

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
 Data File : BF138157.D
 Acq On : 07 Jun 2024 13:36
 Operator : CG\JU
 Sample : P2740-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WCS-TPB

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-BF060524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	20	29	34	rVB	5771637	7727852	81.94%	11.046%
2	5.140	516	519	525	rVB	384706	455322	4.83%	0.651%
3	5.534	580	586	589	rBV	7261189	7957086	84.37%	11.373%
4	6.528	749	755	758	rBV	7231888	8112249	86.02%	11.595%
5	6.904	815	819	822	rBV	3094249	2311849	24.51%	3.304%
6	7.469	909	915	918	rBV	5083341	5202641	55.17%	7.436%
7	8.186	1032	1037	1040	rBV	3728534	3086402	32.73%	4.411%
8	9.263	1214	1220	1223	rBV	10475204	9430699	100.00%	13.480%
9	9.939	1331	1335	1338	rBV	4685385	3661886	38.83%	5.234%
10	10.039	1345	1352	1360	rBV	400264	542376	5.75%	0.775%
11	10.727	1464	1469	1472	rBV	6751737	5946248	63.05%	8.499%
12	11.421	1584	1587	1591	rBV	3738793	3409405	36.15%	4.873%
13	11.951	1673	1677	1682	rBV	480075	468542	4.97%	0.670%
14	12.733	1807	1810	1821	rBV	143272	171659	1.82%	0.245%
15	13.010	1853	1857	1861	rBV	8153636	7604643	80.64%	10.870%
16	13.492	1934	1939	1950	rBV	746041	786529	8.34%	1.124%
17	13.939	2008	2015	2028	rBV7	96761	330939	3.51%	0.473%
18	14.062	2032	2036	2044	rVV	1695795	1512495	16.04%	2.162%
19	15.545	2282	2288	2294	rBV	975620	1244023	13.19%	1.778%

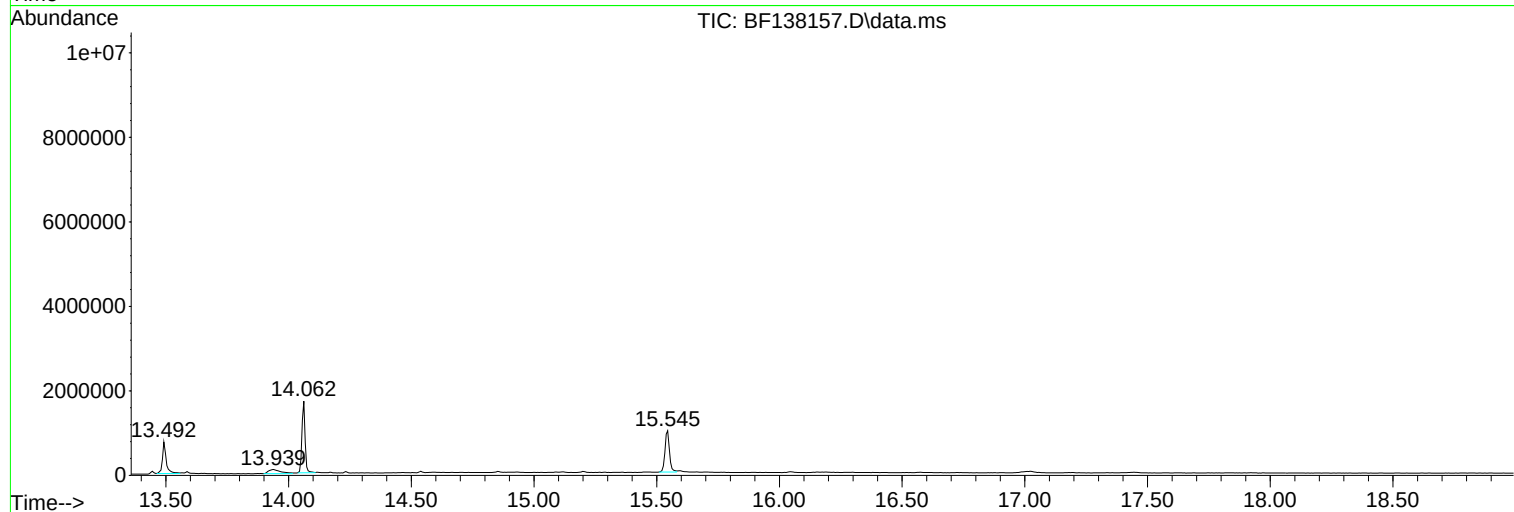
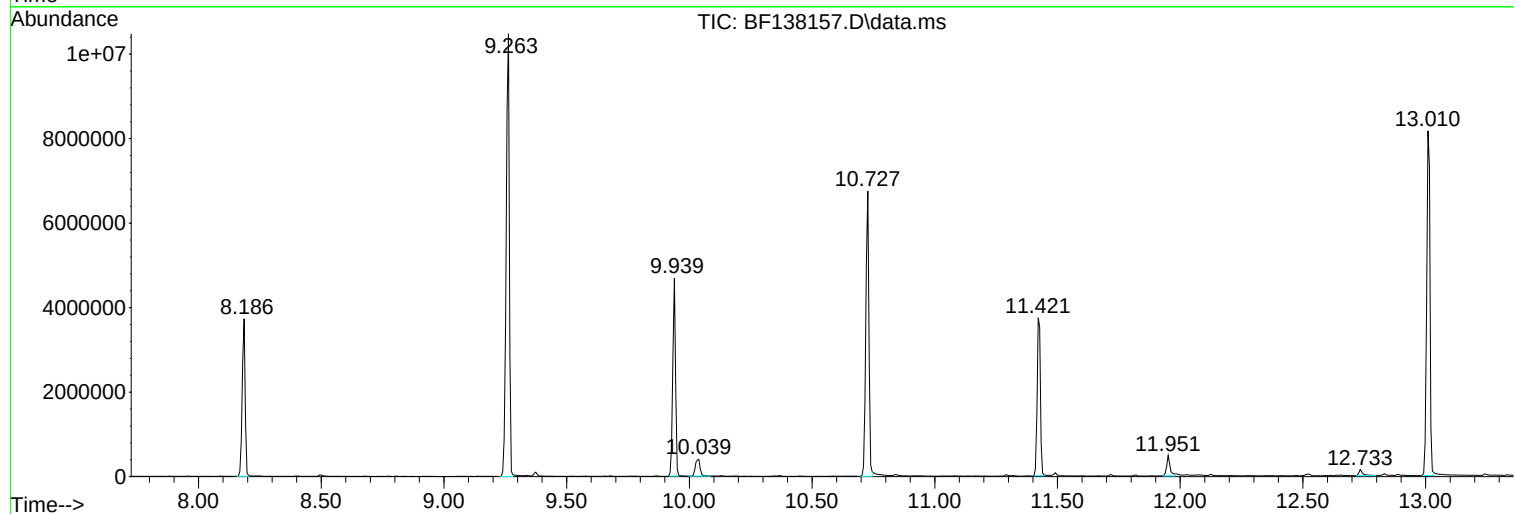
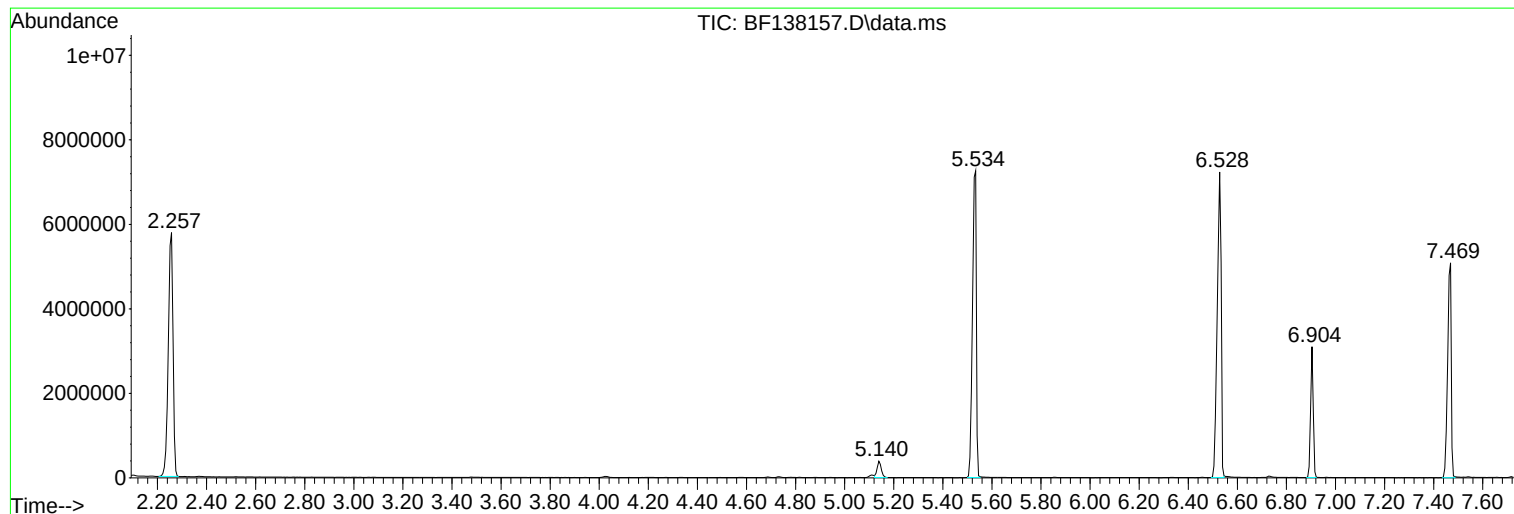
