

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
 Data File : BF132458.D
 Acq On : 17 Feb 2023 19:32
 Operator : CG\JU
 Sample : 01593-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EB-2023-2-16

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132458.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.672	307	312	317	rBV	178954	198660	1.93%	0.279%
2	5.260	408	412	420	rVB	1550478	1743424	16.97%	2.447%
3	5.649	473	478	481	rBV	4018708	3778636	36.78%	5.304%
4	6.319	588	592	596	rBV	1490576	1259490	12.26%	1.768%
5	6.631	641	645	648	rBV	1596945	1455499	14.17%	2.043%
6	6.660	648	650	675	rVB	515179	1555311	15.14%	2.183%
7	7.019	707	711	715	rBV	1640593	1343060	13.07%	1.885%
8	7.590	801	808	811	rBV	3637799	3947422	38.43%	5.541%
9	7.666	815	821	824	rBV	4071831	4420130	43.03%	6.205%
10	7.695	824	826	832	rVB	127554	136006	1.32%	0.191%
11	8.307	926	930	933	rBV	2169579	1727182	16.81%	2.425%
12	8.531	960	968	969	rBV	7347314	10116751	98.48%	14.202%
13	8.560	969	973	980	rVV	8422652	10272528	100.00%	14.421%
14	8.631	980	985	987	rVV2	213046	332157	3.23%	0.466%
15	8.654	987	989	1010	rVB	813072	822743	8.01%	1.155%
16	9.384	1107	1113	1116	rBV	6866646	6671299	64.94%	9.365%
17	9.489	1127	1131	1139	rVB	188870	167291	1.63%	0.235%
