

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032618\
 Data File : BF103924.D
 Acq On : 26 Mar 2018 14:24
 Operator : JU/SJ
 Sample : J1994-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-MW-06-032018

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:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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	2.322	34	40	47	rVB	486540	619838	9.00%	1.486%
2	5.204	527	530	537	rBV	116735	138021	2.00%	0.331%
3	5.598	592	597	600	rBV	2110208	1871474	27.19%	4.488%
4	6.592	762	766	778	rVB	1293951	1143439	16.61%	2.742%
5	6.745	787	792	795	rBV	3423568	3227440	46.88%	7.739%
6	6.975	827	831	834	rBV	1033231	870041	12.64%	2.086%
7	7.134	853	858	861	rBV	3189102	3070922	44.61%	7.364%
8	7.539	921	927	930	rBV	2585561	2737083	39.76%	6.563%
9	8.257	1045	1049	1052	rBV	1312359	1174850	17.07%	2.817%
10	9.333	1226	1232	1235	rBV	4457571	4624155	67.17%	11.088%
11	9.716	1292	1297	1302	rBV	147940	132796	1.93%	0.318%
12	9.928	1329	1333	1336	rBV	89324	71936	1.04%	0.172%
13	10.016	1343	1348	1359	rVB	1533380	1382797	20.09%	3.316%
14	10.427	1411	1418	1421	rBV2	115901	99798	1.45%	0.239%
15	10.810	1478	1483	1486	rBV	2727203	2824667	41.03%	6.773%
16	10.898	1495	1498	1504	rVB	85214	91984	1.34%	0.221%
17	11.510	1598	1602	1605	rBV	1623674	1366296	19.85%	3.276%
18	13.104	1867	1873	1876	rBV	4248954	4933288	71.66%	11.829%
19	13.974	2017	2021	2028	rBV	102554	111058	1.61%	0.266%
20	14.163	2048	2053	2056	rBV	1511535	1375320	19.98%	3.298%
21	15.015	2193	2198	2205	rBV	185946	191222	2.78%	0.459%
22	15.174	2213	2225	2226	rBV2	57268	137583	2.00%	0.330%
23	15.245	2228	2237	2240	rBV	307752	755211	10.97%	1.811%
24	15.304	2241	2247	2248	rBV	397688	640383	9.30%	1.536%
25	15.704	2309	2315	2327	rVB2	832710	1227749	17.83%	2.944%
26	18.374	2711	2769	2770	rBV5	840173	6884070	100.00%	16.507%

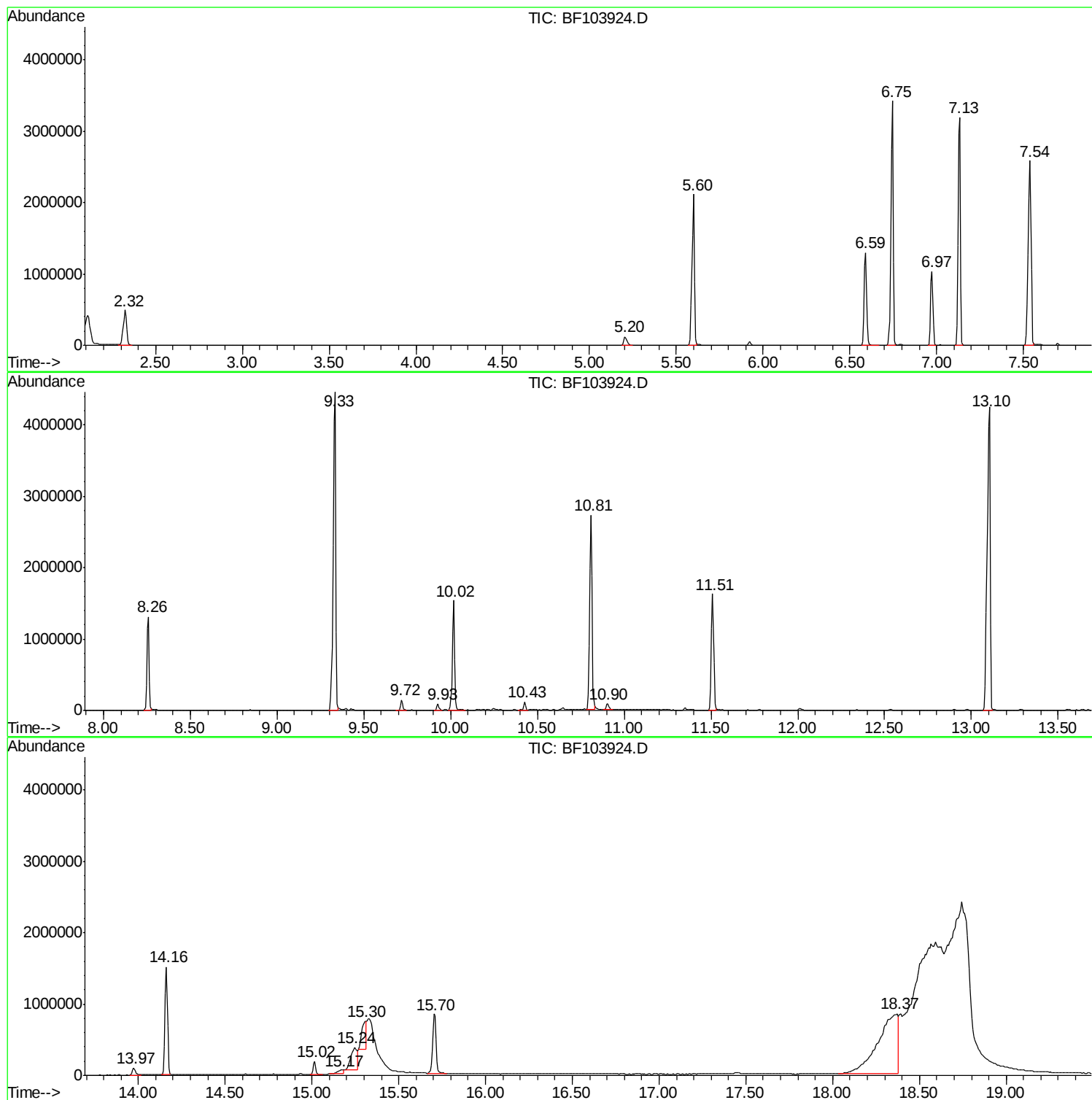
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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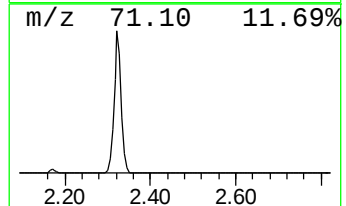
