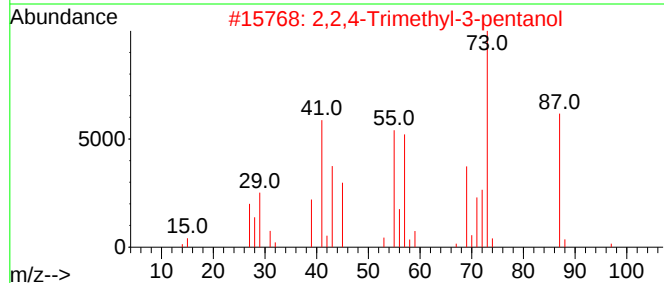
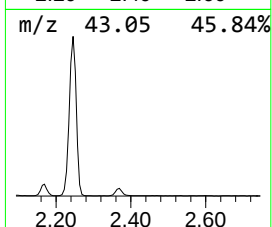
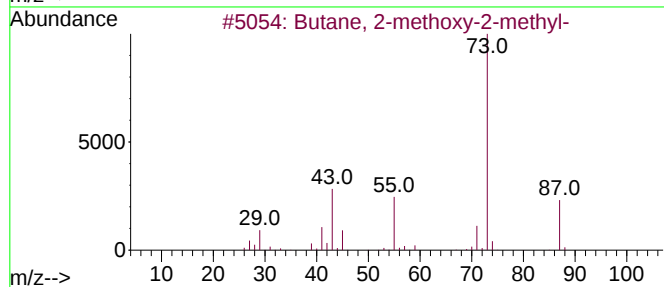
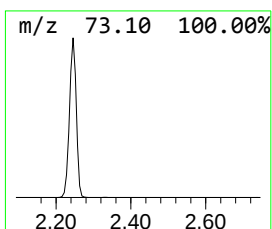
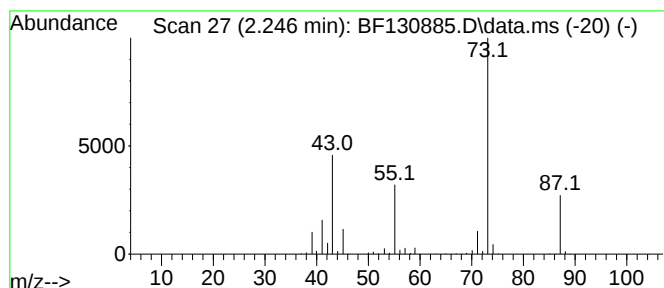
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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	65.86 ng	1549930	1,4-Dichlorobenzene-d4	6.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35



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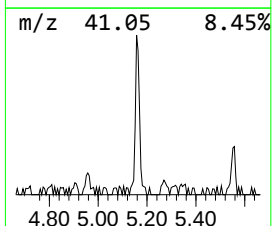
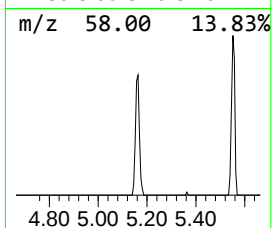
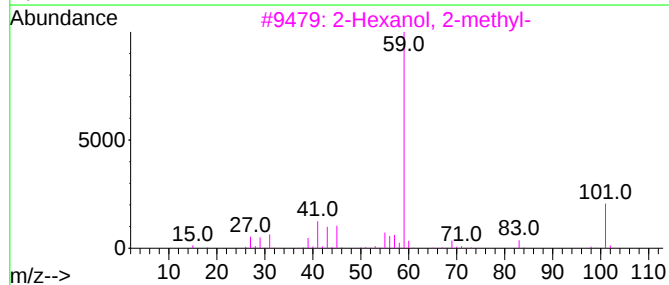
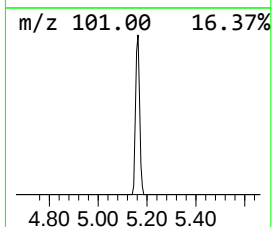
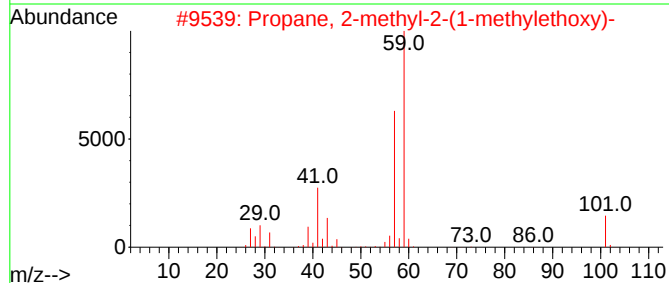
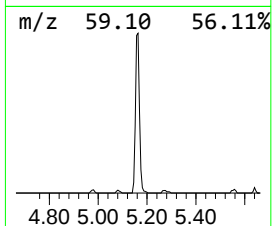
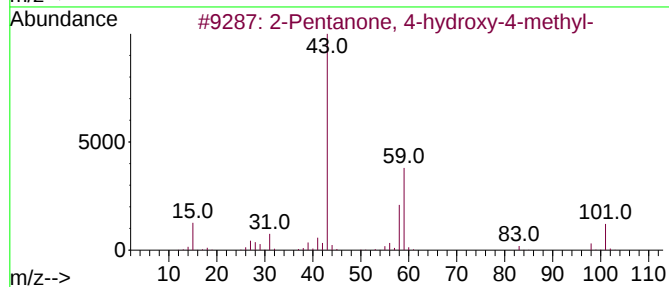