18	10.072	1226	1230	1233	rBV	2337593	2004448	19.51%	2.814%
19	10.866	1360	1365	1368	rBV	4849132	4635537	45.13%	6.507%
20	11.566	1480	1484	1487	rBV	2637377	2145488	20.89%	3.012%
21	12.072	1567	1570	1575	rBV	93151	121288	1.18%	0.170%
22	12.866	1702	1705	1717	rBV2	64385	128086	1.25%	0.180%
23	13.160	1750	1755	1758	rBV	7582663	7653939	74.51%	10.745%
24	14.219	1931	1935	1939	rBV	1967953	1801820	17.54%	2.529%
25	14.307	1944	1950	1958	rBV	1045536	1161349	11.31%	1.630%
26	15.777	2194	2200	2208	rBV	1213873	1635758	15.92%	2.296%

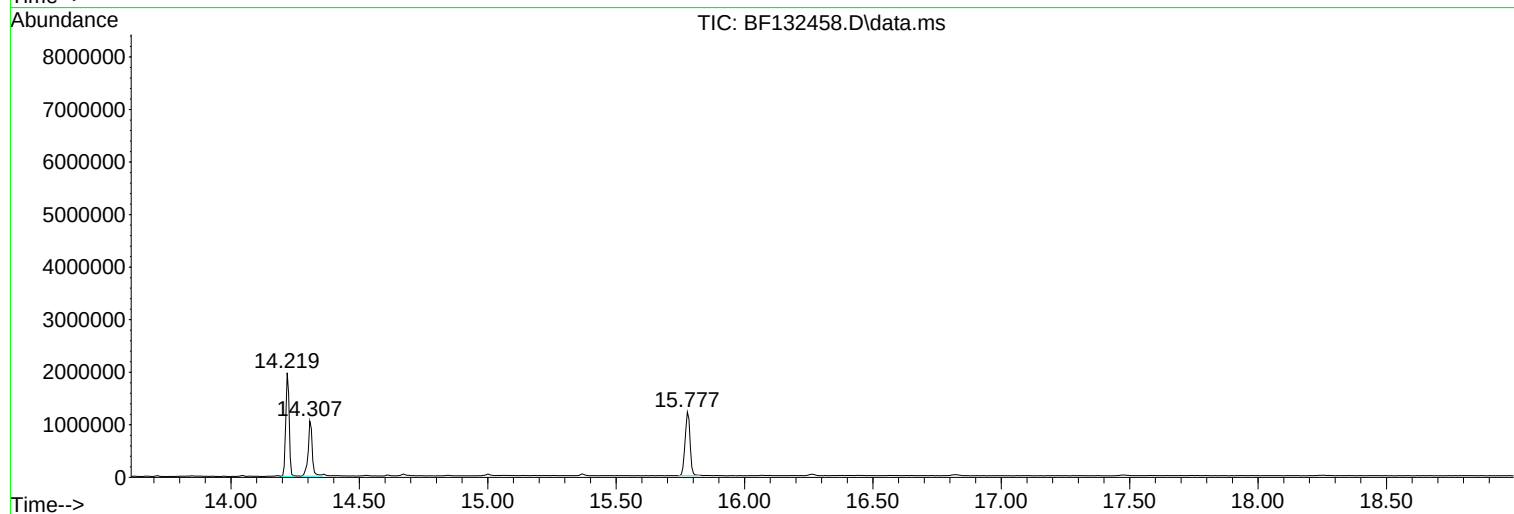
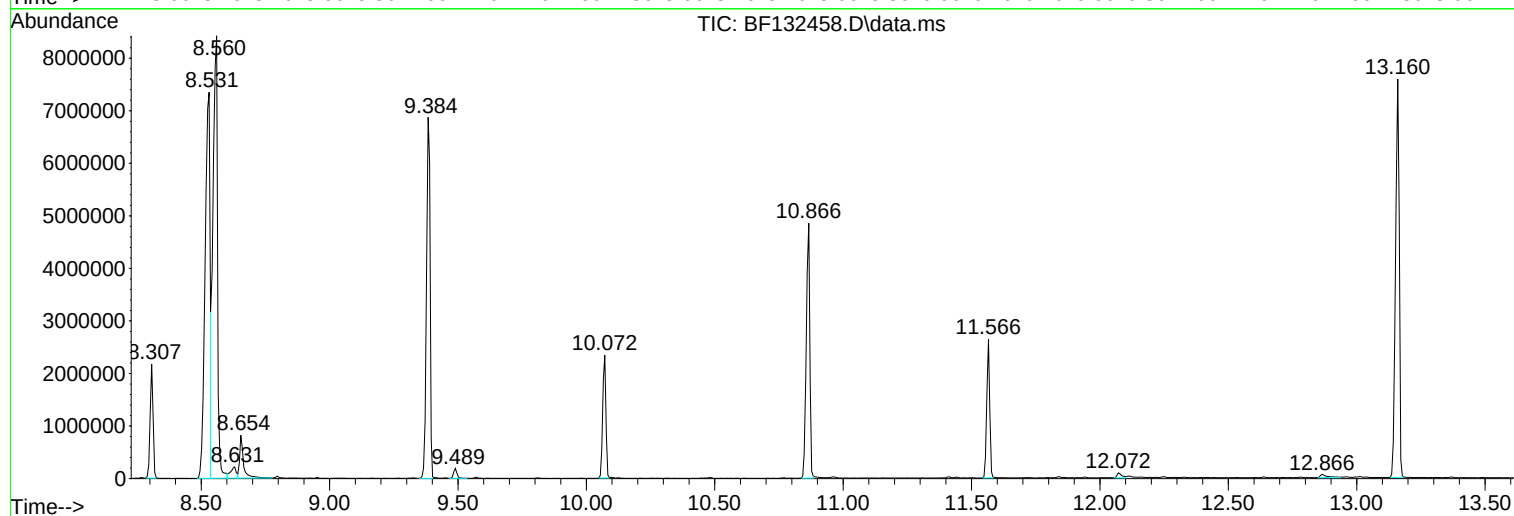
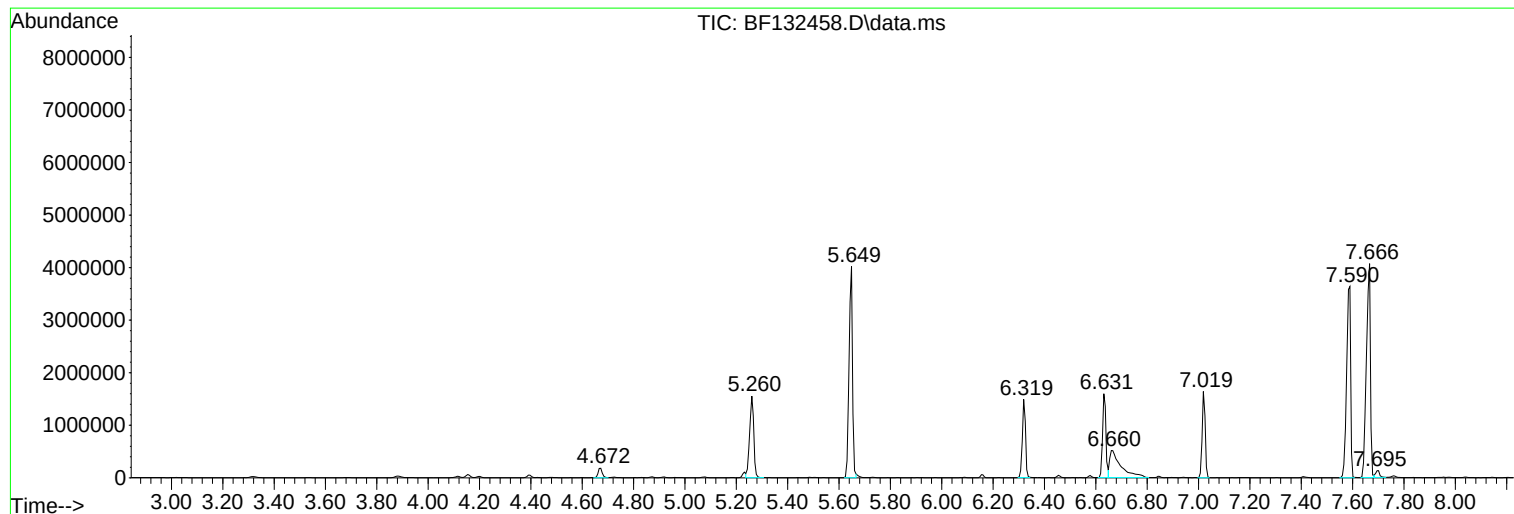
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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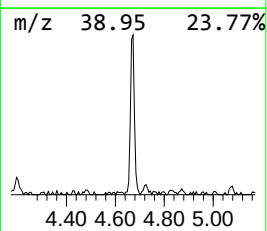
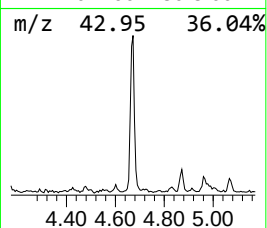
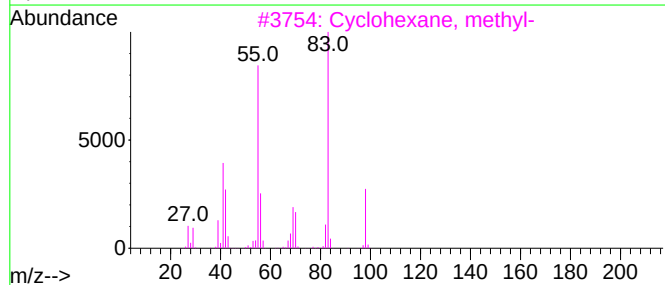
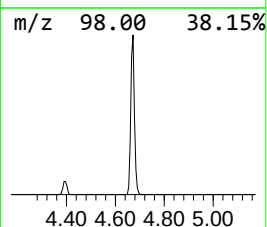
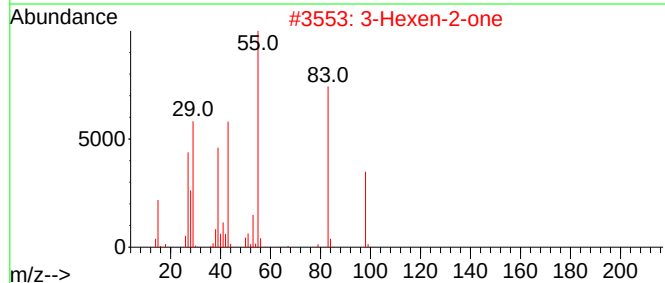
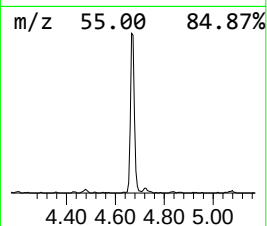
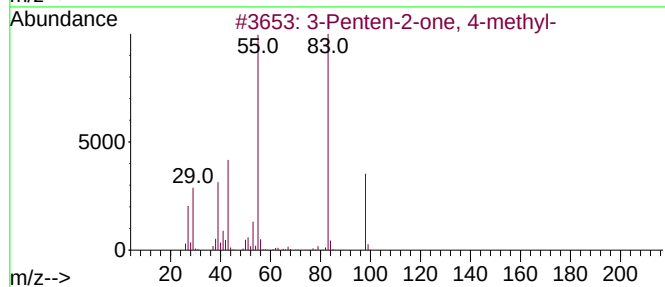
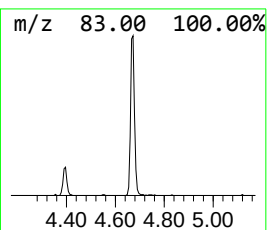
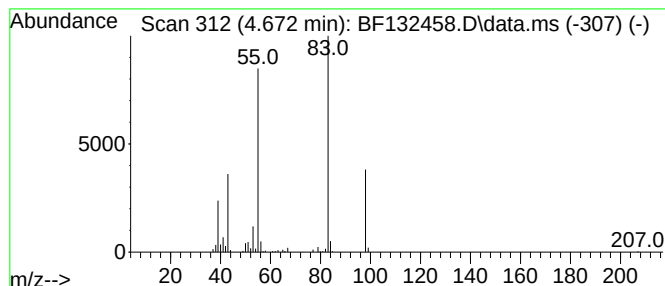
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.672	2.96 ng	198660	1,4-Dichlorobenzene-d4	7.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			Cyclohexane, methyl-	98	C7H14	000108-87-2	80
