

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062518\
 Data File : BF106774.D
 Acq On : 25 Jun 2018 16:37
 Operator : JU/SJ
 Sample : J3573-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-49-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF061918.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.213	484	489	499	rBB	98504	136237	6.36%	0.879%
2	5.607	552	556	560	rBV	1298023	1357110	63.34%	8.751%
3	6.607	721	726	729	rBV	1189064	1444861	67.43%	9.317%
4	6.742	743	749	752	rBV	1290918	1420039	66.27%	9.157%
5	6.960	782	786	789	rBV	373910	311659	14.55%	2.010%
6	7.119	808	813	816	rBV	1190803	1176463	54.91%	7.586%
7	7.525	876	882	885	rBV	898813	987349	46.08%	6.367%
8	8.242	999	1004	1007	rBV	433466	394972	18.43%	2.547%
9	9.319	1181	1187	1190	rBV	1664841	1808359	84.40%	11.661%
10	9.707	1248	1253	1258	rBV	233881	199907	9.33%	1.289%
11	9.907	1284	1287	1298	rBV2	34812	39955	1.86%	0.258%
12	10.001	1298	1303	1309	rVB	537653	480826	22.44%	3.101%
13	10.407	1370	1372	1375	rVB	42969	34509	1.61%	0.223%
14	10.795	1433	1438	1442	rBV	1119898	1255630	58.60%	8.097%
15	10.883	1450	1453	1458	rBV	44322	42261	1.97%	0.273%
16	11.495	1553	1557	1560	rBV	597741	540599	25.23%	3.486%
17	13.083	1821	1827	1830	rBV	1834230	2142719	100.00%	13.817%
