

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100424\
 Data File : BF139668.D
 Acq On : 04 Oct 2024 20:16
 Operator : RC/JU
 Sample : P4242-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-Q

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-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139668.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	5	14	30	rVB	1625038	2611403	100.00%	17.171%
2	5.081	498	508	524	rBV	86963	144611	5.54%	0.951%
3	5.487	571	577	594	rBV	1399620	1822017	69.77%	11.980%
4	6.498	742	749	760	rBV	1294408	1804340	69.09%	11.864%
5	6.863	806	811	816	rBV	409438	493916	18.91%	3.248%
6	7.428	901	907	912	rBV	867733	1136421	43.52%	7.472%
7	8.145	1024	1029	1034	rBV	473517	575380	22.03%	3.783%
8	9.222	1206	1212	1217	rBV	1431523	1816762	69.57%	11.946%
9	9.898	1322	1327	1332	rBV	452720	548687	21.01%	3.608%
10	10.610	1443	1448	1456	rBV	146845	181041	6.93%	1.190%
11	10.686	1456	1461	1478	rVV	706714	908455	34.79%	5.973%
12	11.386	1575	1580	1587	rBV	408648	517973	19.84%	3.406%
13	11.910	1664	1669	1683	rBV3	31898	92301	3.53%	0.607%
14	12.969	1843	1849	1854	rBV	1233002	1550116	59.36%	10.192%
15	13.445	1926	1930	1936	rBV	41261	56955	2.18%	0.374%
16	14.021	2021	2028	2040	rBV	369318	538116	20.61%	3.538%
17	15.492	2273	2278	2293	rVB	240854	410166	15.71%	2.697%

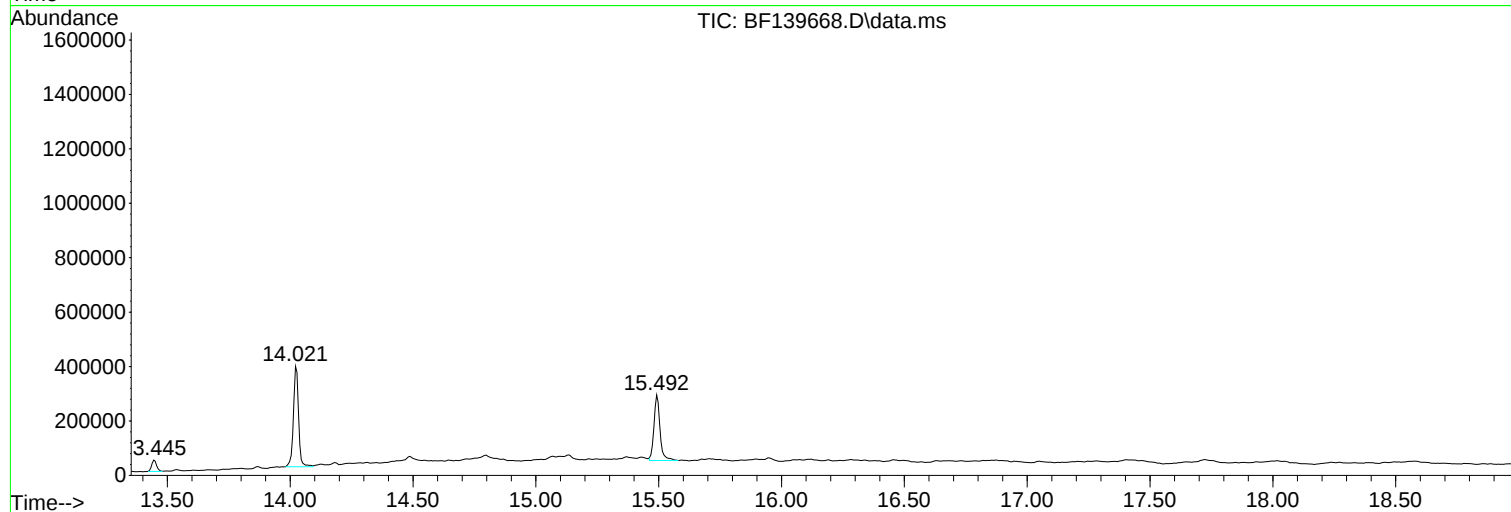
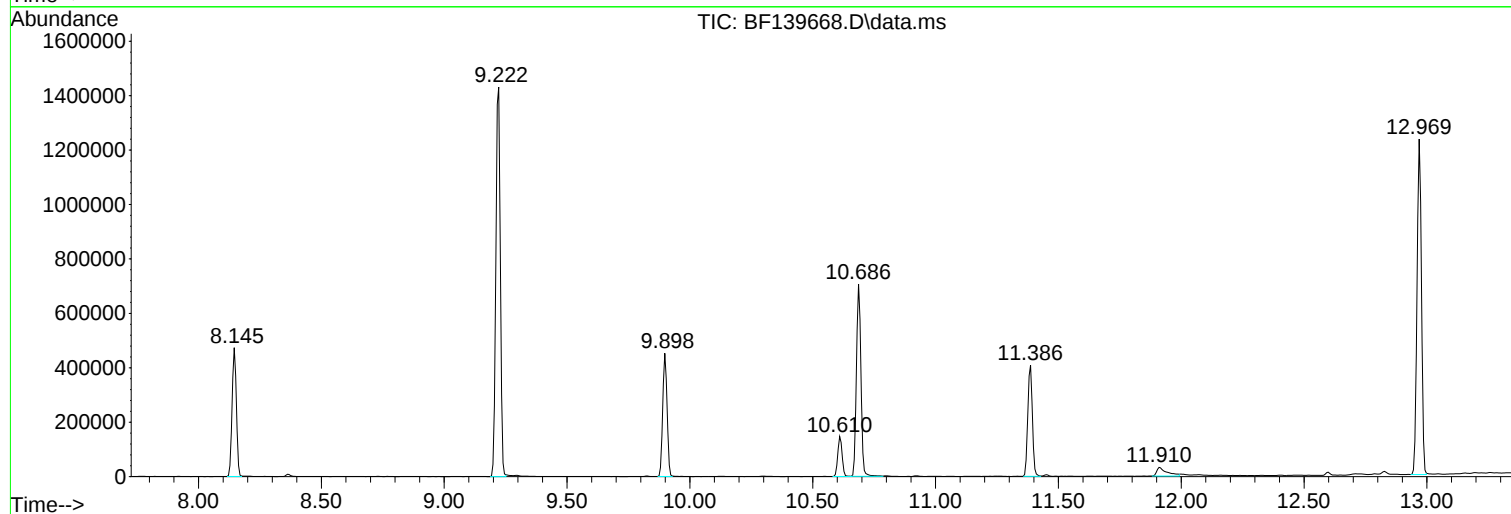
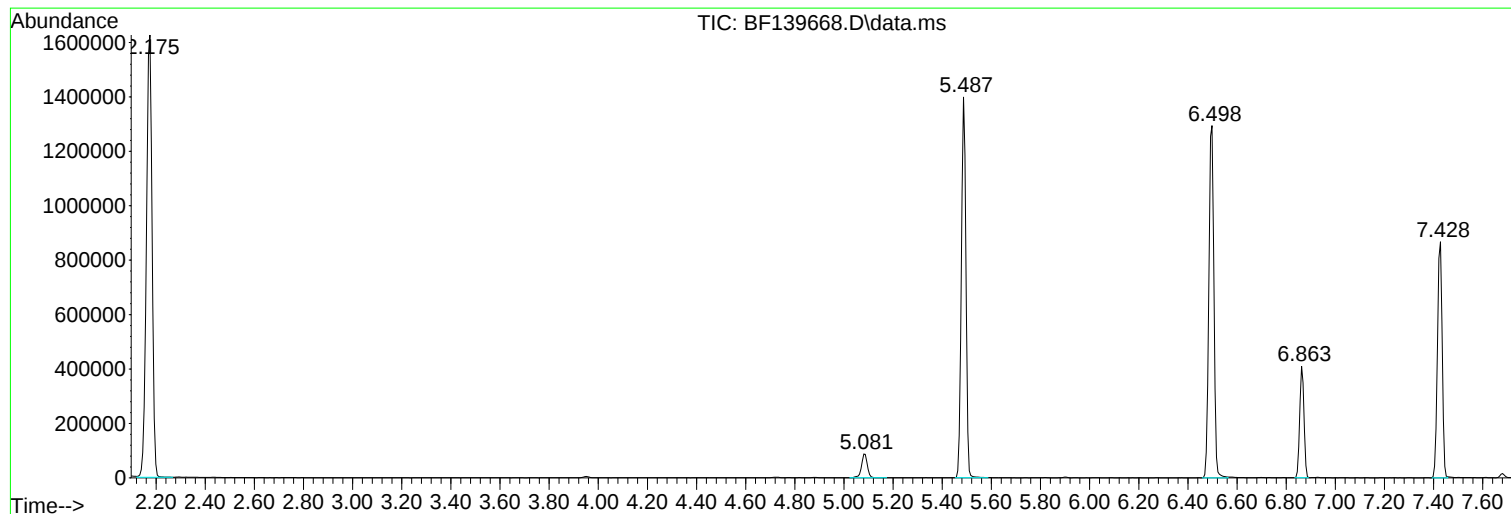