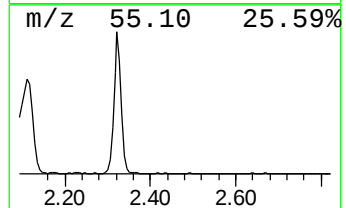
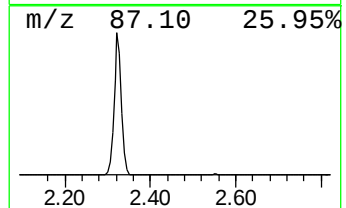
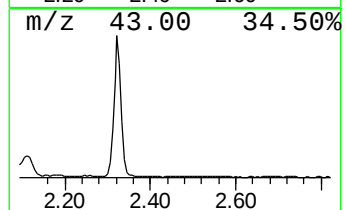
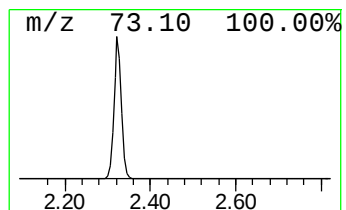
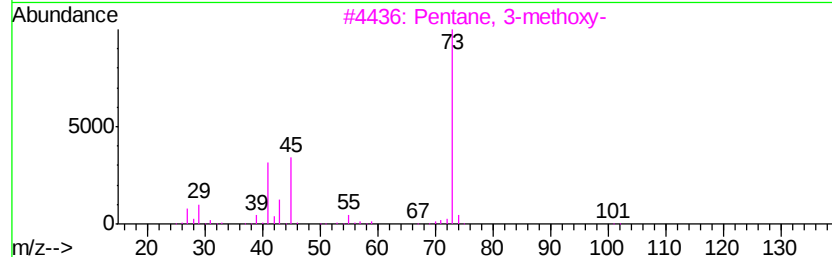
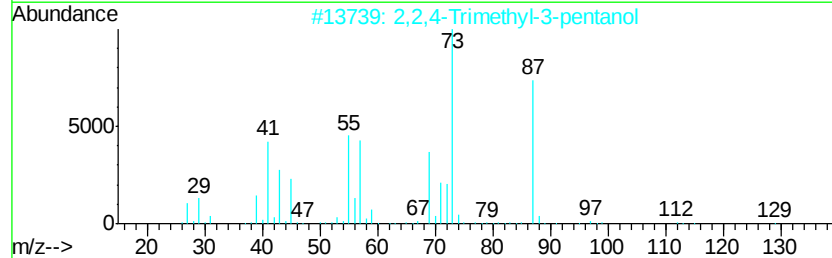
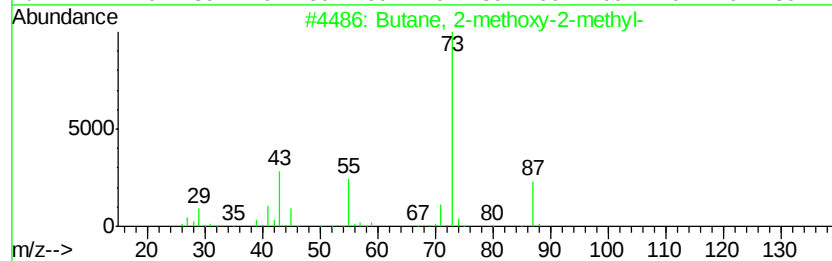
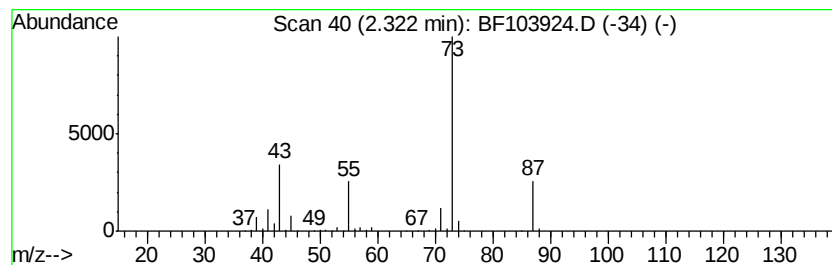
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	14.25 ng	619838	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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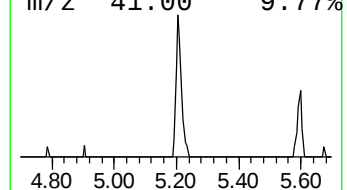
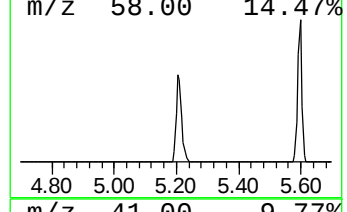
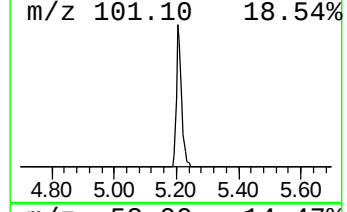
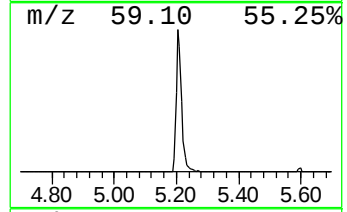
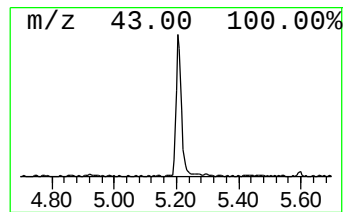
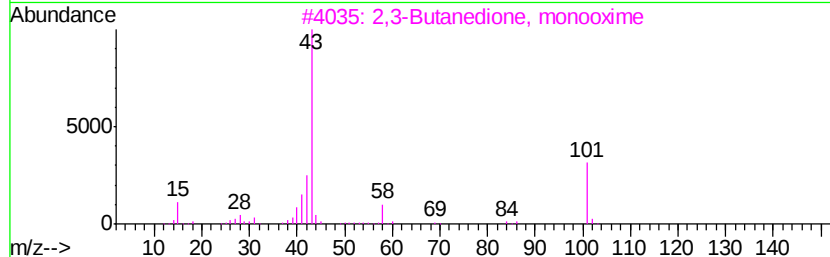
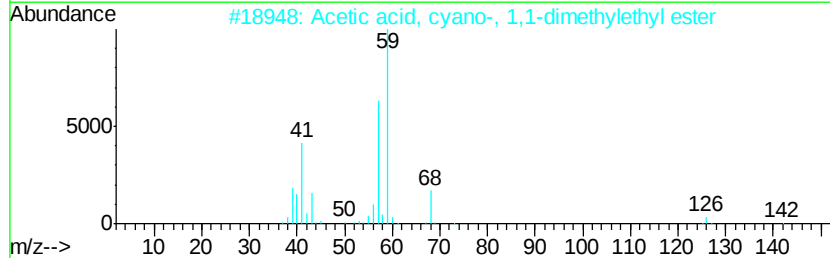
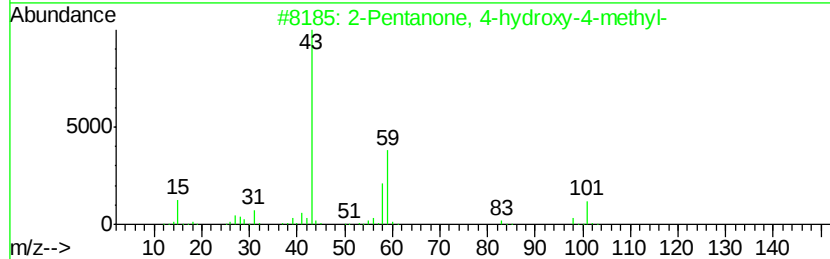
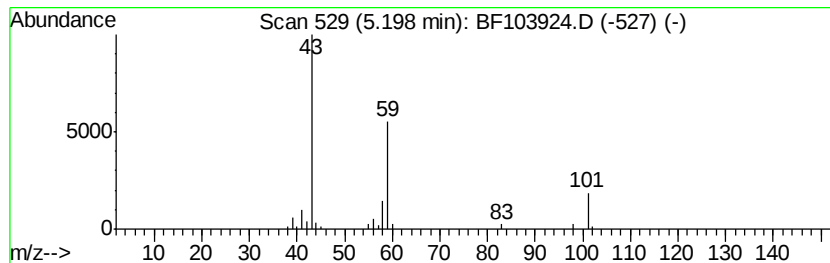
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.17 ng	138021	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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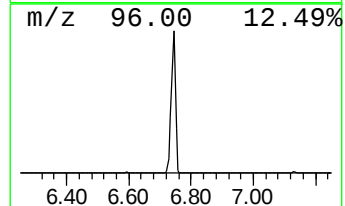