18	13.601	1910	1915	1917	rBV	227766	212674	9.93%	1.371%
19	13.960	1972	1976	1982	rBV	208831	194832	9.09%	1.256%
20	14.154	2005	2009	2013	rVB	536771	476304	22.23%	3.071%
21	14.289	2029	2032	2041	rBV5	27231	39747	1.85%	0.256%
22	14.424	2052	2055	2060	rVB	73484	62896	2.94%	0.406%
23	14.624	2084	2089	2094	rBV2	36997	55098	2.57%	0.355%
24	15.095	2165	2169	2173	rBV	37486	39359	1.84%	0.254%
25	15.707	2268	2273	2279	rBV	289659	383642	17.90%	2.474%
26	16.218	2355	2360	2366	rBV7	11376	22232	1.04%	0.143%
27	16.748	2446	2450	2456	rVB	13261	22768	1.06%	0.147%
28	17.877	2638	2642	2647	rBV6	11674	23007	1.07%	0.148%
29	18.306	2711	2715	2723	rVB8	14353	33737	1.57%	0.218%
30	18.489	2739	2746	2756	rVB6	41211	89846	4.19%	0.579%
31	18.718	2779	2785	2786	rBV5	18212	27491	1.28%	0.177%
32	18.806	2796	2800	2808	rVB9	22160	50787	2.37%	0.327%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

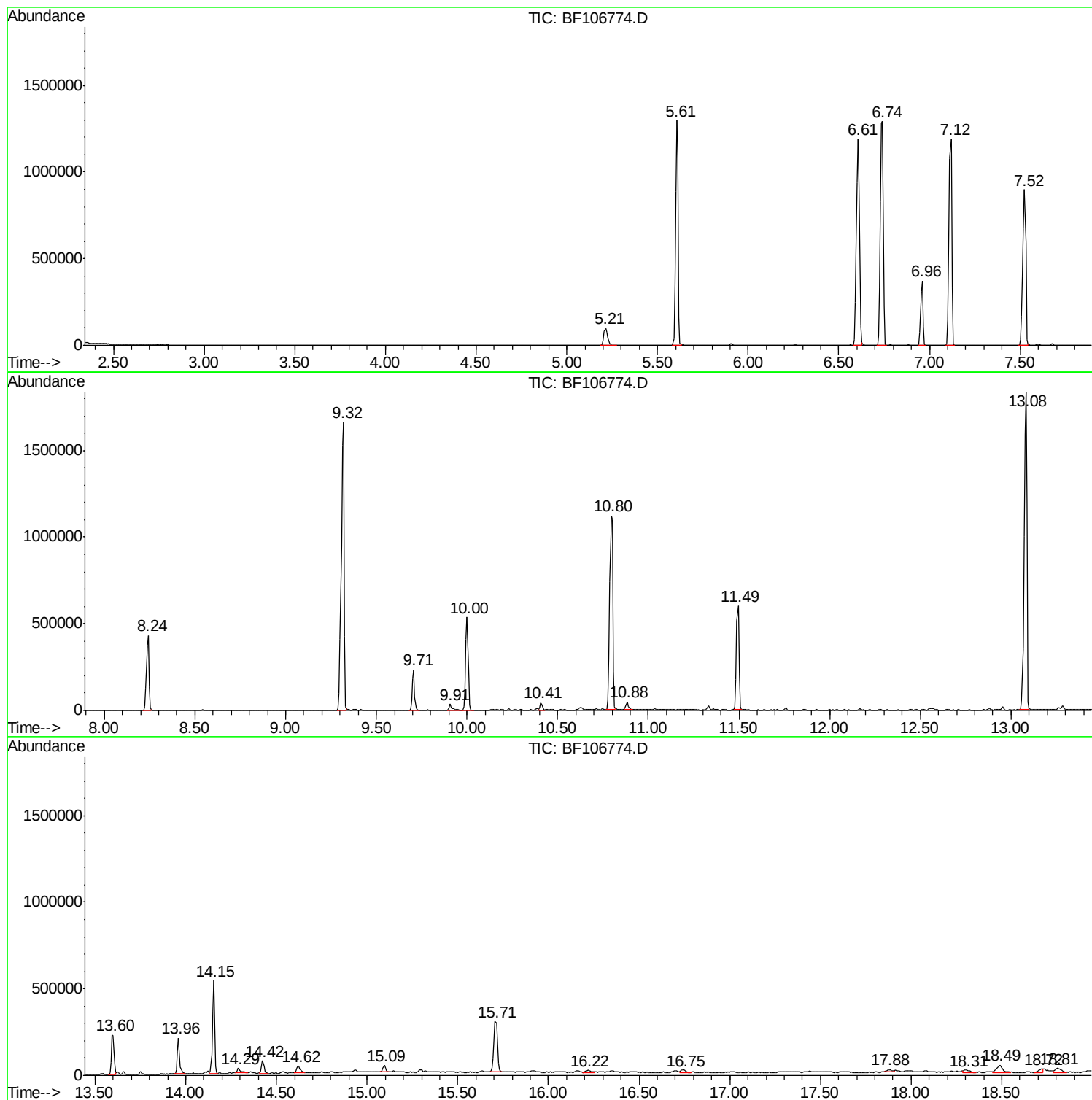
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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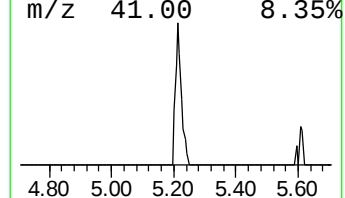
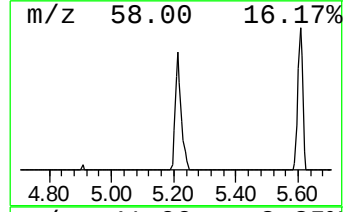
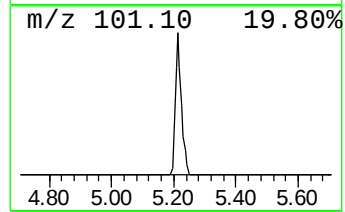
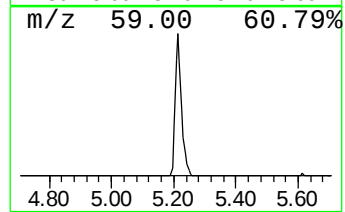
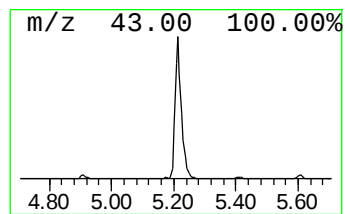