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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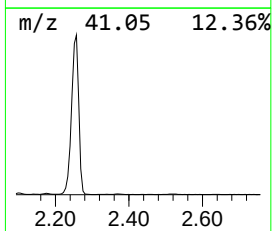
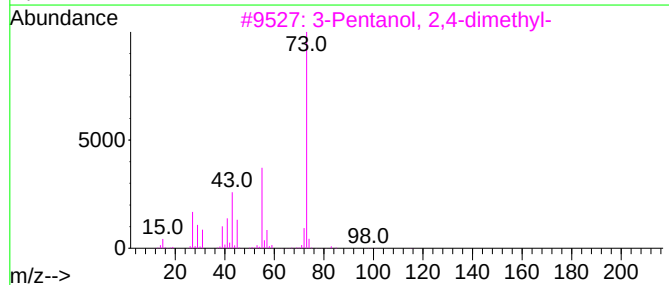
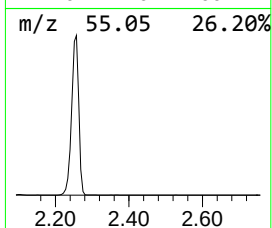
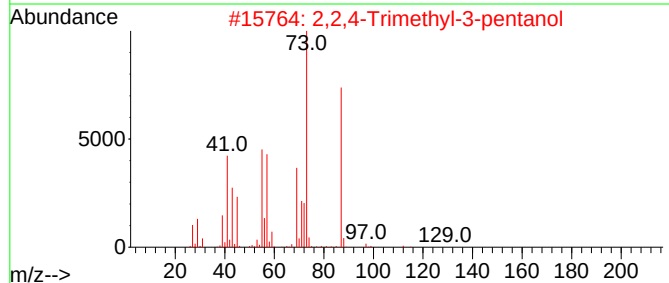
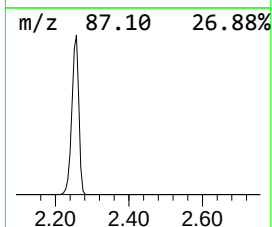
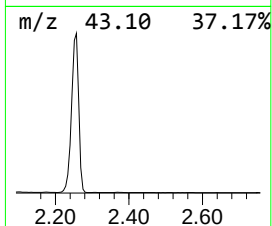
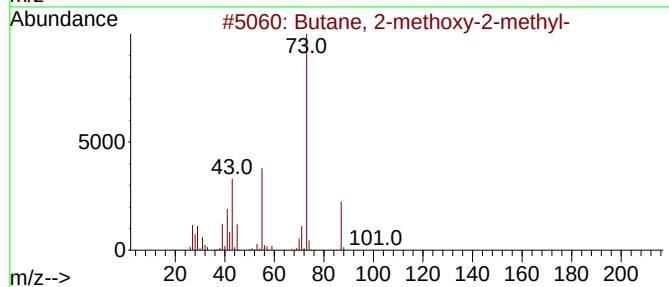
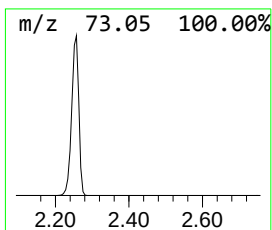
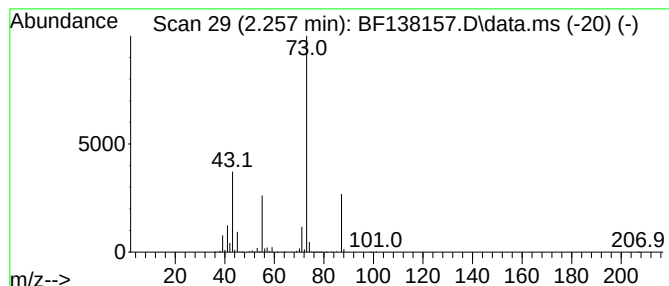
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	66.85 ng	7727850	1,4-Dichlorobenzene-d4	6.904

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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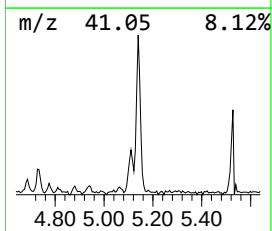
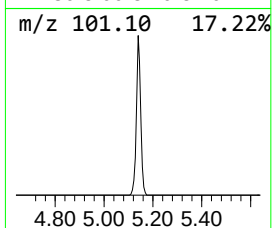
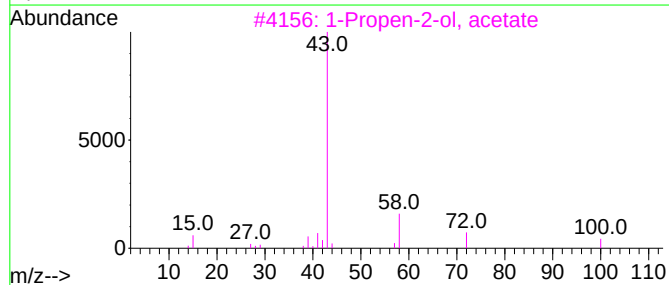
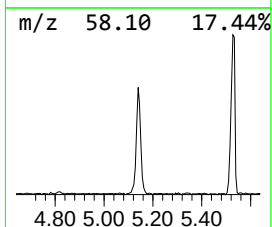