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100424\
Data File : BF139668.D
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Operator : RC/JU
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Instrument :
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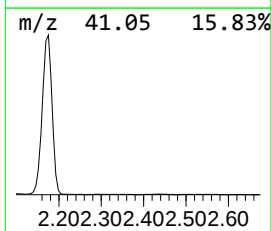
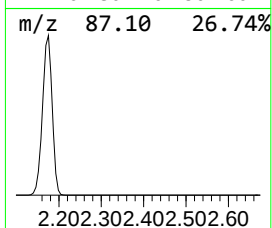
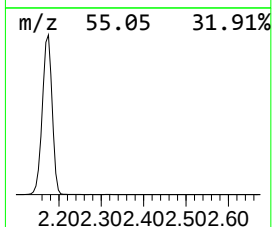
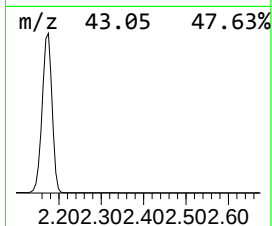
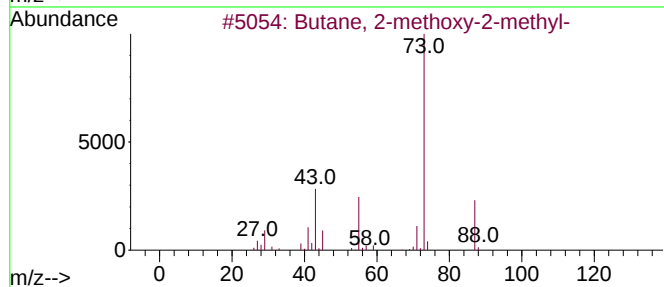
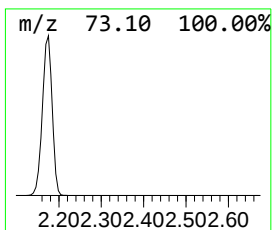
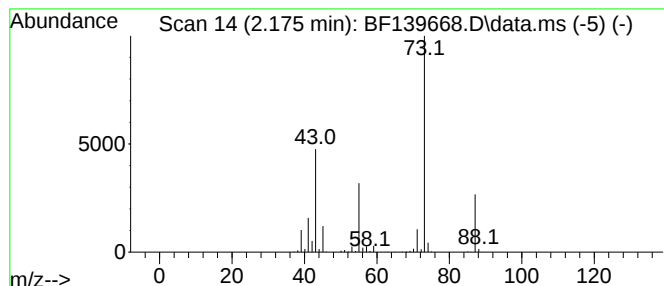
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	105.74 ng	2611400	1,4-Dichlorobenzene-d4	6.863