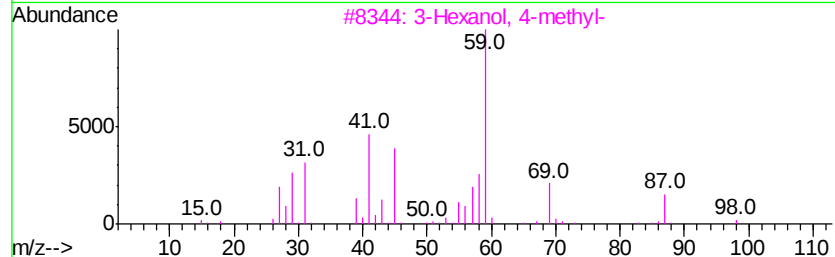
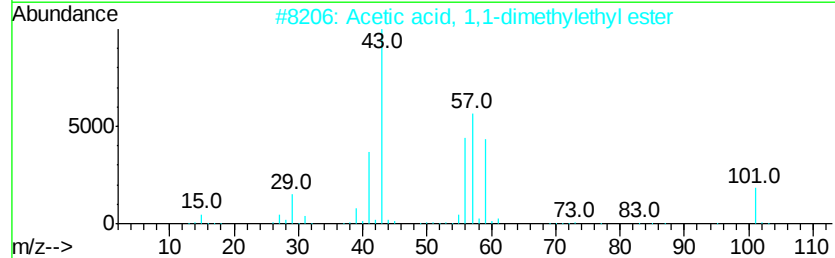
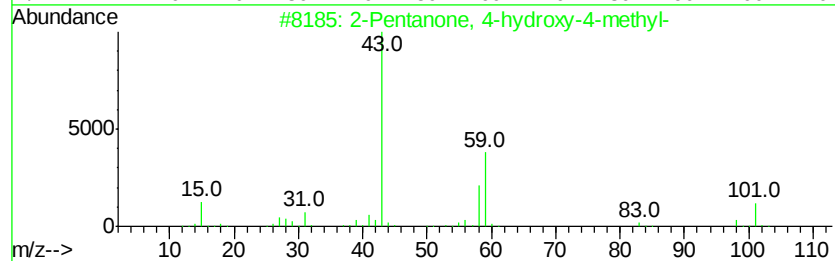
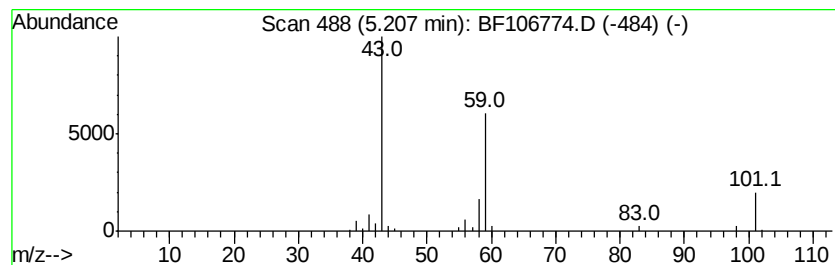
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	8.74 ng	136237	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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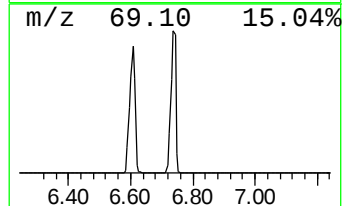
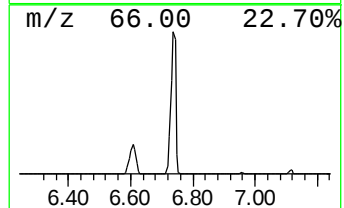
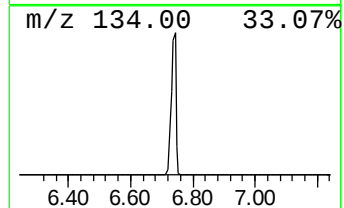
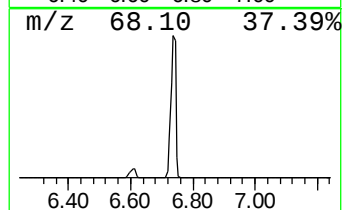
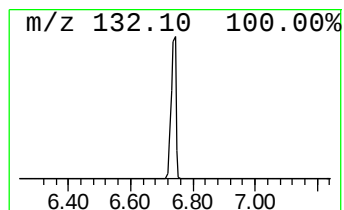
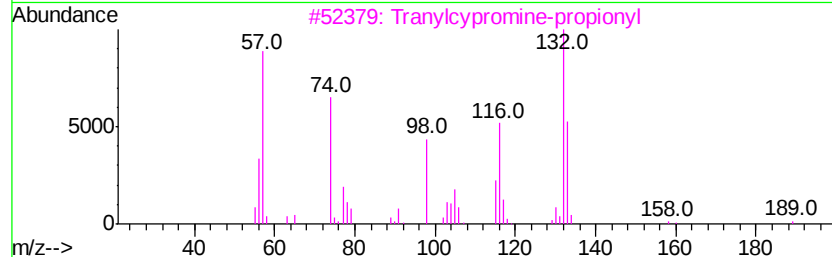
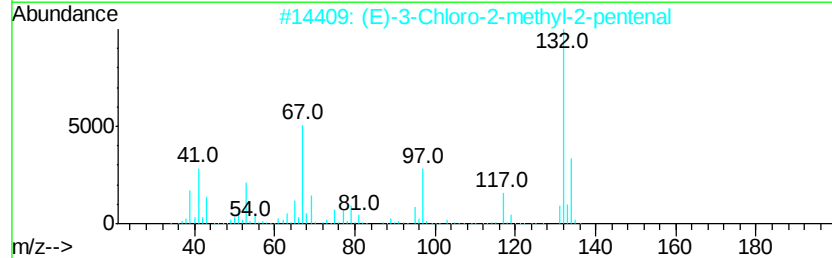
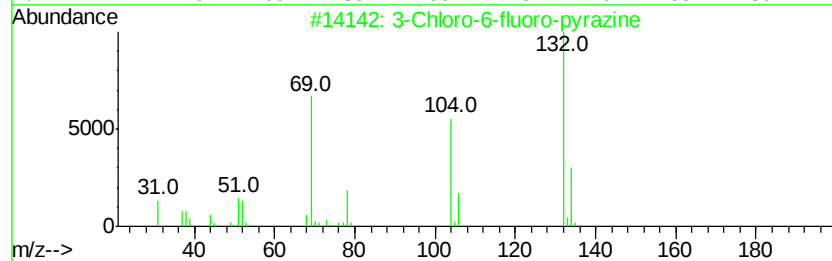
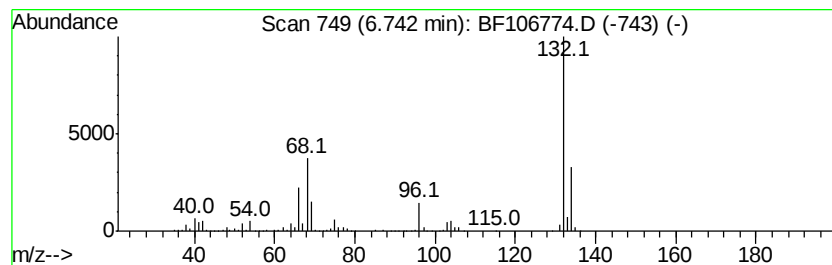
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	91.13 ng	1420040	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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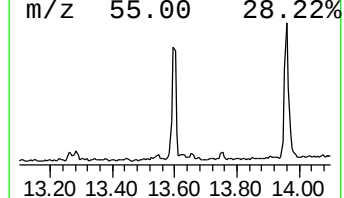
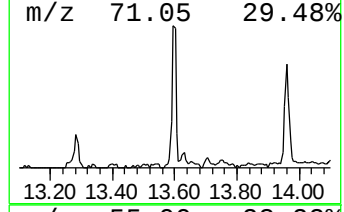
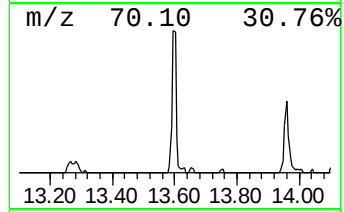
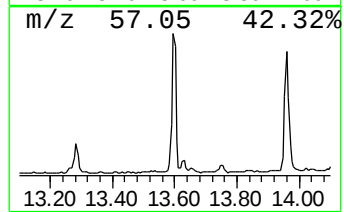
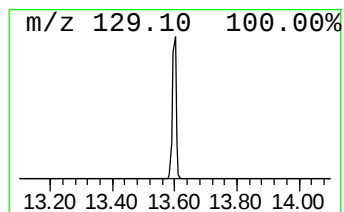
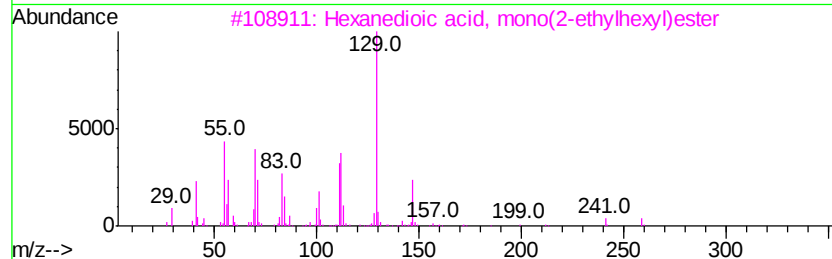
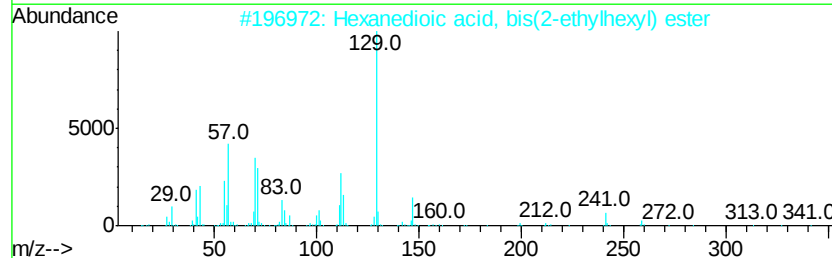
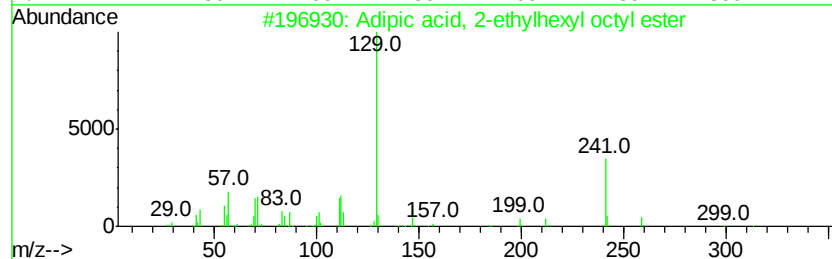
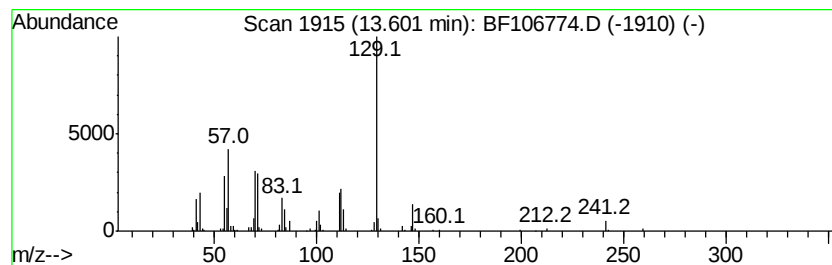