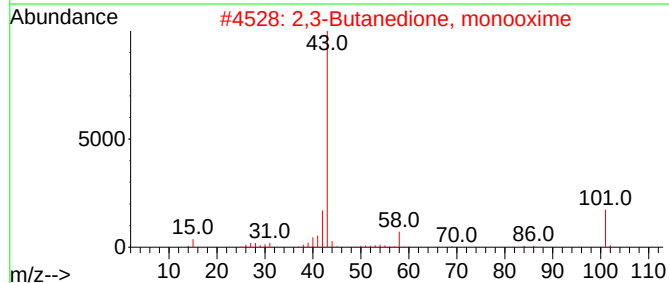
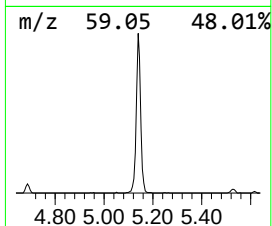
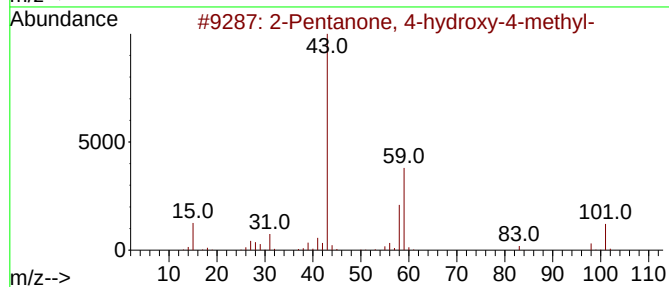
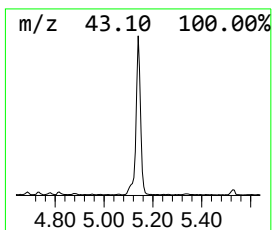
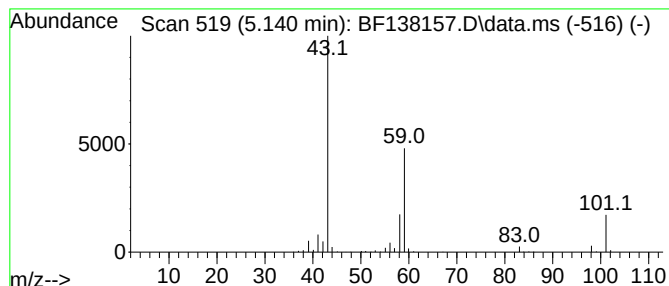
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	3.94 ng	455322	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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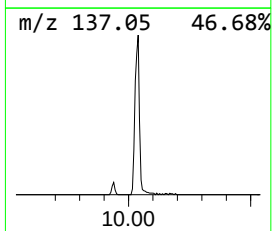
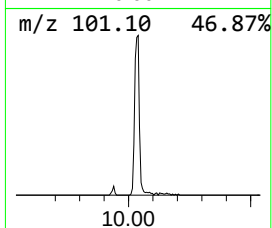
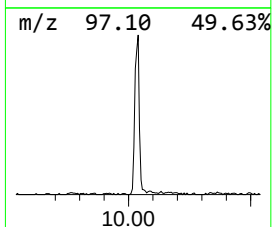
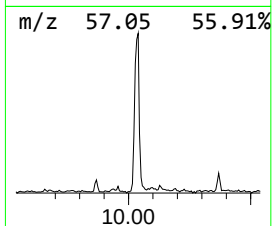
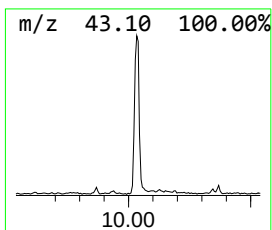
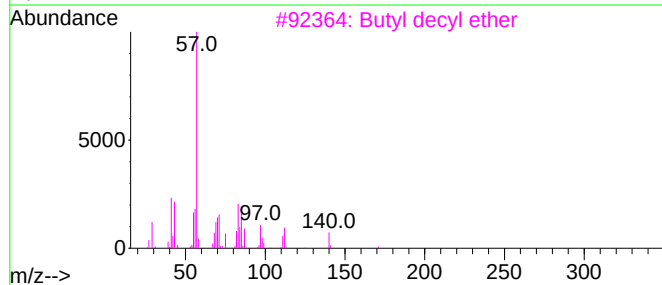
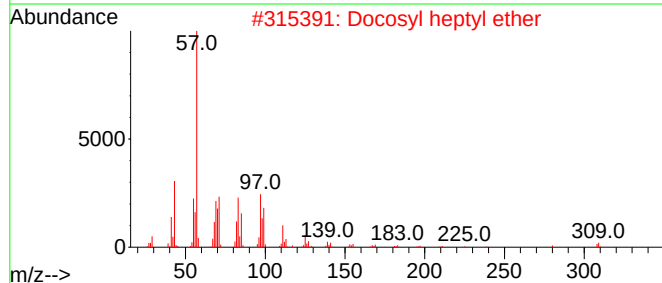
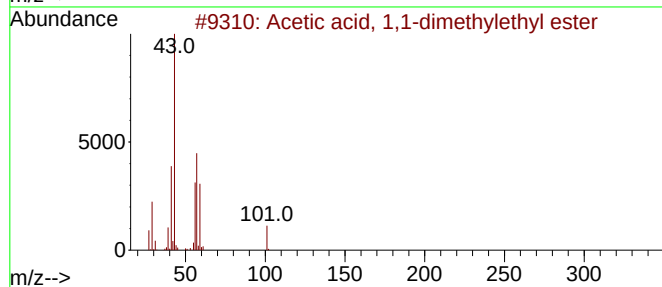
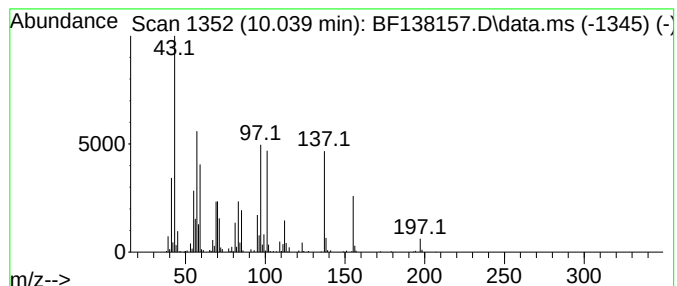