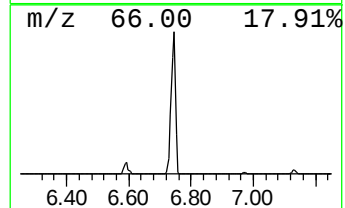
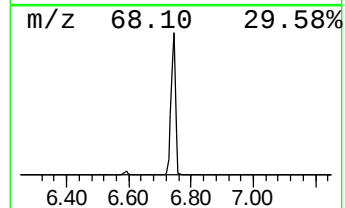
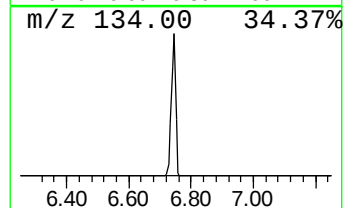
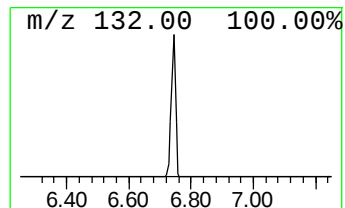
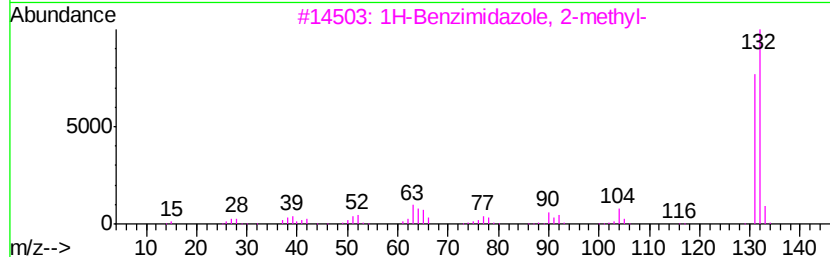
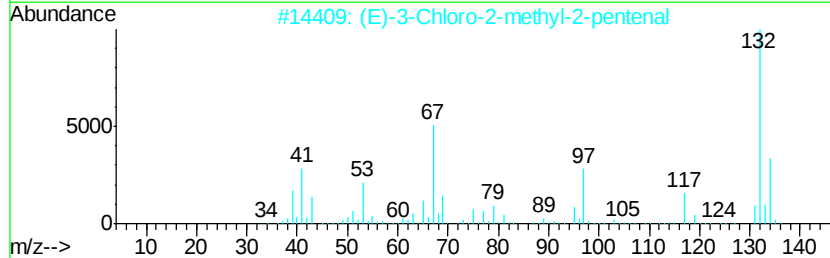
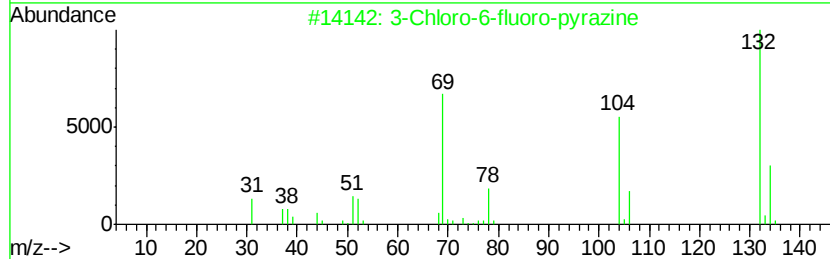
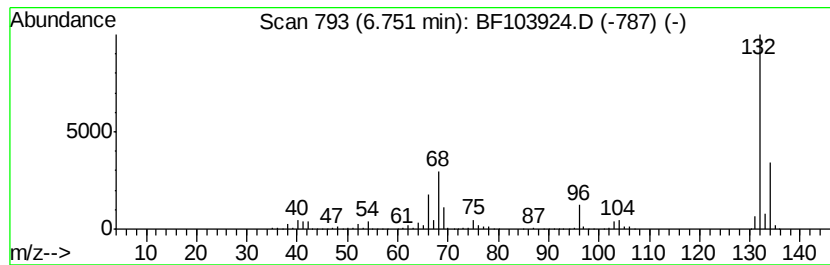
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Peak Number 3 unknown6.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	74.19 ng	3227440	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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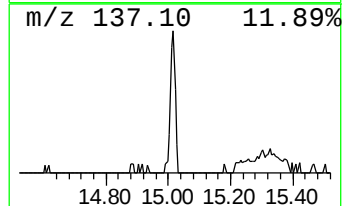
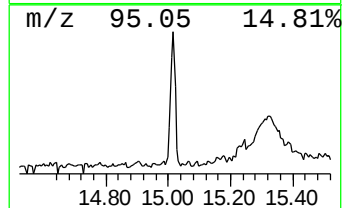
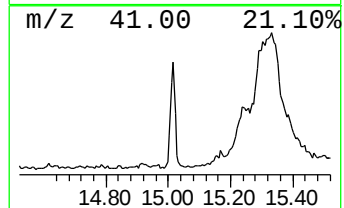
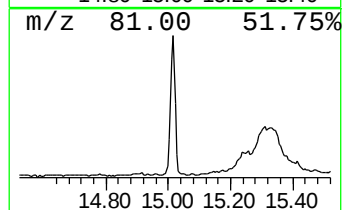
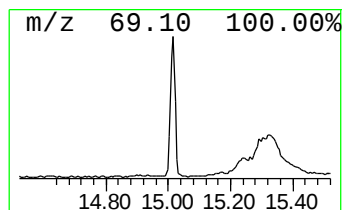
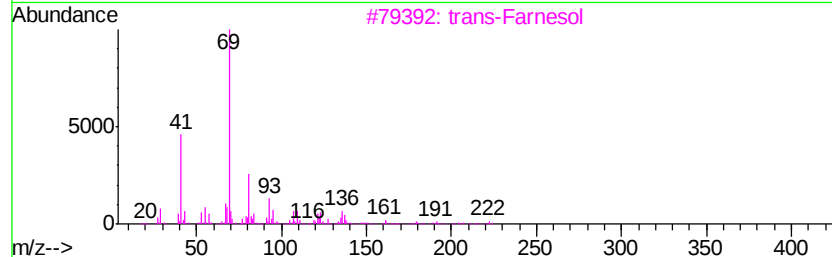
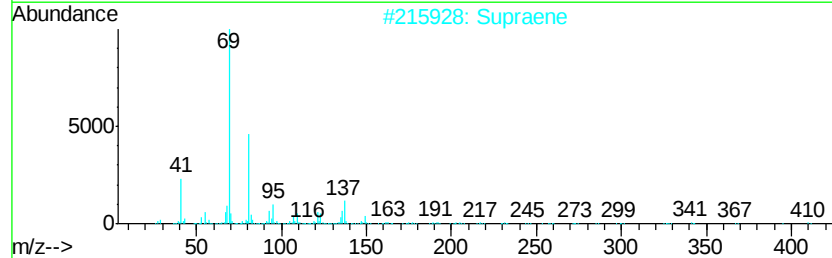
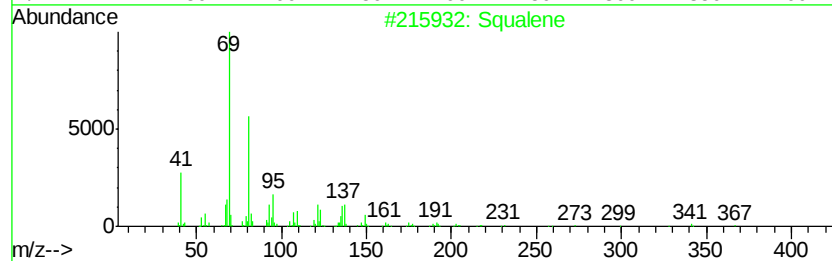