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Adipic acid, 2-ethylhexyl o... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	8.93 ng	212674	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2		Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
3		Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68
4		Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	64
5		Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	59



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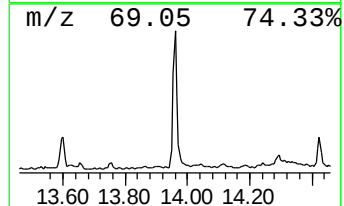
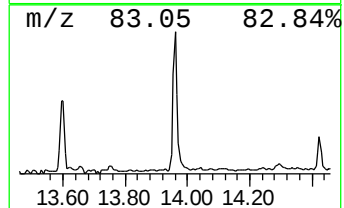
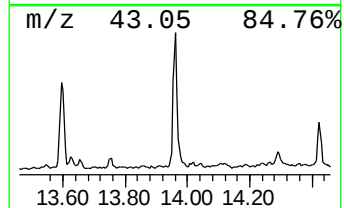
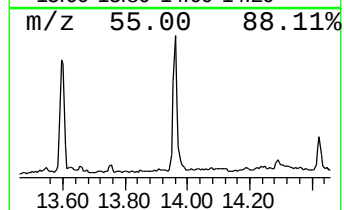
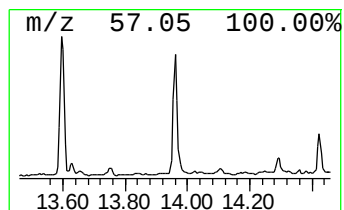
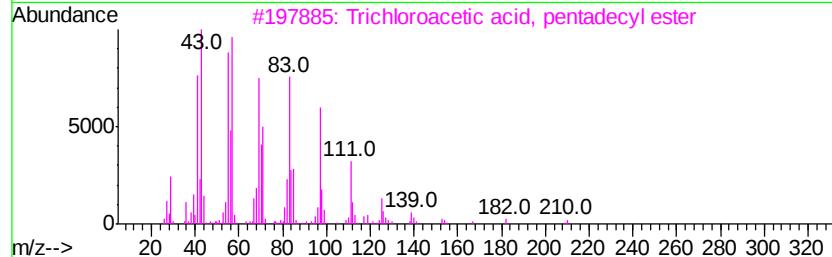
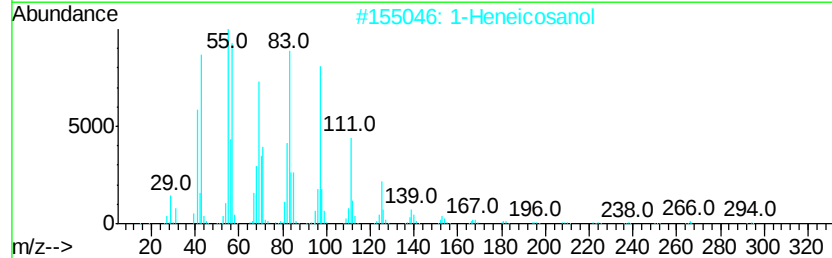
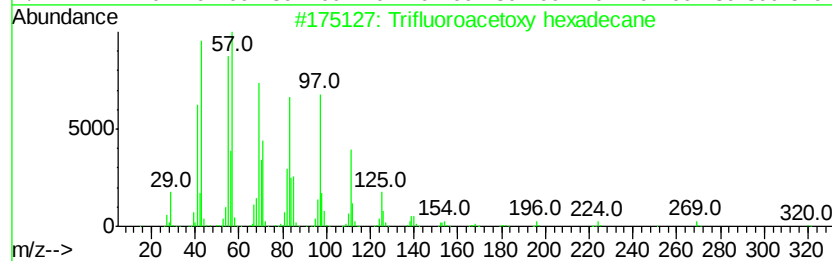
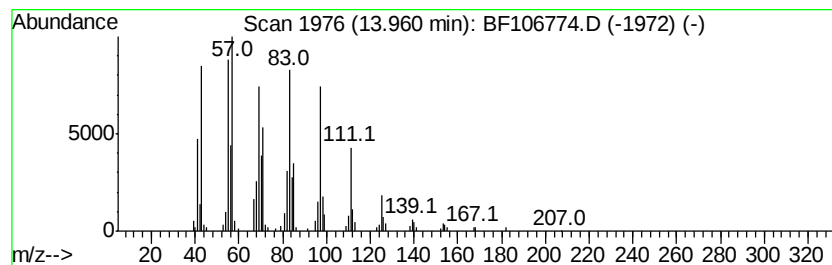
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.96	8.18 ng	194832	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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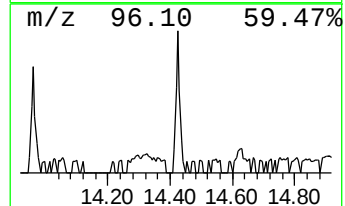
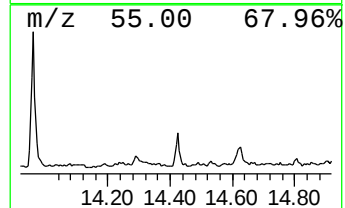
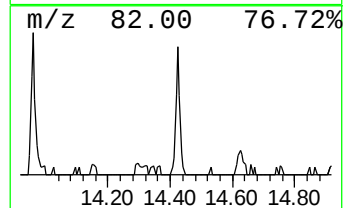
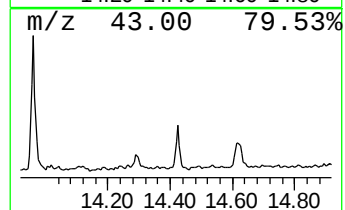
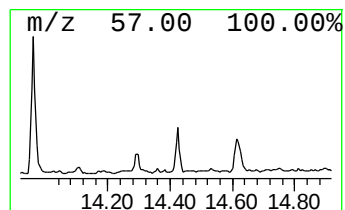