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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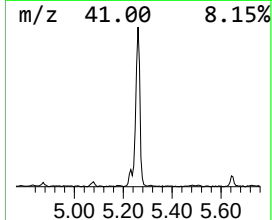
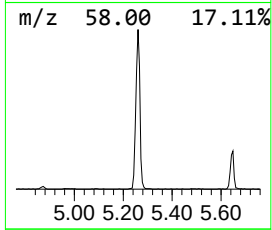
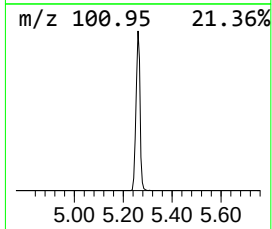
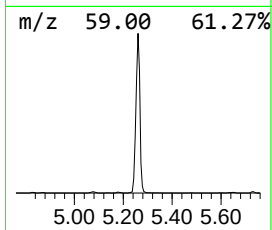
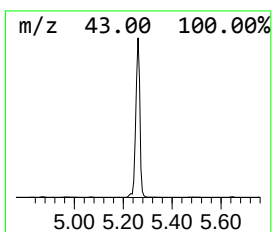
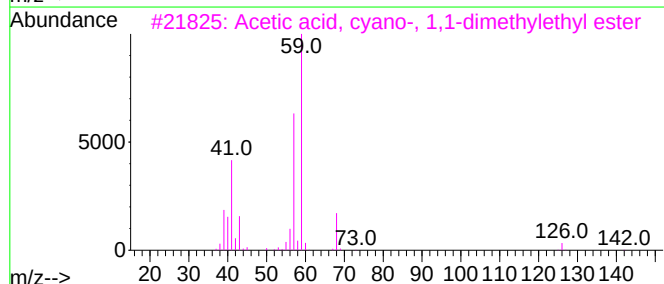
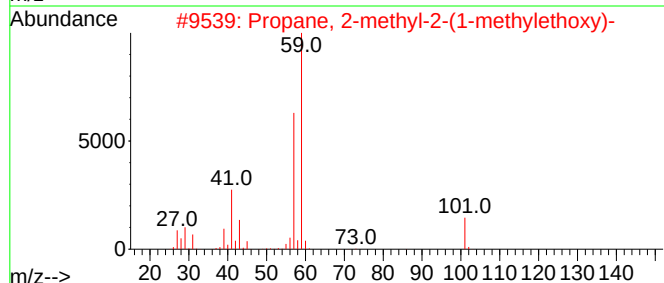
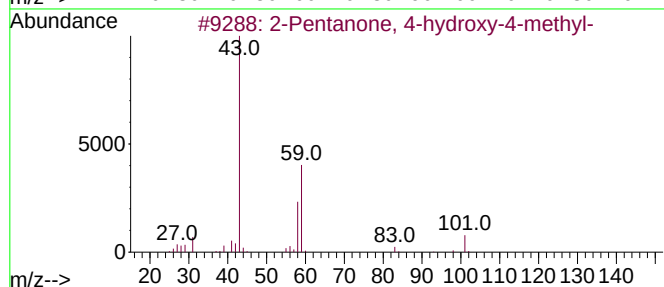
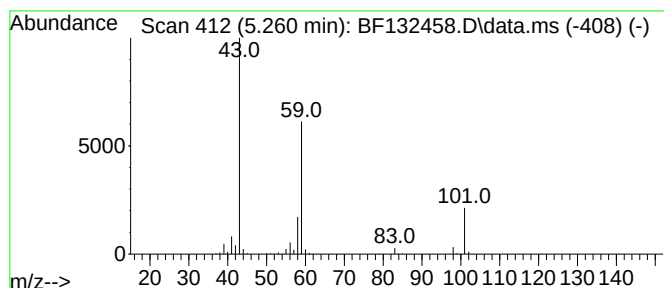
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.260	25.96 ng	1743420	1,4-Dichlorobenzene-d4	7.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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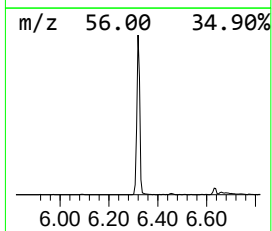
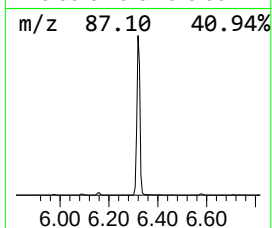
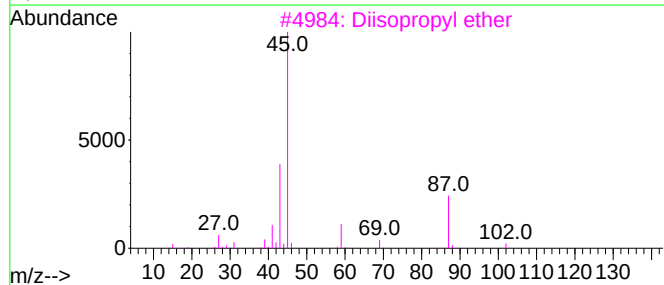
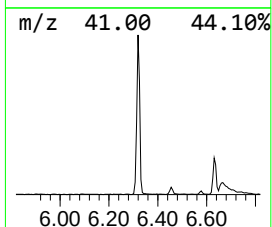
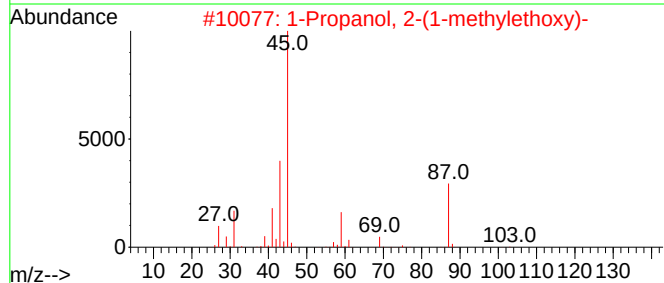
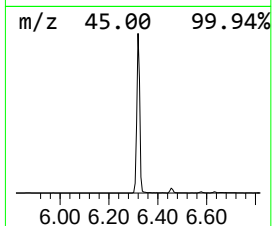
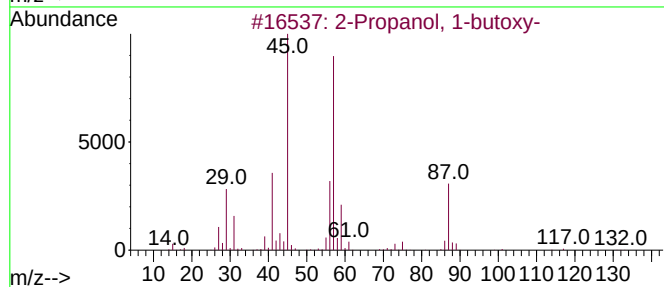
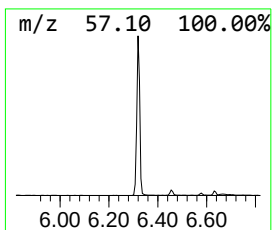
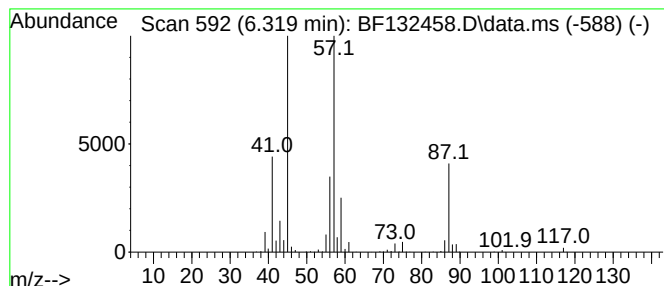
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Propanol, 1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.319	18.76 ng	1259490	1,4-Dichlorobenzene-d4	7.019