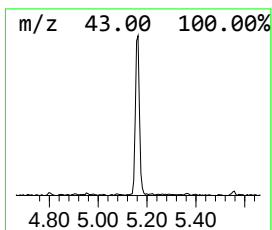
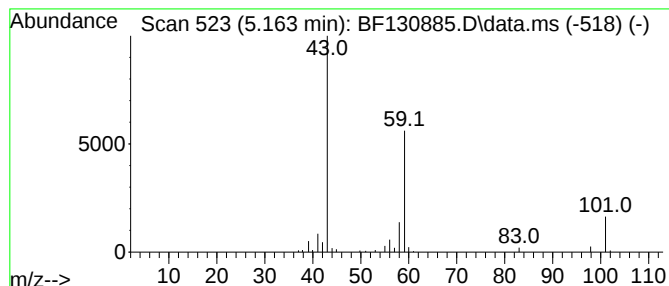
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	5.06 ng	119033	1,4-Dichlorobenzene-d4	6.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23		



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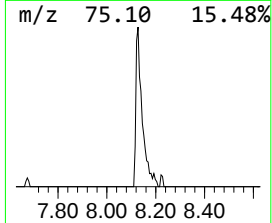
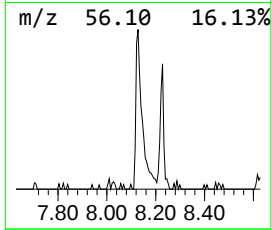
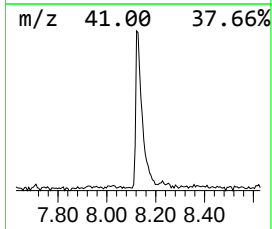
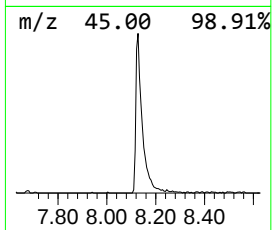
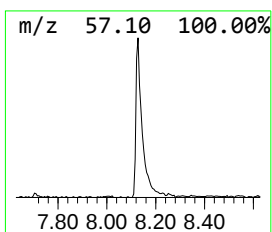
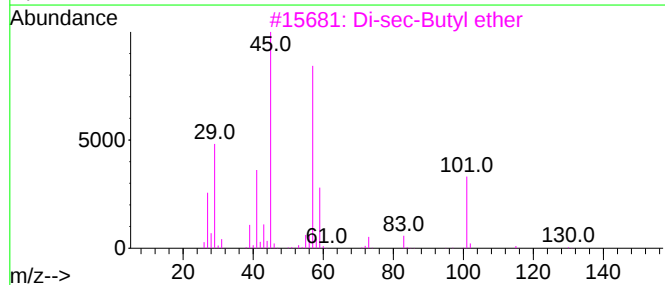
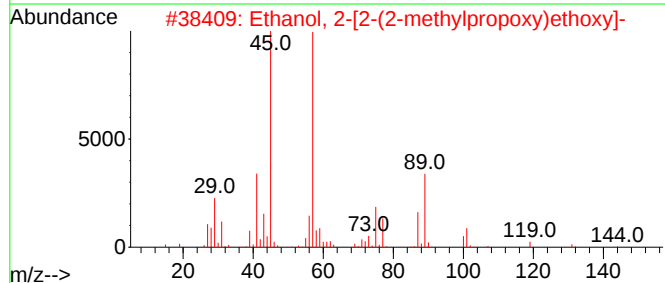
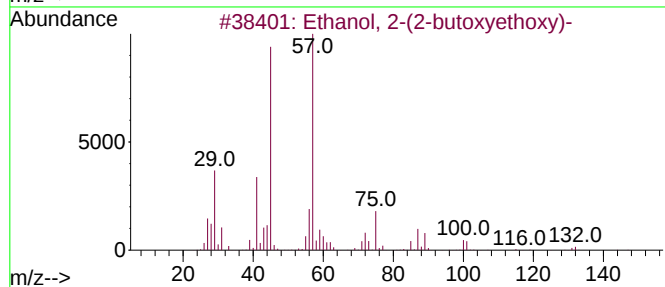
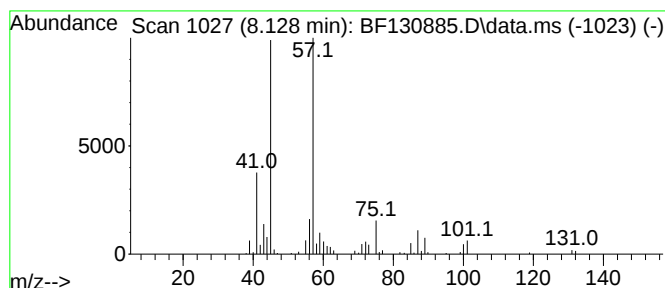
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.128	8.99 ng	258180	Naphthalene-d8	8.228