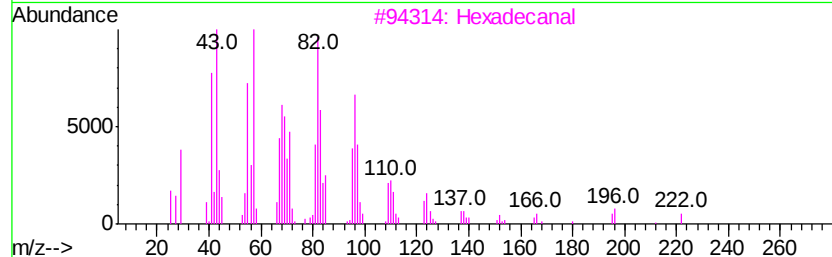
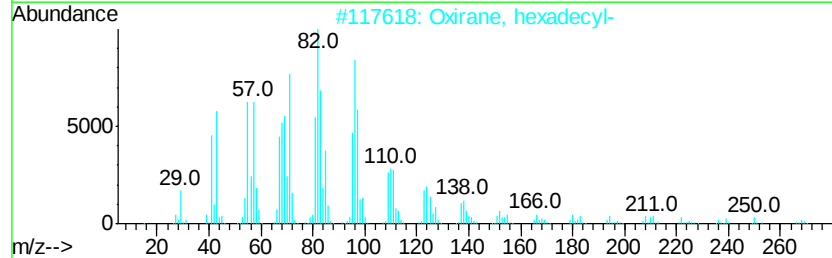
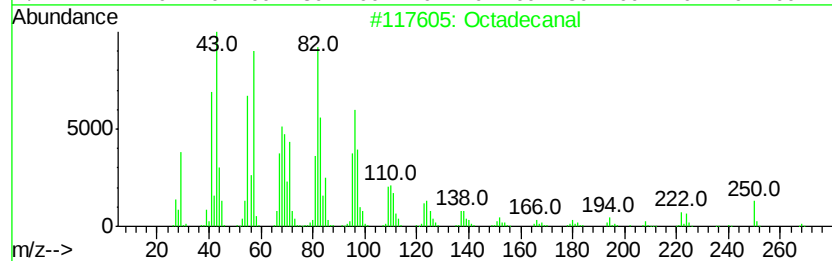
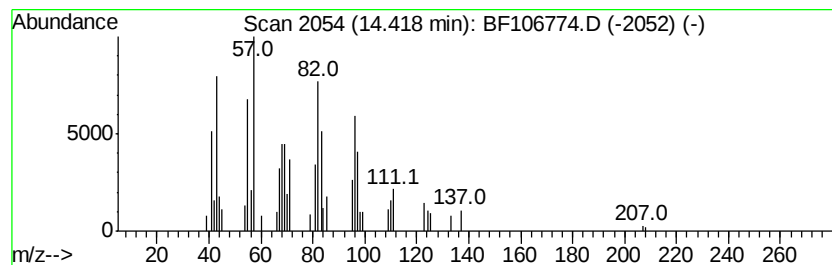
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.64 ng	62896	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal		268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91
3	Hexadecanal		240	C16H32O	000629-80-1	91
4	Heptadecanal		254	C17H34O	1000376-70-0	91
5	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062518\
Data File : BF106774.D
Acq On : 25 Jun 2018 16:37
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49-COMP

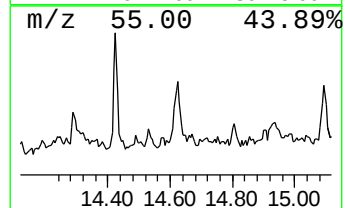
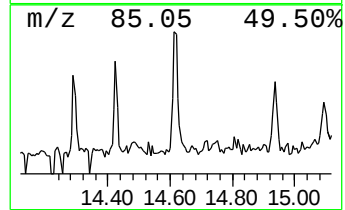
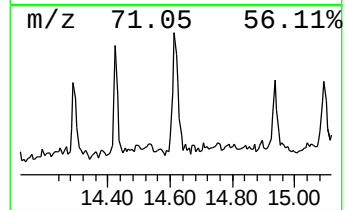
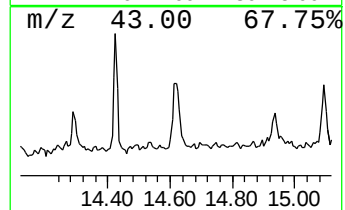
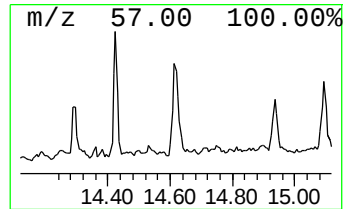
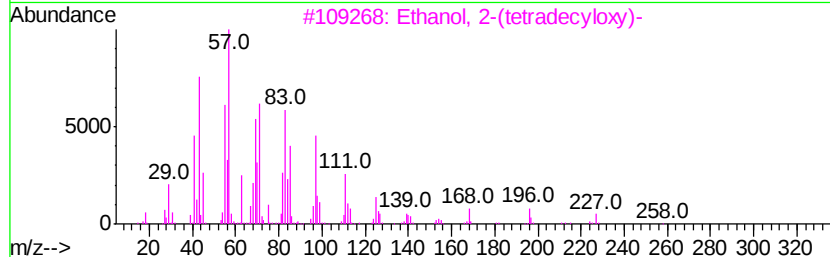
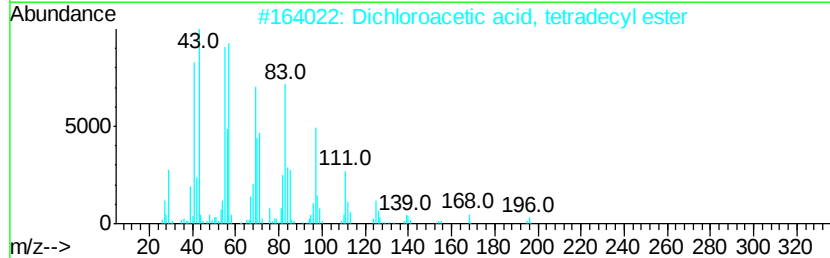
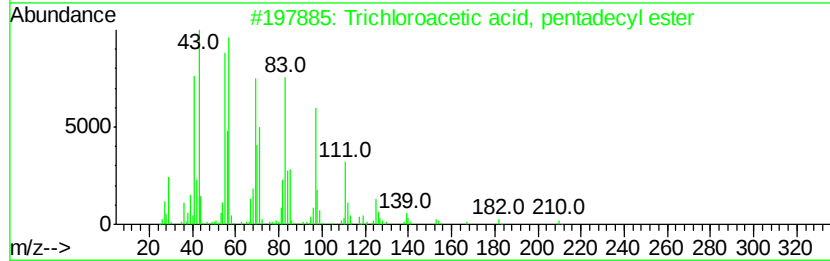
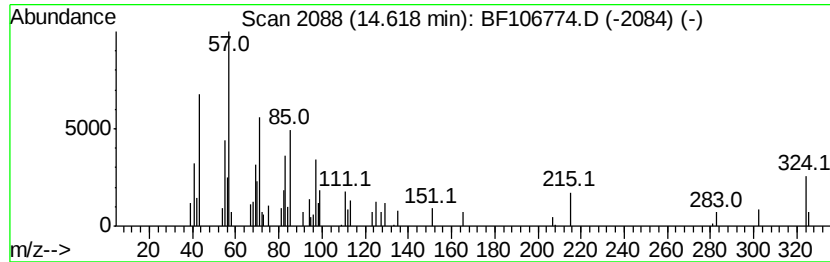
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.31 ng	55098	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	60
2		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	60
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	58
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	53