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Peak Number 3 unknown10.039 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.039	2.96 ng	542376	Acenaphthene-d10	9.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2	Docosyl heptyl ether	424	C29H60O	1000406-39-7	10
3	Butyl decyl ether	214	C14H30O	1000406-40-2	10
4	Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	10
5	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10



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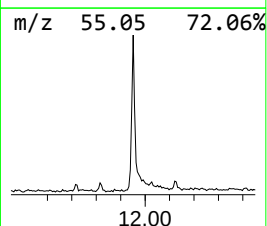
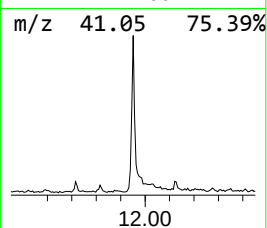
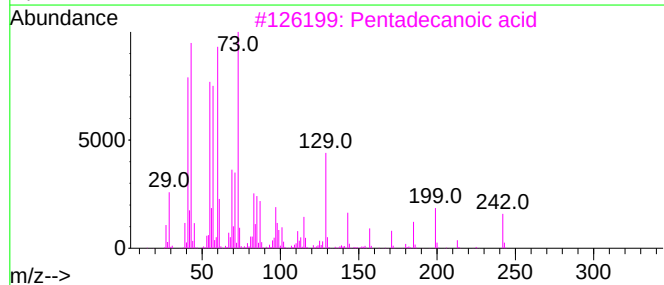
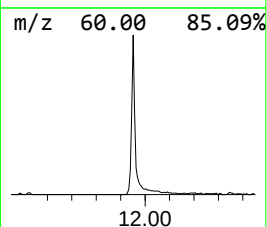
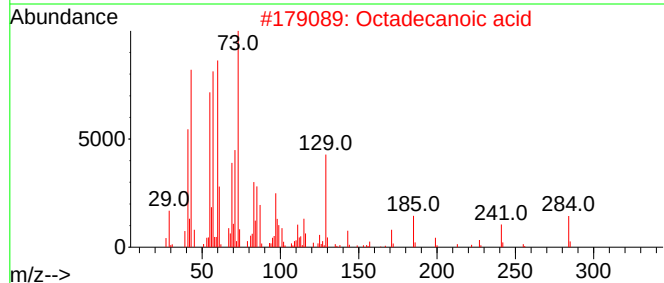
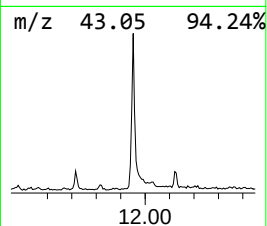
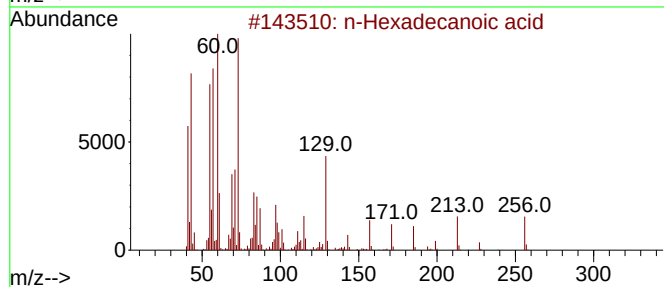
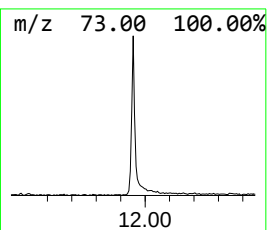