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2		1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
3		Diisopropyl ether	102	C6H14O	000108-20-3	42
4		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
5		Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	40



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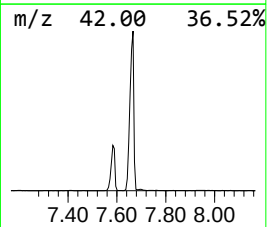
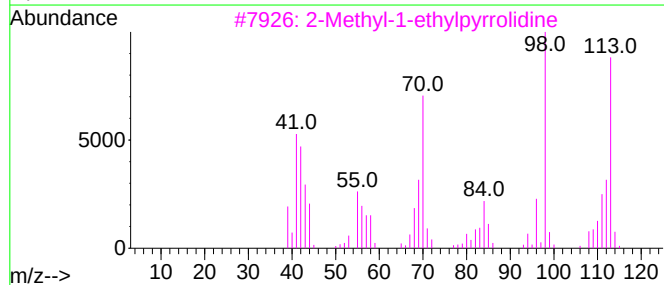
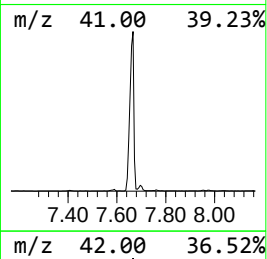
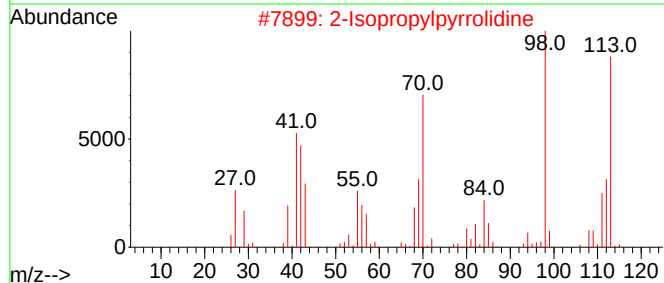
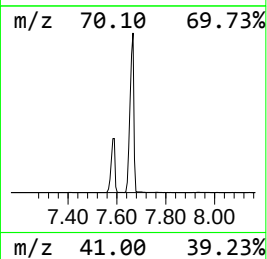
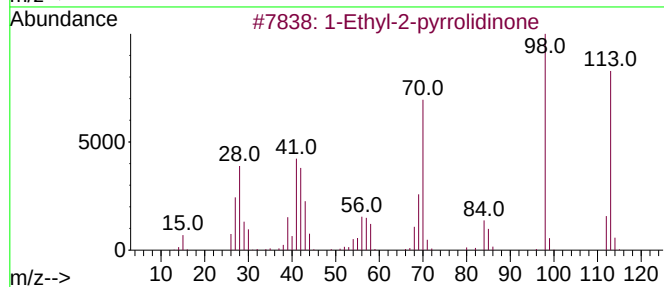
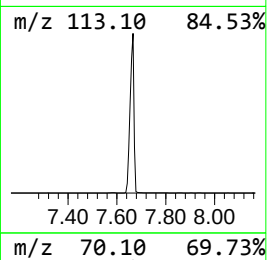
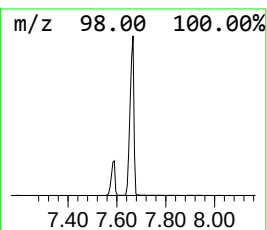
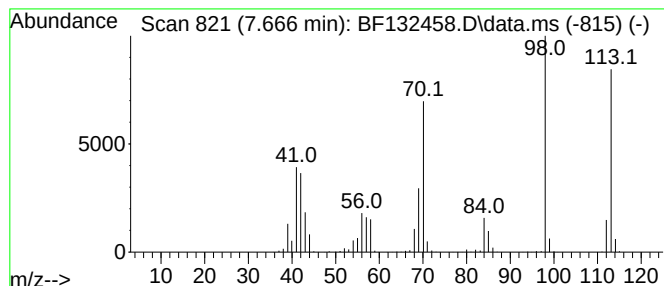
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Peak Number 4 1-Ethyl-2-pyrrolidinone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.666	51.18 ng	4420130	Naphthalene-d8	8.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-2-pyrrolidinone	113	C6H11NO	002687-91-4	96
2			2-Isopropylpyrrolidine	113	C7H15N	1010424-35-0	87
3			2-Methyl-1-ethylpyrrolidine	113	C7H15N	000765-79-7	87
4			(E)-3-(Dimethylamino)-2-pentene	113	C7H15N	032317-47-8	59
5			3-Penten-2-one, 4-(methylamino)-	113	C6H11NO	014092-14-9	50