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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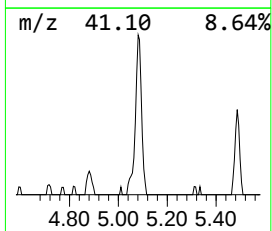
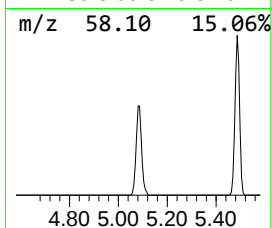
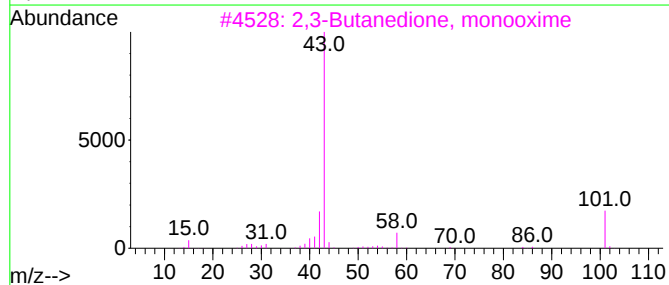
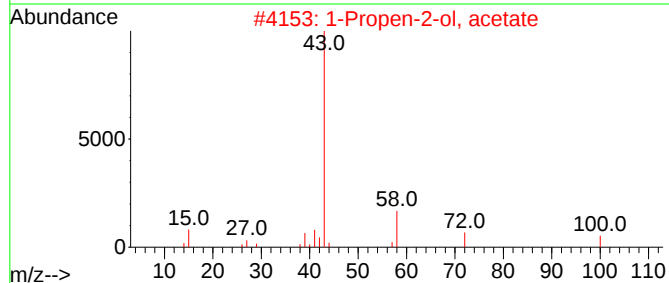
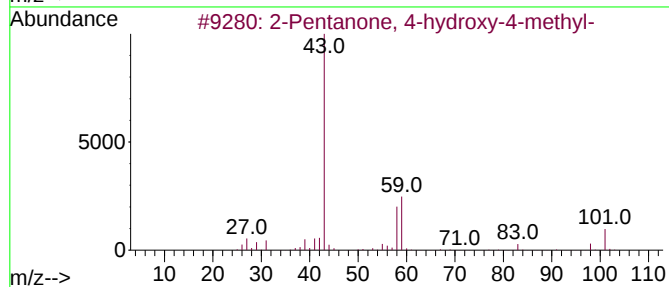
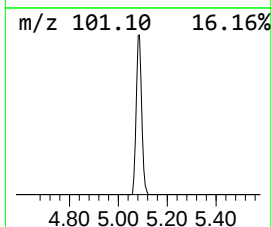
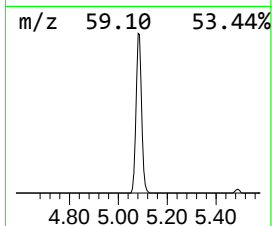
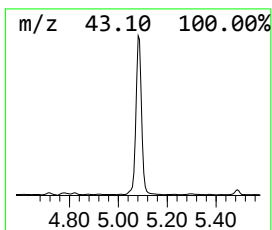
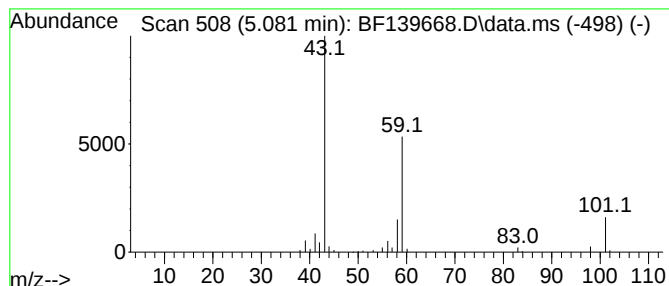
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	5.86 ng	144611	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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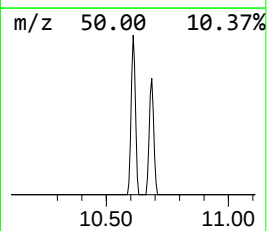
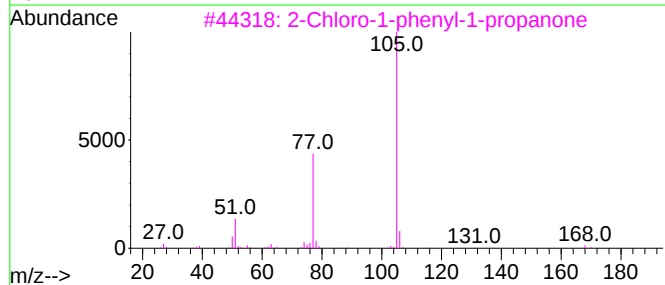