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2		Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
3		Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5		Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



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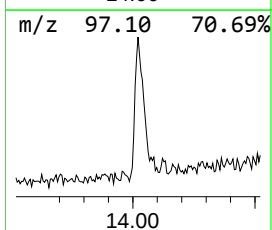
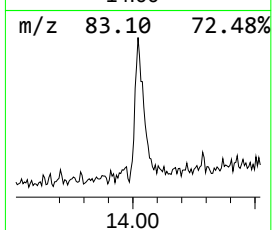
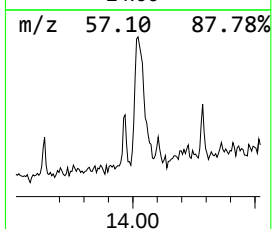
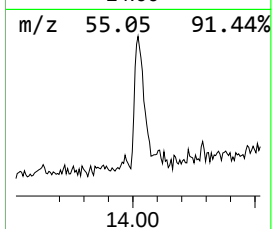
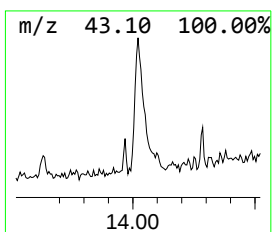
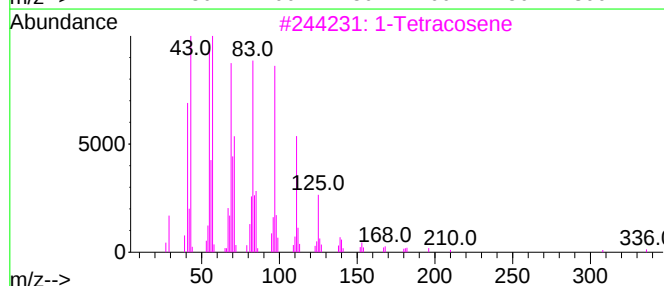
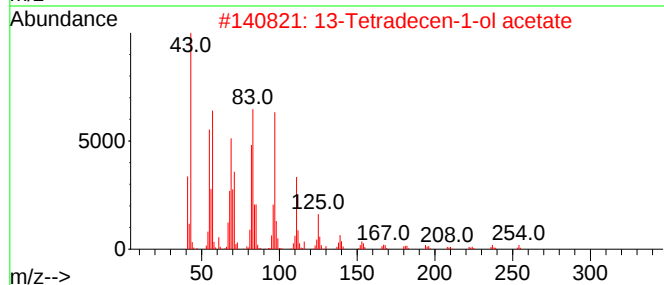
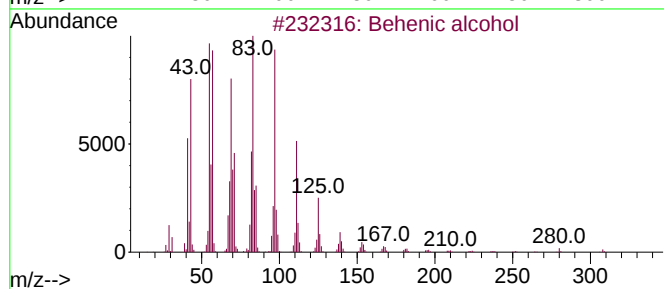
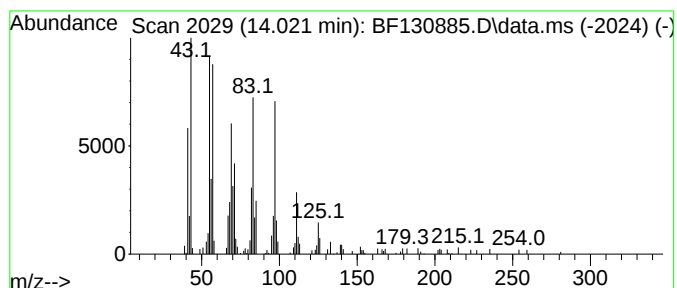
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Peak Number 5 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.021	10.37 ng	222905	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