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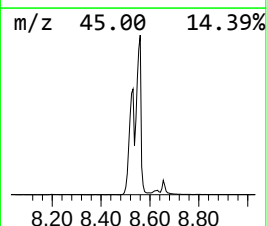
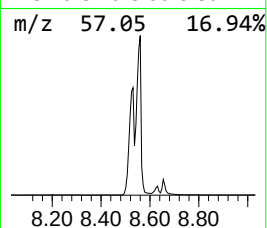
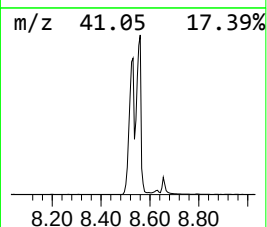
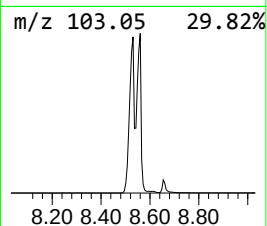
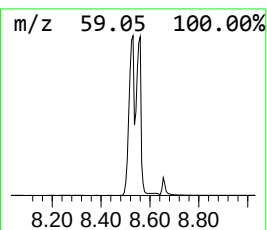
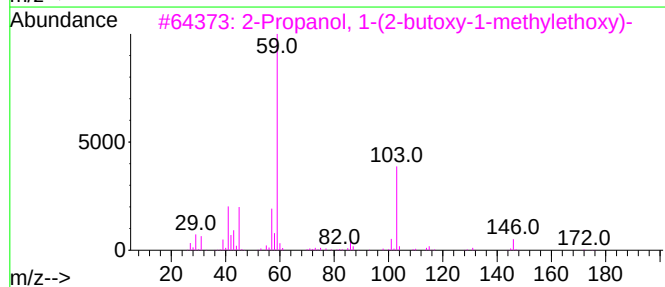
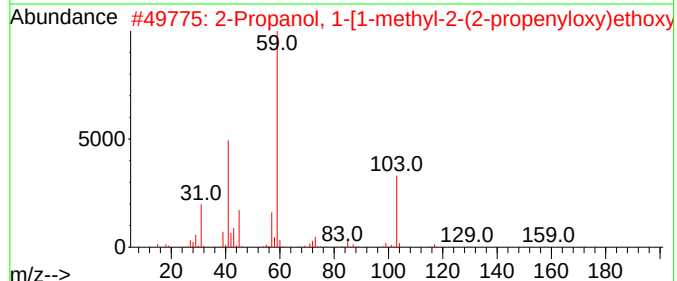
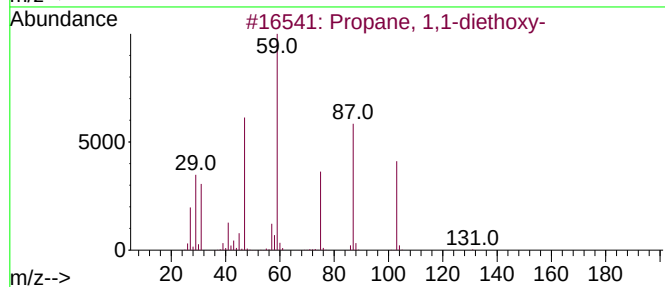
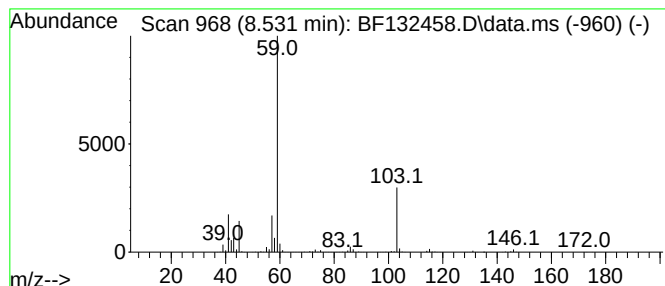
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Propane, 1,1-diethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.531	117.15 ng	10116800	Naphthalene-d8	8.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	78
2			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	74
3			2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
4			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
5			Methane, diethoxy-	104	C5H12O2	000462-95-3	72



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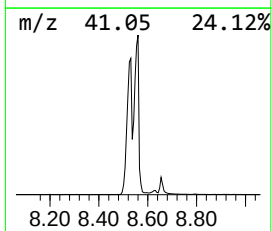
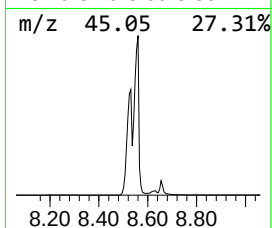
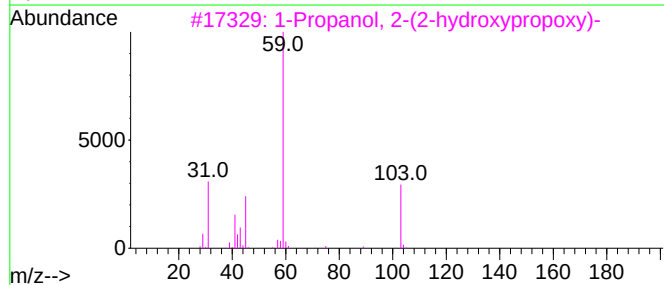
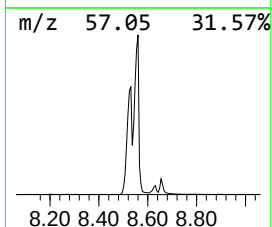
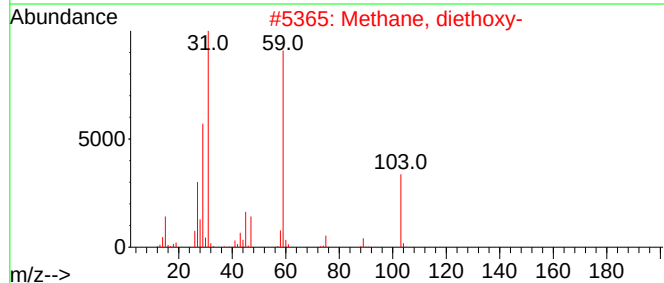
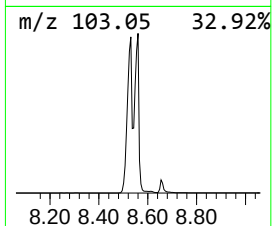
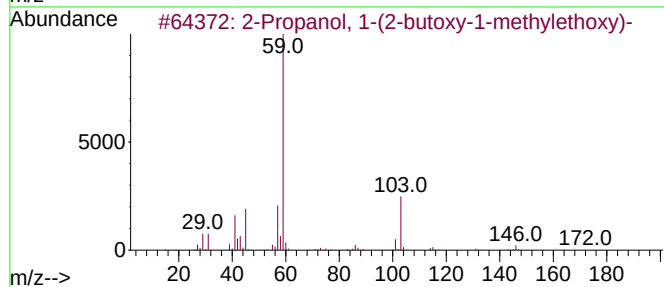
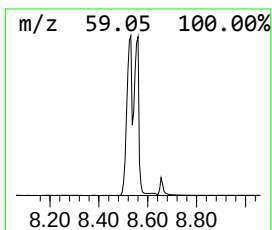