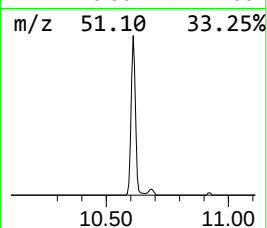
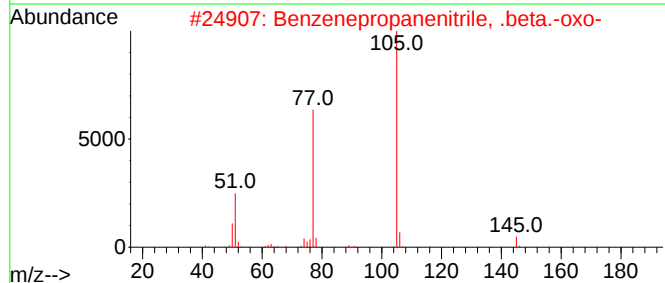
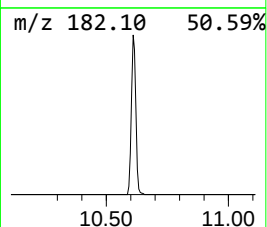
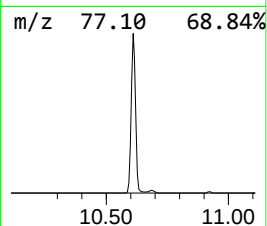
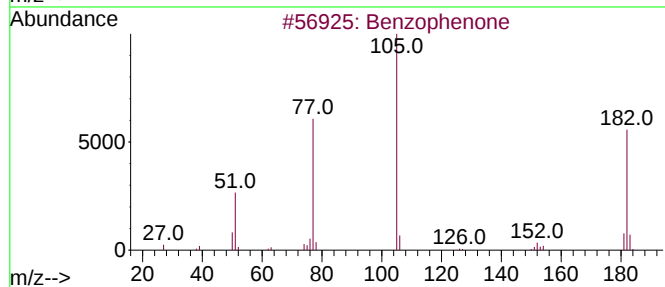
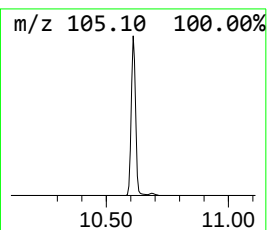
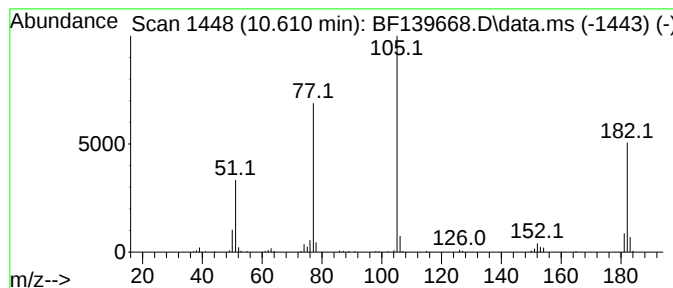
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	6.60 ng	181041	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
3			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50



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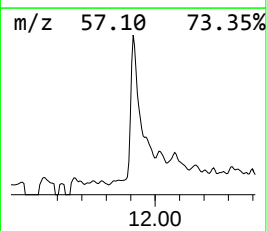
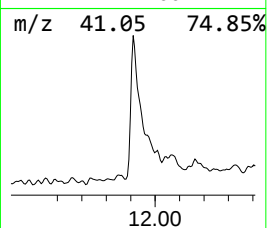
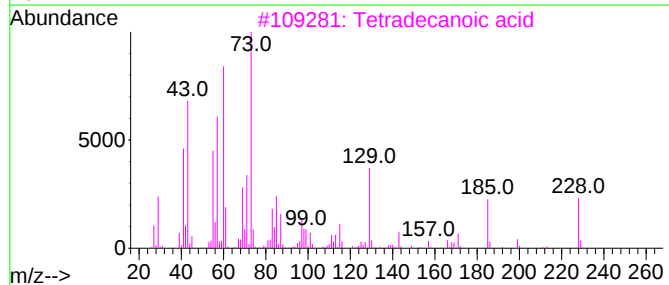
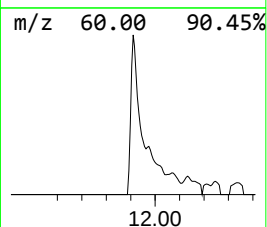
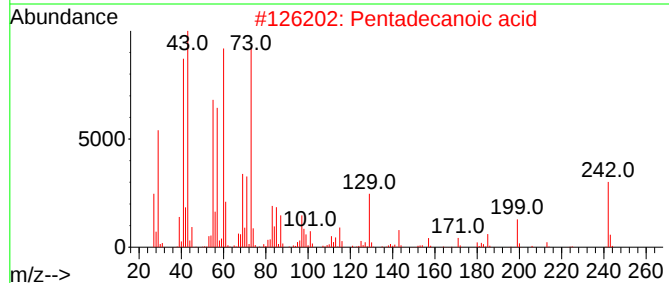