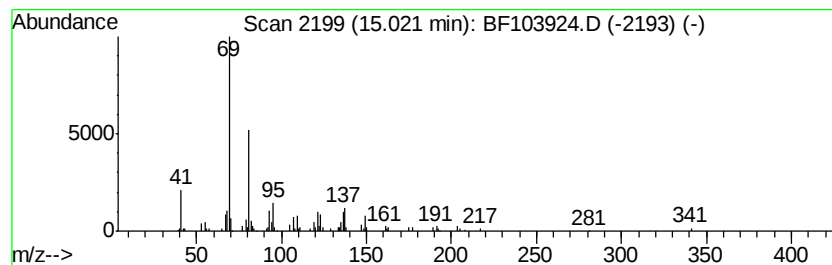
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Peak Number 5 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.12 ng	191222	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	94
2		Supraene	410	C30H50	007683-64-9	87
3		trans-Farnesol	222	C15H26O	000106-28-5	59
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



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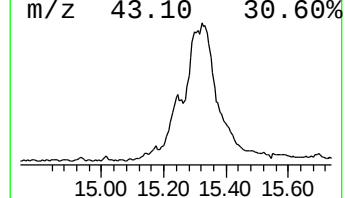
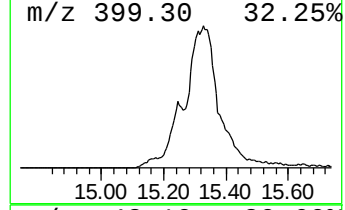
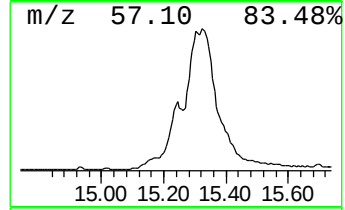
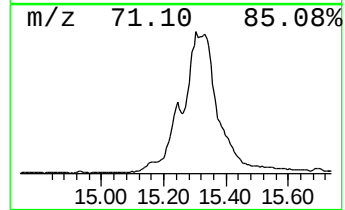
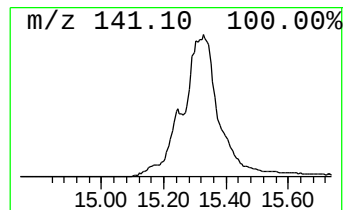
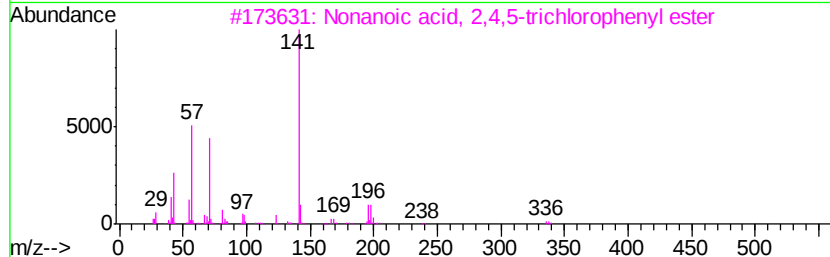
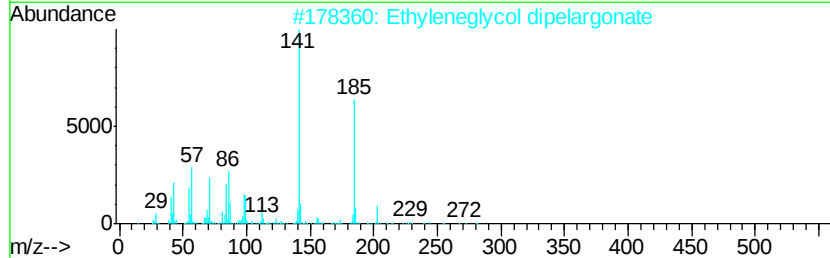
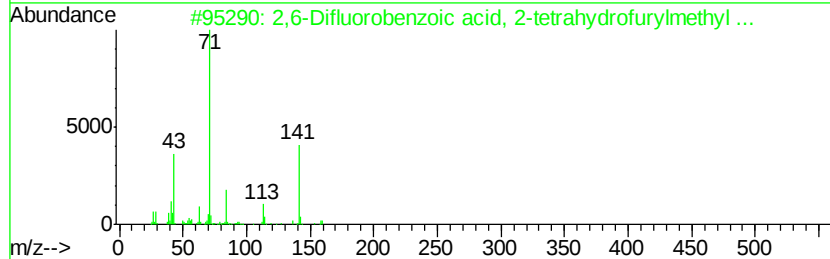
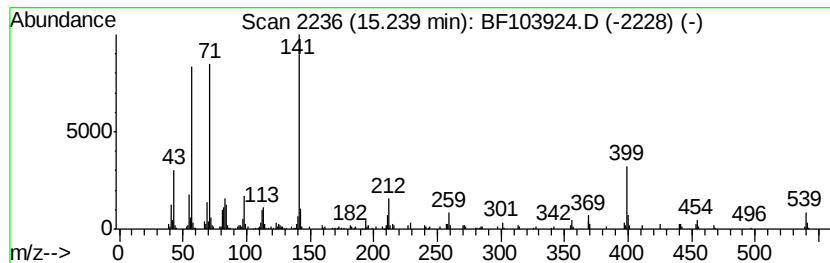
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Peak Number 7 unknown15.24 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	12.30 ng	755211	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6-Difluorobenzoic acid, 2-tetr...	242	C12H12F2O3	1000293-47-9	35