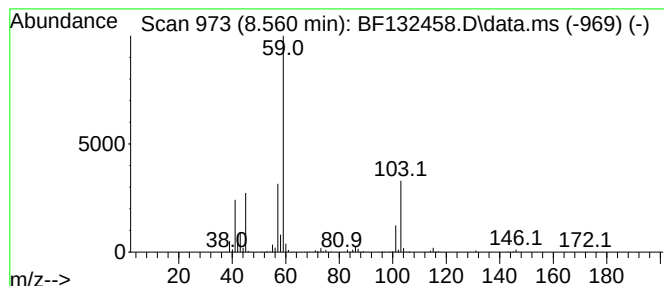
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.560	118.95 ng	10272500	Naphthalene-d8	8.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78		
2	Methane, diethoxy-	104	C5H12O2	000462-95-3	72		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64		
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132458.D
Acq On : 17 Feb 2023 19:32
Operator : CG\JU
Sample : 01593-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-2023-2-16

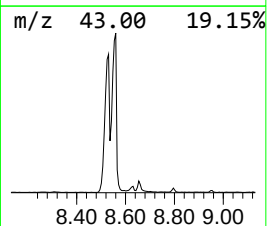
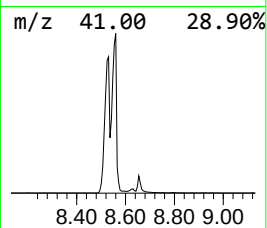
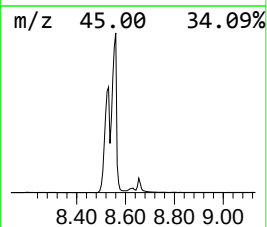
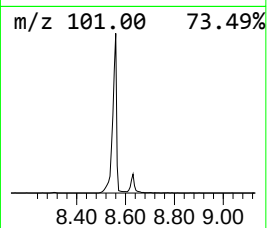
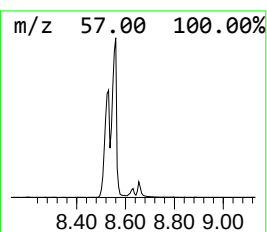
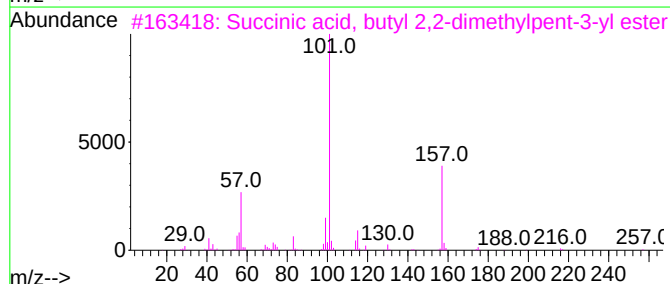
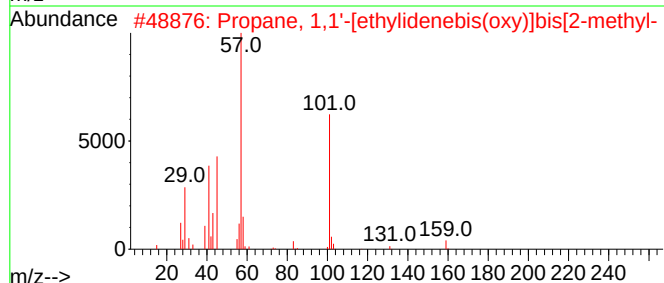
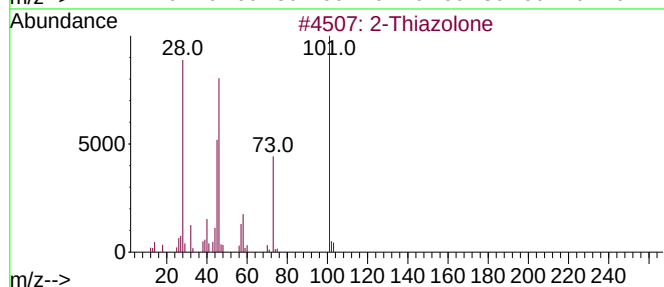
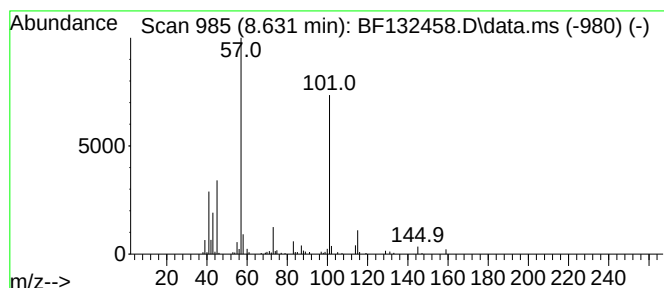
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Thiazolone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.631	3.85 ng	332157	Naphthalene-d8	8.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Thiazolone	101	C3H3NOS	1010432-90-5	53
2			Propane, 1,1'-[ethylidenebis(oxy...]	174	C10H22O2	005669-09-0	42
3			Succinic acid, butyl 2,2-dimethy...	272	C15H28O4	1000381-73-1	40