5		1-Tricosene	322	C23H46	018835-32-0	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062518\
Data File : BF106774.D
Acq On : 25 Jun 2018 16:37
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49-COMP

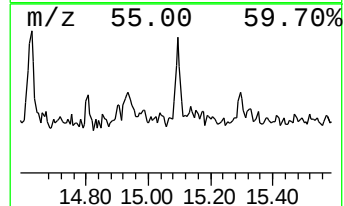
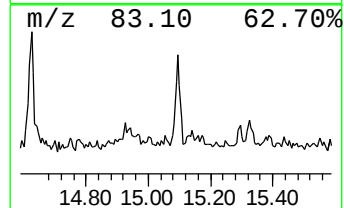
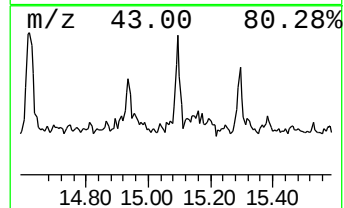
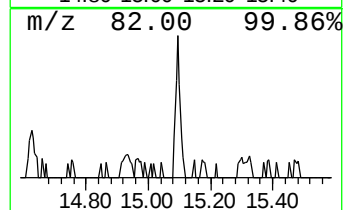
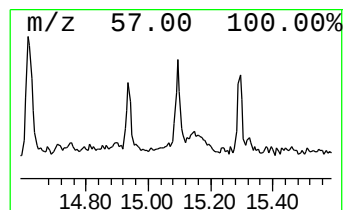
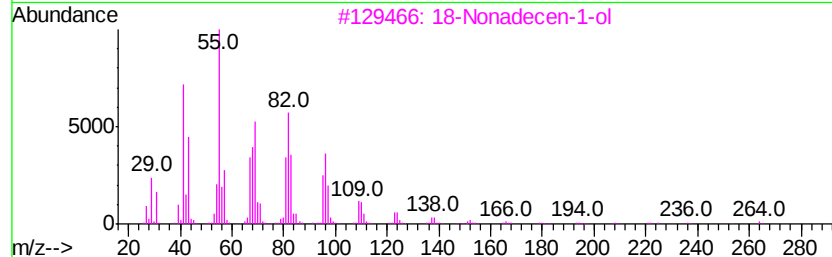
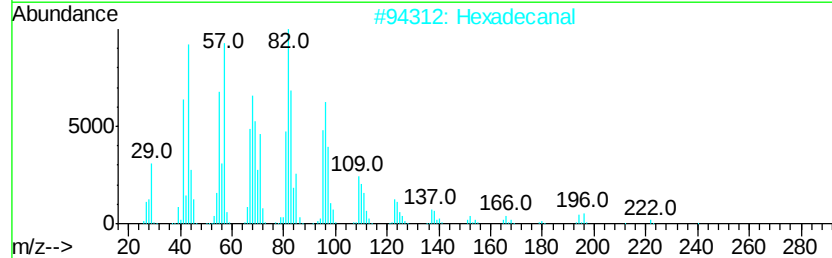
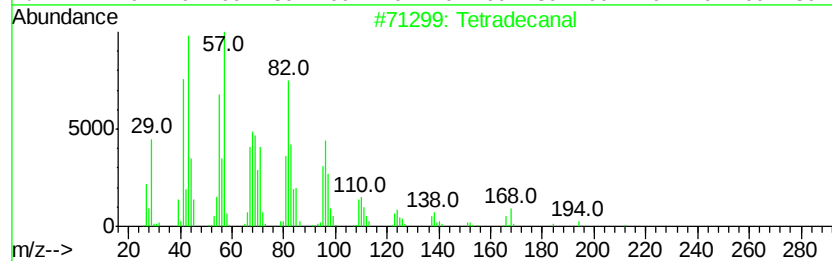
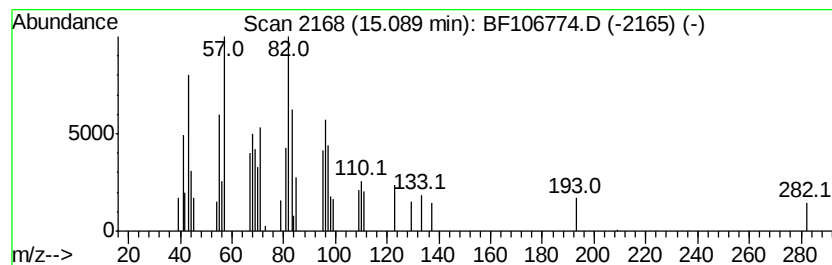
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tetradecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.05 ng	39359	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecanal	212	C14H28O	000124-25-4	90
2		Hexadecanal	240	C16H32O	000629-80-1	83
3		18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	64
4		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	64
5		1,15-Pentadecanediol	244	C15H32O2	014722-40-8	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062518\
Data File : BF106774.D
Acq On : 25 Jun 2018 16:37
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49-COMP

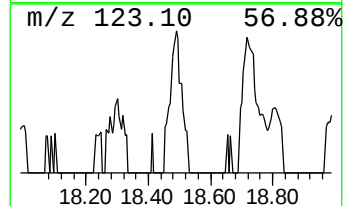
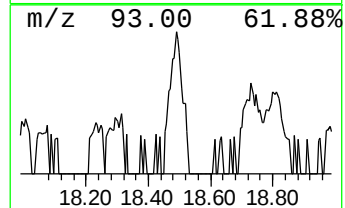