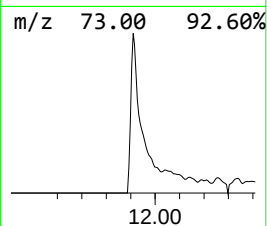
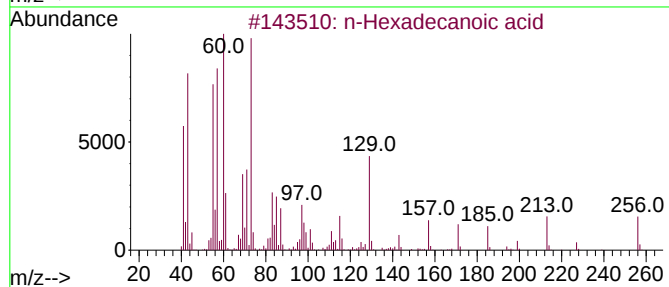
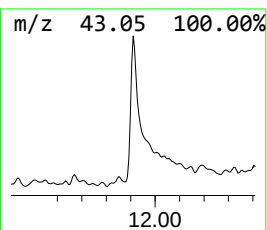
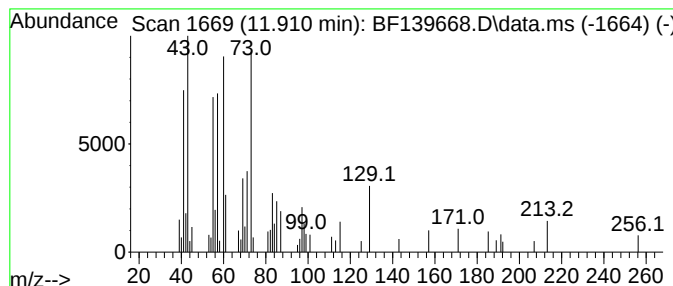
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.56 ng	92301	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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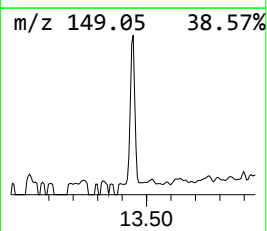
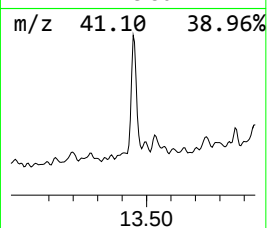
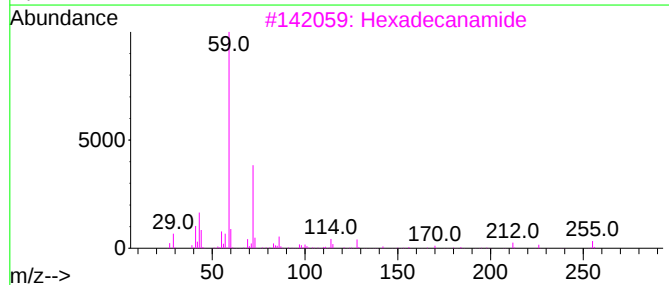
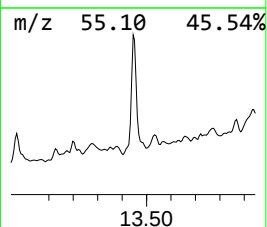
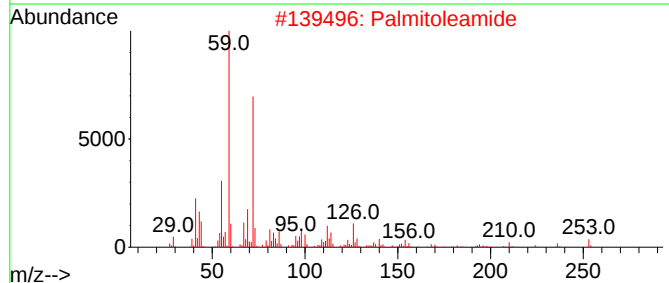
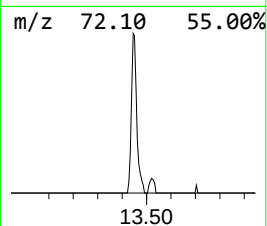
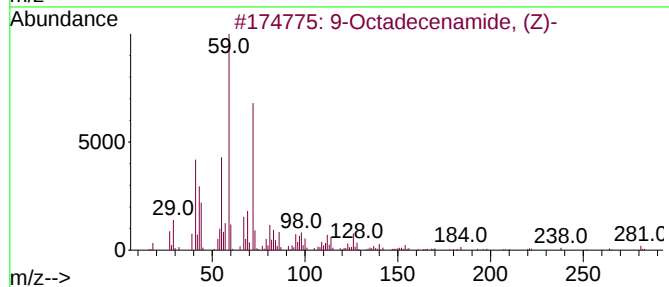
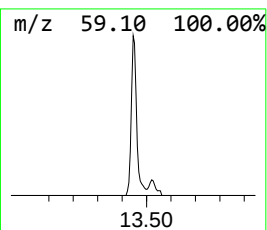
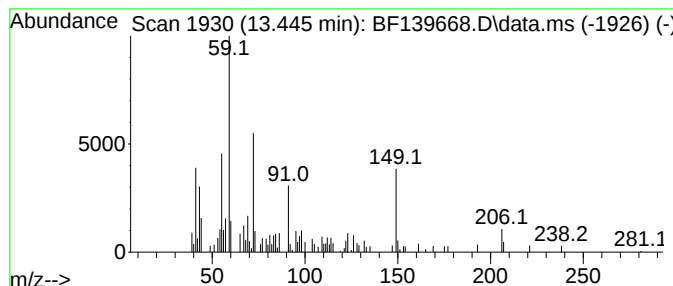
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	2.12 ng	56955	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
2			Palmitoleamide	253	C16H31NO	106010-22-4	52
3			Hexadecanamide	255	C16H33NO	000629-54-9	50
4			Tetradecanamide	227	C14H29NO	000638-58-4	50
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50



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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...	2.175	105.7	ng	2611400	1	6.863	493916	20.0
2-Pentanone, 4-...	5.081	5.9	ng	144611	1	6.863	493916	20.0
Benzophenone	10.610	6.6	ng	181041	3	9.898	548687	20.0
n-Hexadecanoic ...	11.910	3.6	ng	92301	4	11.386	517973	20.0
9-Octadecenamid...	13.445	2.1	ng	56955	5	14.021	538116	20.0