4			Succinic acid, butyl 2,4-dimethy...	272	C15H28O4	1000349-35-6	38
5			1,3-Dioxolane, 4,5-dimethyl-2-pe...	312	C20H40O2	056599-61-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132458.D
Acq On : 17 Feb 2023 19:32
Operator : CG\JU
Sample : 01593-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-2023-2-16

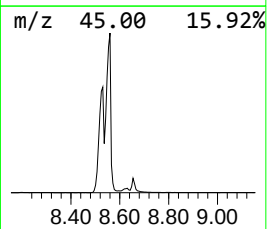
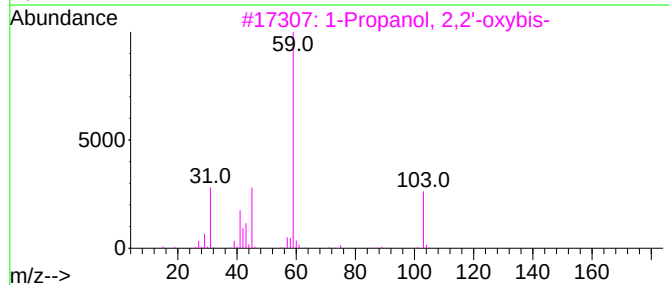
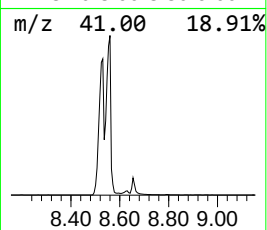
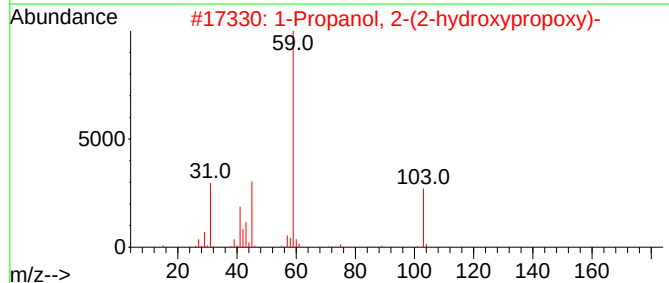
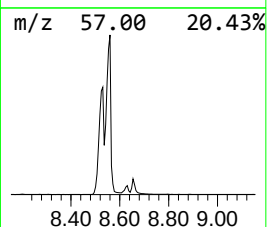
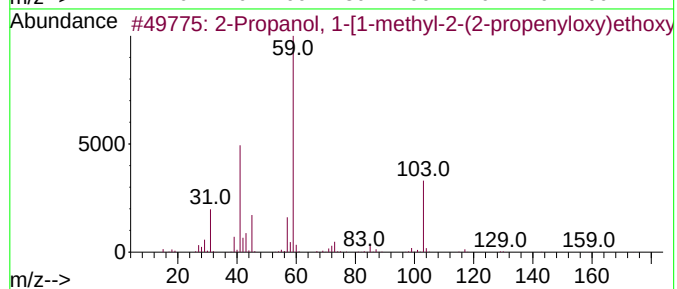
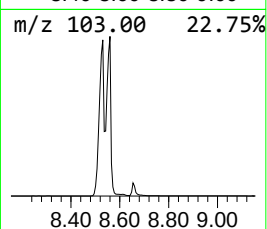
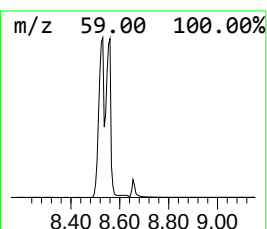
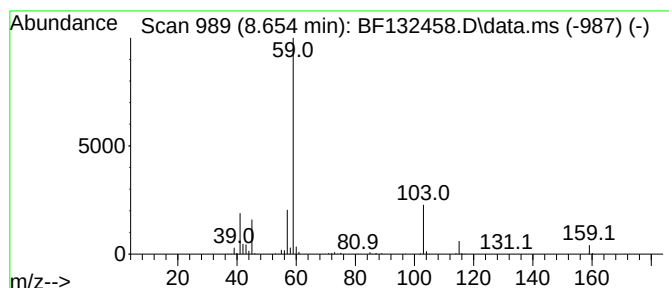
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.654	9.53 ng	822743	Naphthalene-d8	8.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78		
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64		
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	64		
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132458.D
Acq On : 17 Feb 2023 19:32
Operator : CG\JU
Sample : 01593-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-2023-2-16

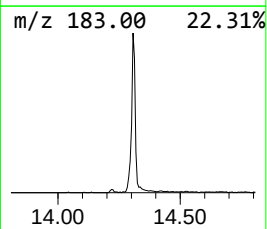
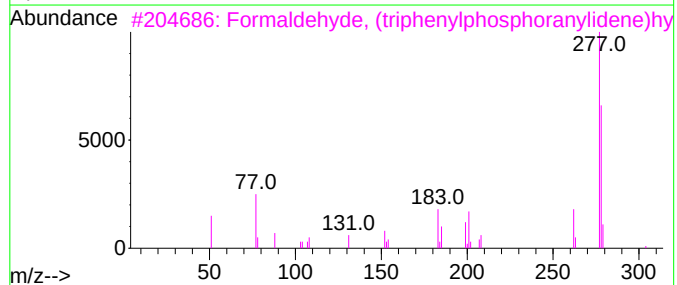
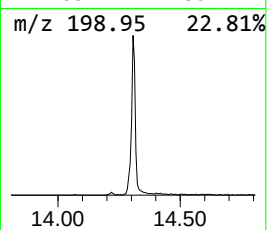