2		Ethylene glycol dipelargonate	342	C20H38O4	015805-87-5	25
3		Nonanoic acid, 2,4,5-trichloroph...	336	C15H19Cl3O2	1000360-67-3	25
4		l-Methionine, N-neopentylloxycarb...	473	C26H51NO4S	1000328-79-3	22
5		Benzhydrazide, 2,6-difluoro-N2-(...	317	C13H8F5N3O	1000266-89-5	22



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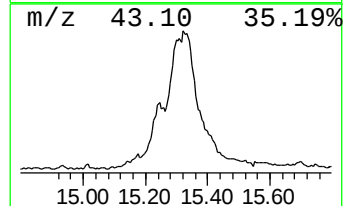
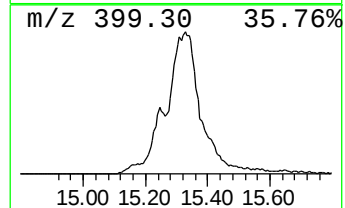
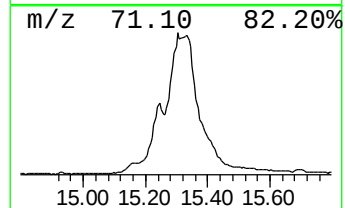
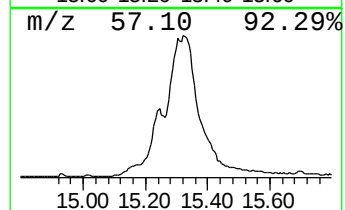
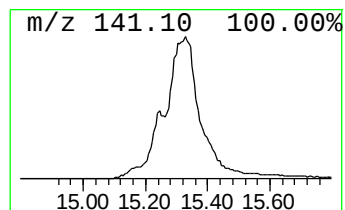
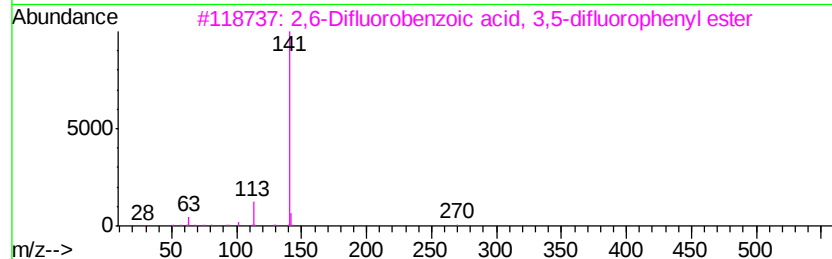
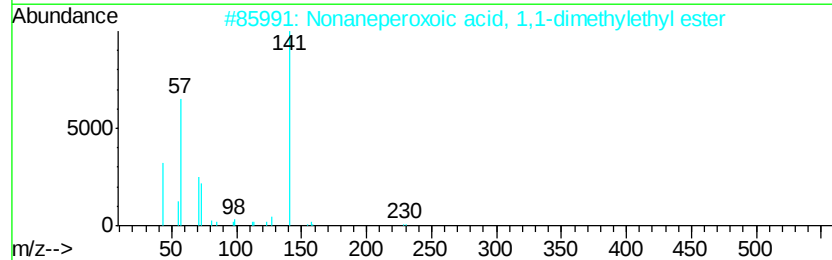
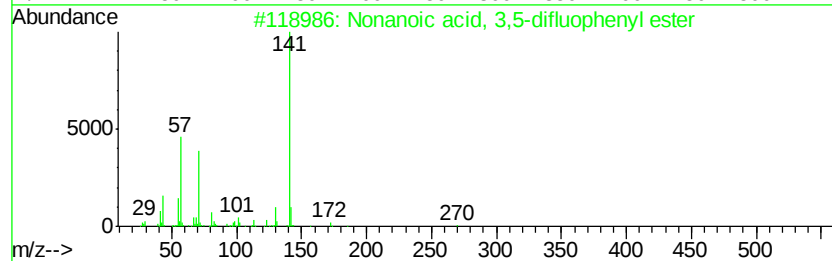
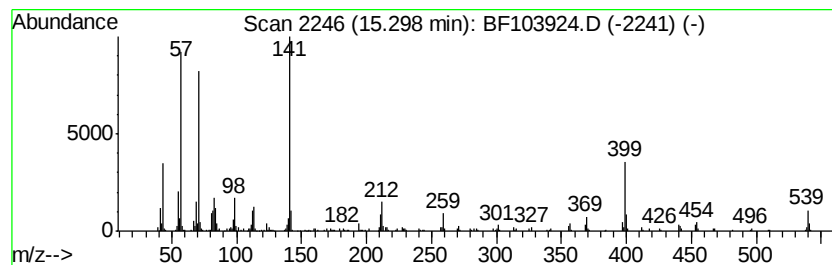
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonanoic acid, 3,5-difluoph... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	10.43 ng	640383	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid, 3,5-difluophenyl ...	270	C15H20F2O2	1000358-02-3	59