3			1-Tetracosene	336	C24H48	010192-32-2	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			1-Docosene	308	C22H44	001599-67-3	91



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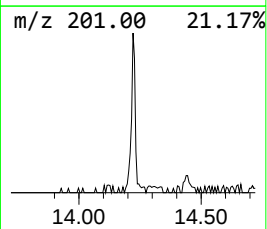
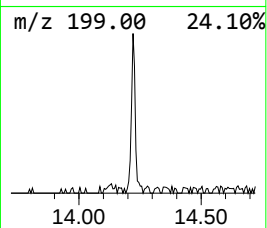
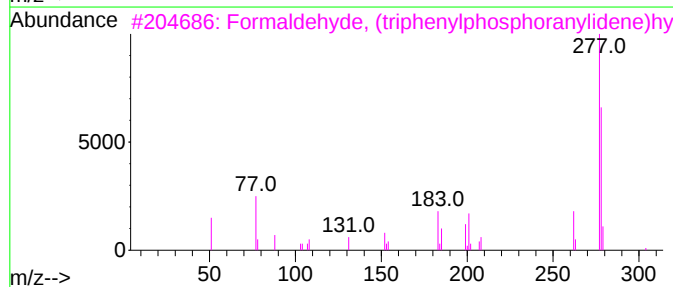
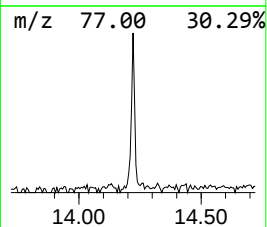
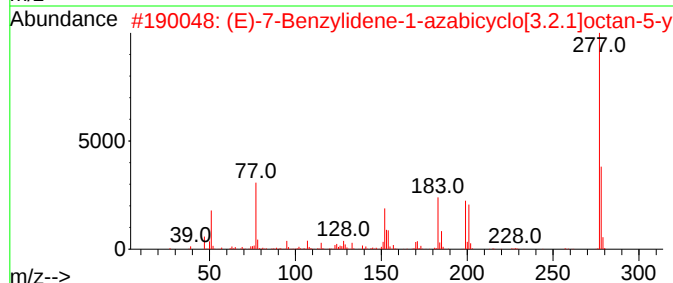
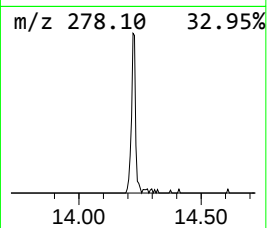
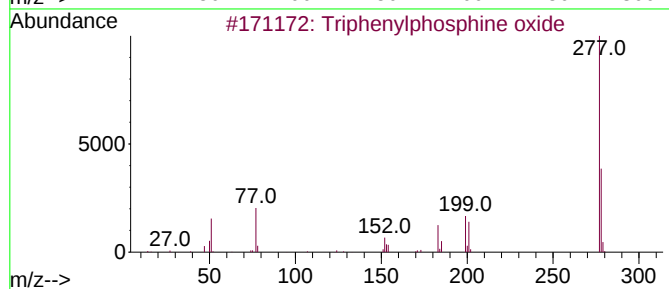
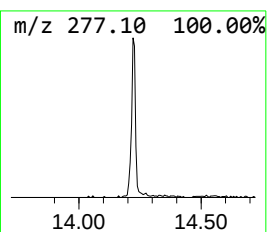
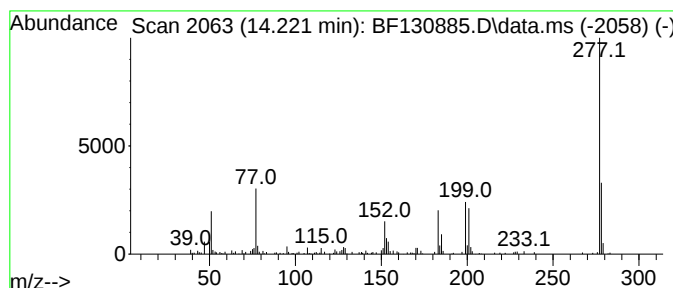
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	5.43 ng	116723	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	62