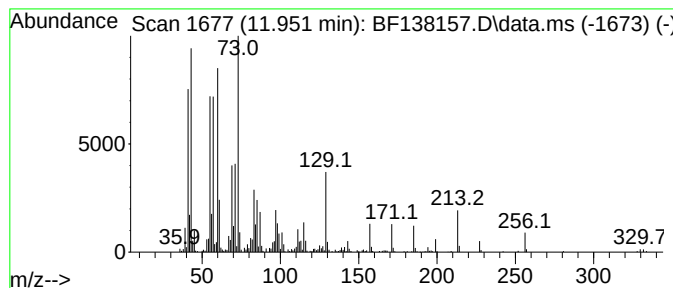
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.951	2.75 ng	468542	Phenanthrene-d10		11.421	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Octadecanoic acid		284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
4	Tridecanoic acid		214	C13H26O2	000638-53-9	81
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	76



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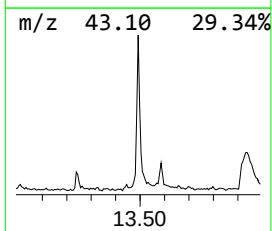
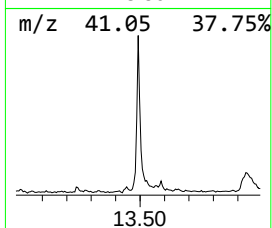
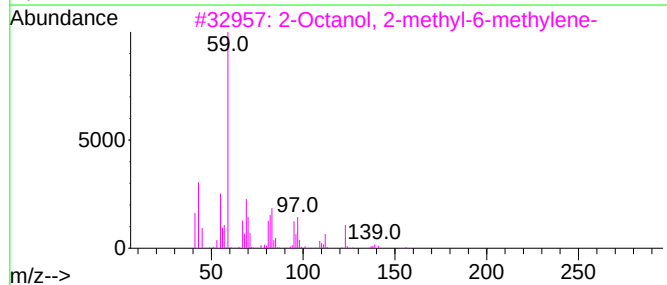
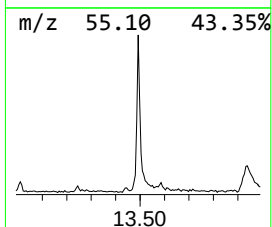
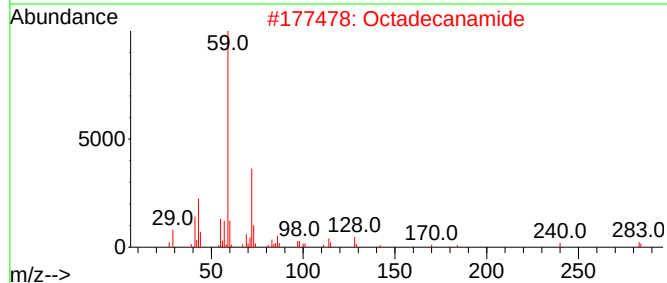
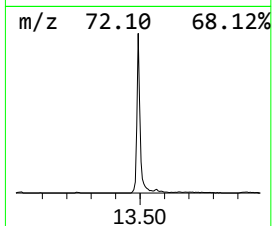
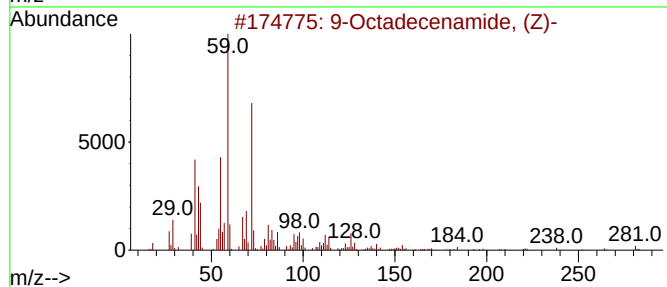
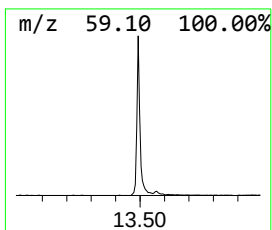
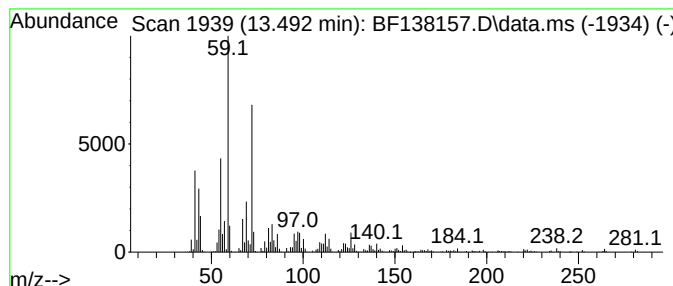