2		Nonaneperoxoic acid, 1,1-dimethy...	230	C13H26O3	022913-02-6	25
3		2,6-Difluorobenzoic acid, 3,5-di...	270	C13H6F4O2	1000292-62-1	22
4		2,6-Difluorobenzoic acid, 3-meth...	226	C12H12F2O2	1000292-58-2	22
5		Fumaric acid, 2,4-dichlorophenyl...	302	C13H12Cl2O4	1000345-33-5	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103924.D
Acq On : 26 Mar 2018 14:24
Operator : JU/SJ
Sample : J1994-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-MW-06-032018

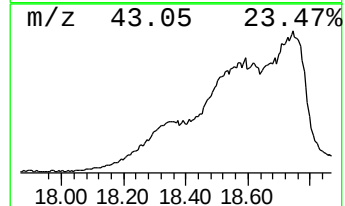
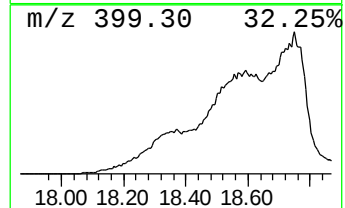
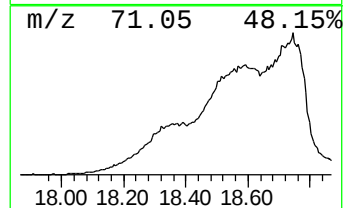
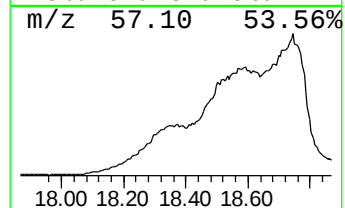
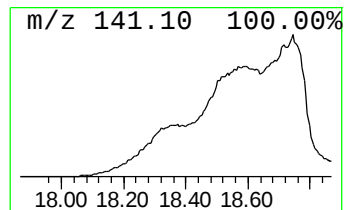
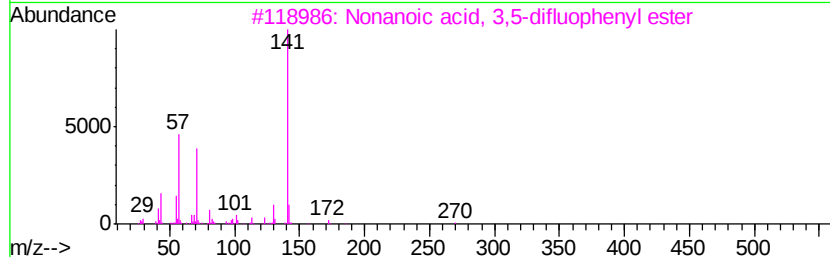
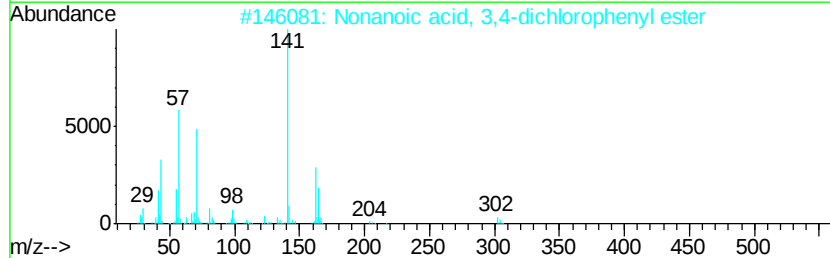
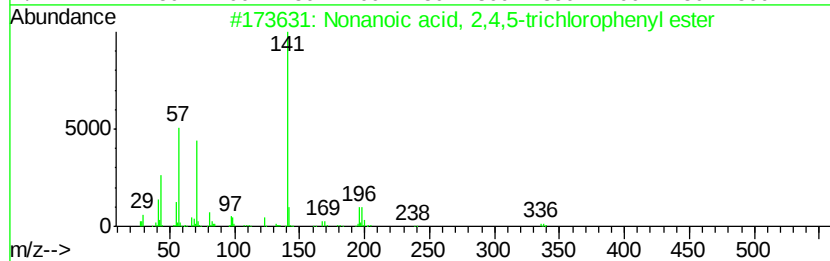
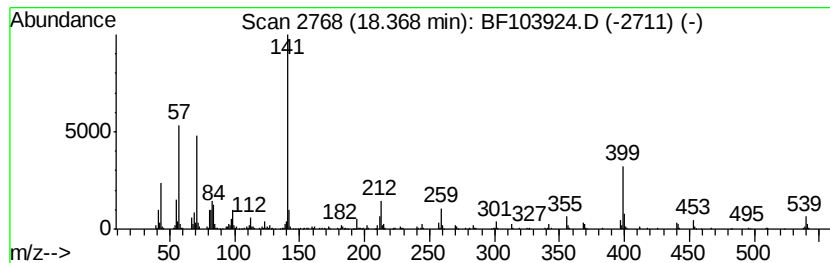
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid, 2,4,5-trichl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	112.14 ng	6884070	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid, 2,4,5-trichloroph...	336	C15H19Cl3O2	1000360-67-3	53
2		Nonanoic acid, 3,4-dichloropheny...	302	C15H20Cl2O2	1000358-02-7	53
3		Nonanoic acid, 3,5-difluophenyl ...	270	C15H20F2O2	1000358-02-3	53
4		Nonanoic acid, pentafluorophenyl...	324	C15H17F5O2	1000360-66-5	42
5		Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032618\
Data File : BF103924.D
Acq On : 26 Mar 2018 14:24
Operator : JU/SJ
Sample : J1994-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-MW-06-032018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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
Butane, 2-methoxy...	2.32	14.3	ng	619838	1	6.97	870041	20.0
2-Pentanone, 4-hy...	5.20	3.2	ng	138021	1	6.97	870041	20.0
unknown6.75	6.75	74.2	ng	3227440	1	6.97	870041	20.0
Squalene	15.02	3.1	ng	191222	6	15.71	1227750	20.0
unknown15.24	15.24	12.3	ng	755211	6	15.71	1227750	20.0
Nonanoic acid, 3,...	15.30	10.4	ng	640383	6	15.71	1227750	20.0
Nonanoic acid, 2,...	18.37	112.1	ng	6884070	6	15.71	1227750	20.0