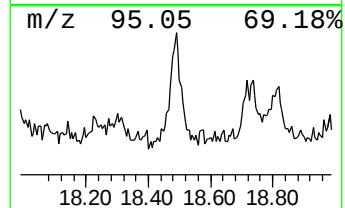
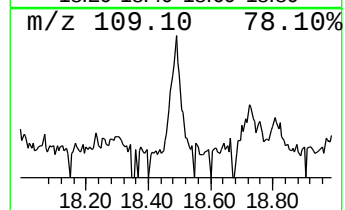
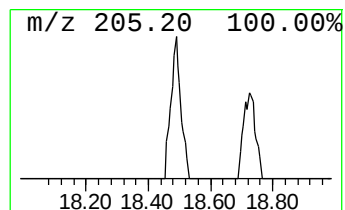
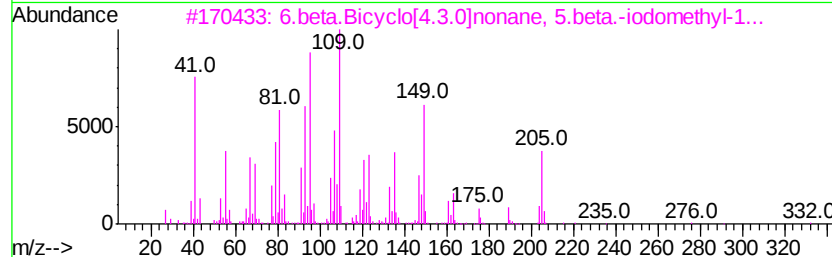
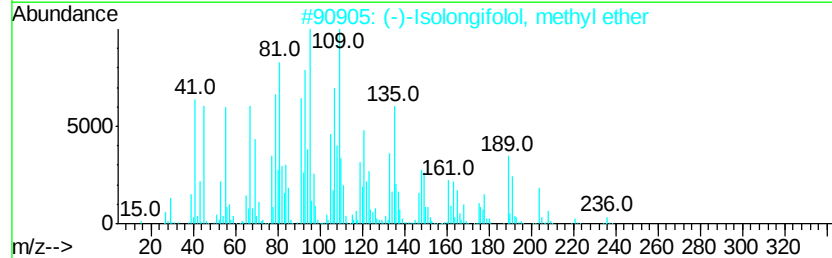
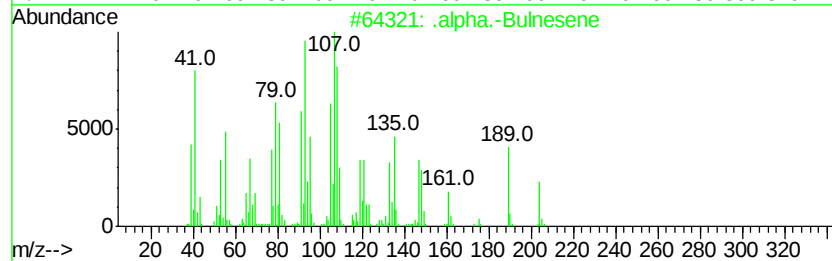
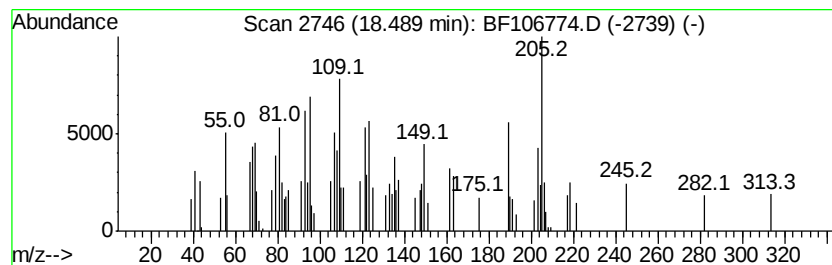
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 .alpha.-Bulnesene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	4.68 ng	89846	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Bulnesene	204	C15H24	1000374-19-9	55
2		(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	38
3		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	38
4		2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	35
5		Longifolenaldehyde	220	C15H24O	019890-84-7	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062518\
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Acq On : 25 Jun 2018 16:37
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49-COMP

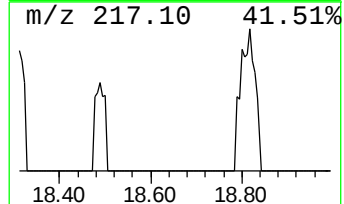
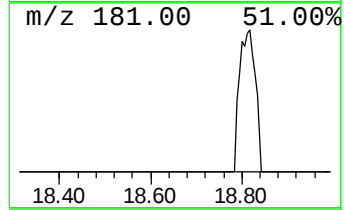
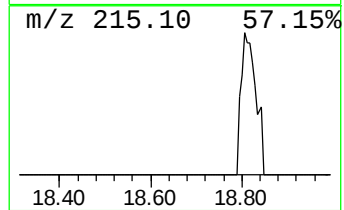
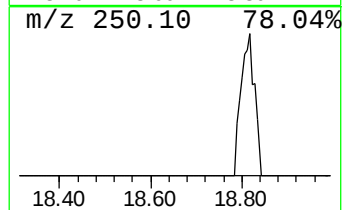
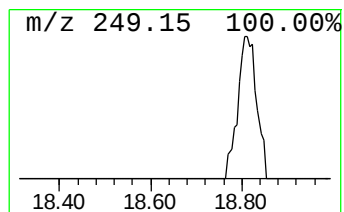
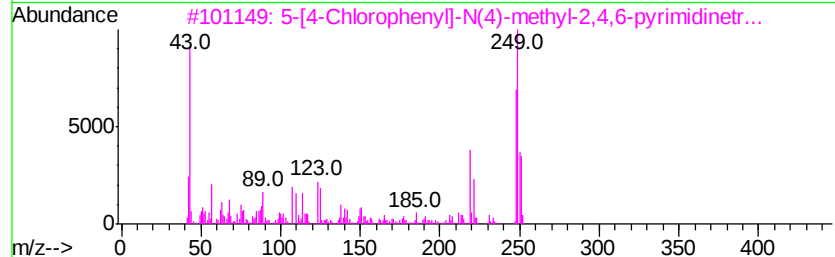
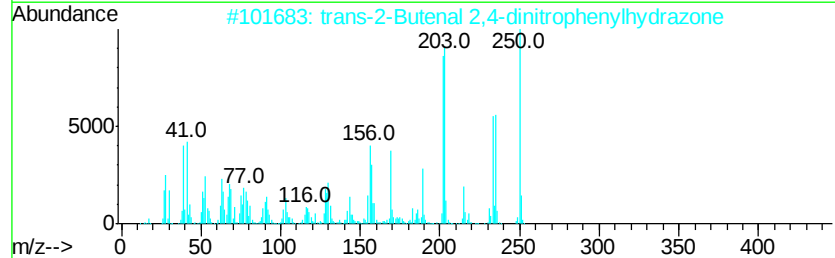