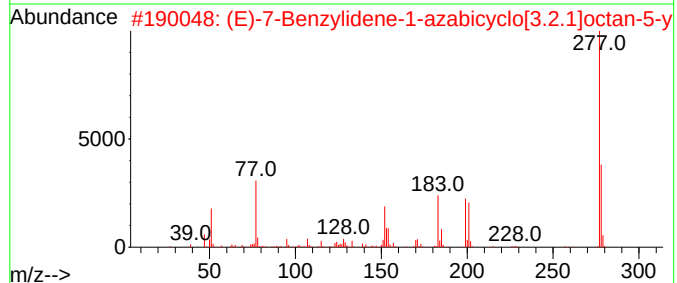
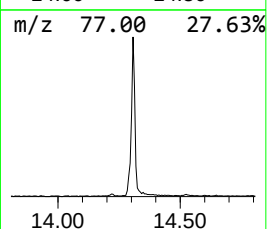
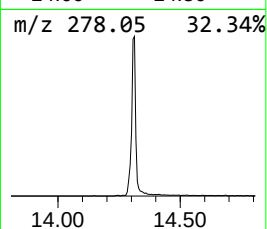
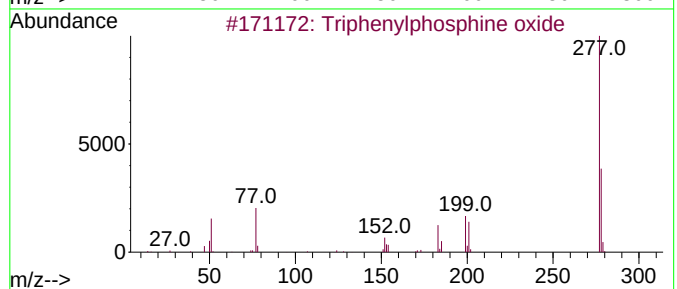
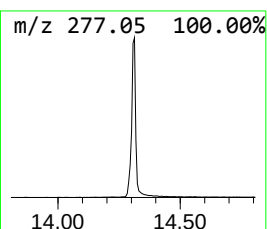
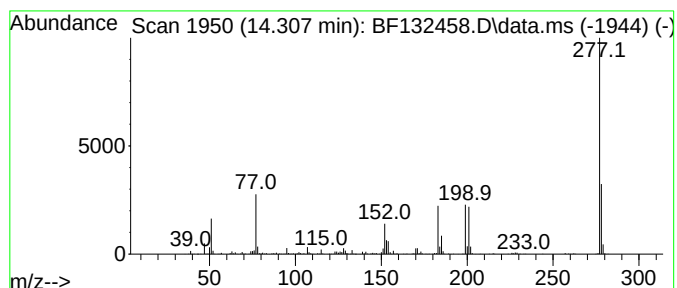
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.307	12.89 ng	1161350	Chrysene-d12	14.219

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	43
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132458.D
Acq On : 17 Feb 2023 19:32
Operator : CG\JU
Sample : 01593-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-2023-2-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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-Penten-2-one,...	4.672	3.0	ng	198660	1	7.019	1343060	20.0
2-Pentanone, 4-...	5.260	26.0	ng	1743420	1	7.019	1343060	20.0
2-Propanol, 1-b...	6.319	18.8	ng	1259490	1	7.019	1343060	20.0
1-Ethyl-2-pyrro...	7.666	51.2	ng	4420130	2	8.307	1727180	20.0
Propane, 1,1-di...	8.531	117.2	ng	10116800	2	8.307	1727180	20.0
2-Propanol, 1-(...	8.560	119.0	ng	10272500	2	8.307	1727180	20.0
2-Thiazolone	8.631	3.9	ng	332157	2	8.307	1727180	20.0
2-Propanol, 1-[...	8.654	9.5	ng	822743	2	8.307	1727180	20.0
Triphenylphosph...	14.307	12.9	ng	1161350	5	14.219	1801820	20.0