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	10.40 ng	786529	Chrysene-d12	14.062

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99	
2	Octadecanamide	283	C18H37NO	000124-26-5	53	
3	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	45	
4	2-Propanol, 1-(isooctyloxy)-2-me...	202	C12H26O2	056282-27-0	43	
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	38	



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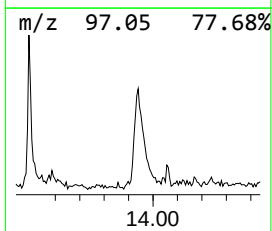
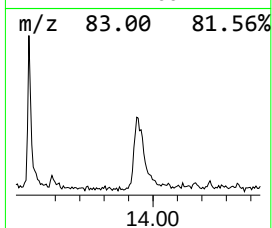
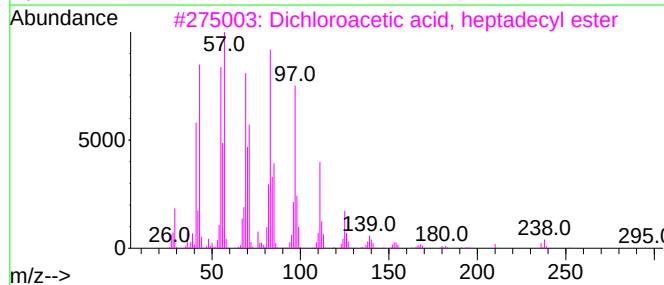
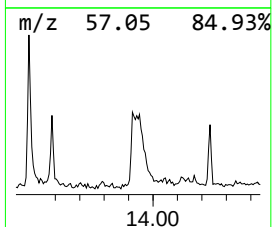
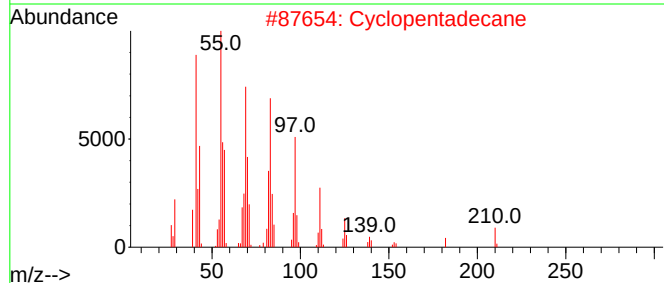
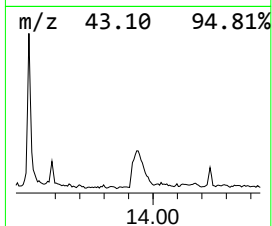
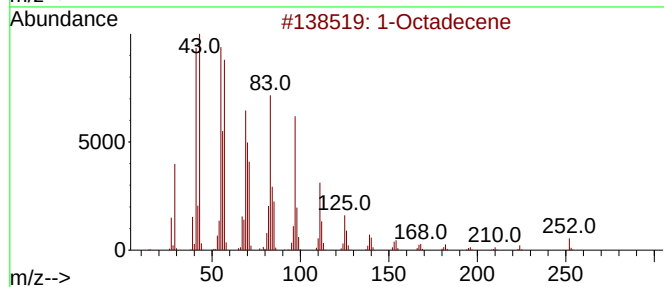
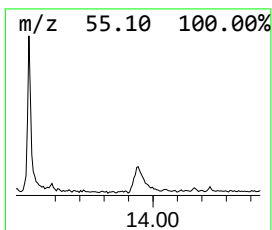
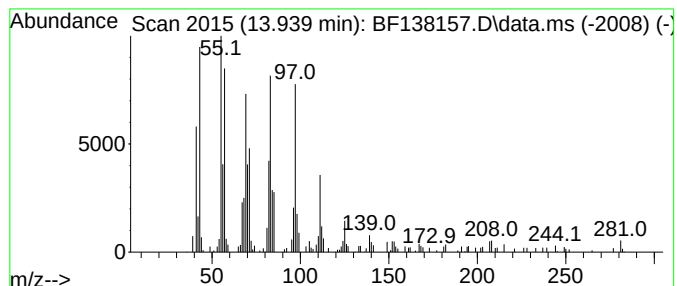
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	4.38 ng	330939	Chrysene-d12	14.062

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	98
2			Cyclopentadecane	210	C15H30	000295-48-7	96
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
Data File : BF138157.D
Acq On : 07 Jun 2024 13:36
Operator : CG\JU
Sample : P2740-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.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...	2.257	66.8	ng	7727850	1	6.904	2311850	20.0
2-Pentanone, 4-...	5.140	3.9	ng	455322	1	6.904	2311850	20.0
unknown10.039	10.039	3.0	ng	542376	3	9.939	3661890	20.0
n-Hexadecanoic ...	11.951	2.8	ng	468542	4	11.421	3409410	20.0
9-Octadecenamid...	13.492	10.4	ng	786529	5	14.062	1512500	20.0
1-Octadecene	13.939	4.4	ng	330939	5	14.062	1512500	20.0