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130885.D
Acq On : 31 Oct 2022 18:15
Operator : CG\JU
Sample : N5355-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5518-1

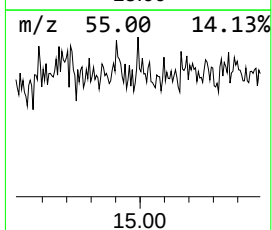
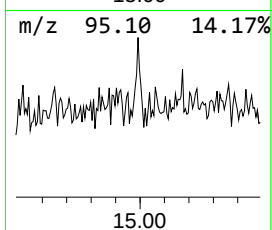
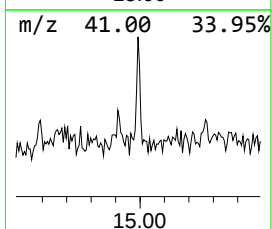
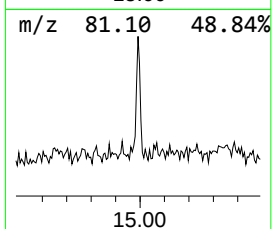
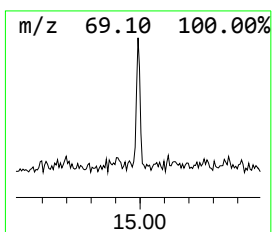
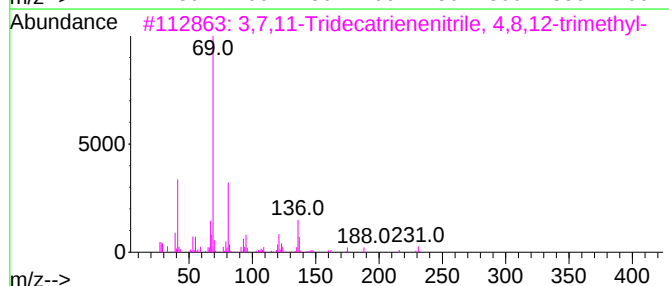
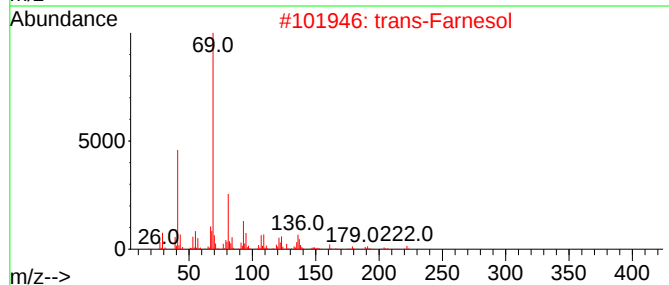
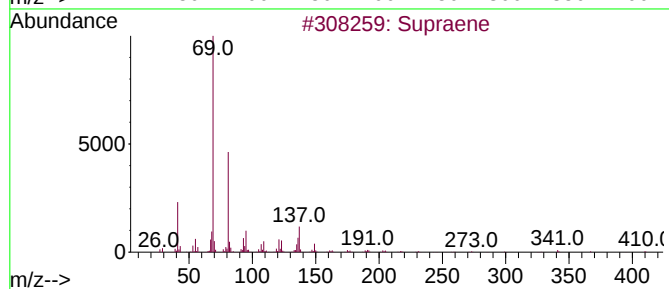
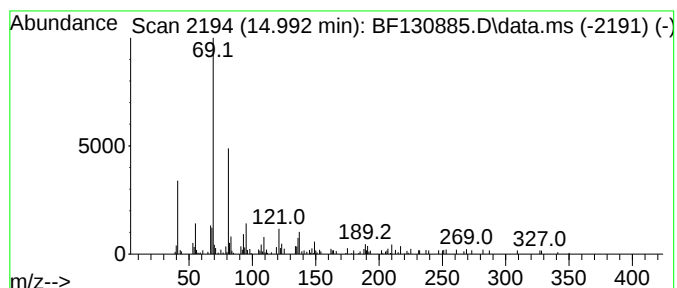
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	2.01 ng	38021	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			trans-Farnesol	222	C15H26O	000106-28-5	58
3			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	56
4			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	56
5			1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130885.D
Acq On : 31 Oct 2022 18:15
Operator : CG\JU
Sample : N5355-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5518-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Buten-2-one, ...	2.169	2.8	ng	66798	1	6.939	470639	20.0
Butane, 2-metho...	2.246	65.9	ng	1549930	1	6.939	470639	20.0
2-Pentanone, 4-...	5.163	5.1	ng	119033	1	6.939	470639	20.0
Ethanol, 2-(2-b...	8.128	9.0	ng	258180	2	8.228	574430	20.0
Behenic alcohol	14.021	10.4	ng	222905	5	14.127	429753	20.0
Triphenylphosph...	14.221	5.4	ng	116723	5	14.127	429753	20.0
Supraene	14.992	2.0	ng	38021	6	15.645	378868	20.0