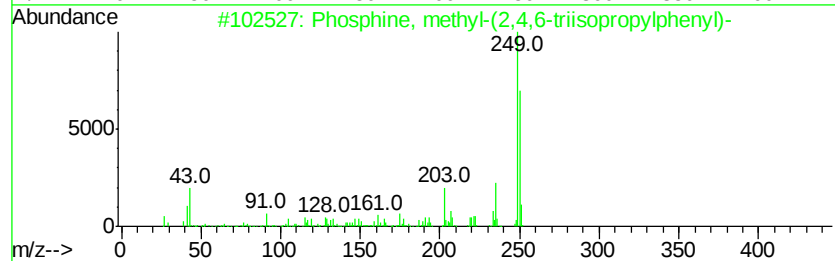
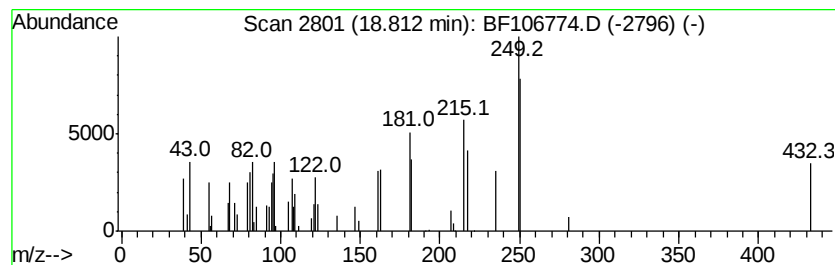
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown18.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.81	2.65 ng	50787	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phosphine, methyl-(2,4,6-triisopropylphenyl)-	250	C16H27P	158748-69-7	35
2		trans-2-Butenal 2,4-dinitrophenylhydrazone	250	C10H10N4O4	018318-80-4	18
3		5-[4-Chlorophenyl]-N(4)-methyl-2,4,6-pyrimidinetr...	249	C11H12ClN5	1000212-53-8	18
4		12H-Benzo[alpha]phenothiazine	249	C16H11NS	000225-83-2	16
5		2-Benzoyl-1,3-indanedione	250	C16H10O3	001785-95-1	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062518\
Data File : BF106774.D
Acq On : 25 Jun 2018 16:37
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	8.7	ng	136237	1	6.96	311659	20.0
unknown6.74	6.74	91.1	ng	1420040	1	6.96	311659	20.0
Adipic acid, 2-et...	13.60	8.9	ng	212674	5	14.15	476304	20.0
Trifluoroacetoxy ...	13.96	8.2	ng	194832	5	14.15	476304	20.0
Octadecanal	14.42	2.6	ng	62896	5	14.15	476304	20.0
Trichloroacetic a...	14.62	2.3	ng	55098	5	14.15	476304	20.0
Tetradecanal	15.09	2.0	ng	39359	6	15.71	383642	20.0
.alpha.-Bulnesene	18.49	4.7	ng	89846	6	15.71	383642	20.0
unknown18.81	18.81	2.6	ng	50787	6	15.71	383642	20.0