

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100592.D
 Acq On : 15 Nov 2017 17:05
 Operator : SJ/JU
 Sample : I6448-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EPE-120-2(10-12)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	2.210	17	21	27	rVB2	26064	38634	1.19%	0.138%
2	5.116	511	515	526	rBV	427573	636403	19.67%	2.276%
3	5.510	576	582	585	rBV	2852760	3038958	93.92%	10.869%
4	6.510	746	752	759	rBV	2477131	3201019	98.93%	11.448%
5	6.657	771	777	780	rBV	2889297	3046206	94.14%	10.895%
6	6.886	812	816	819	rBV	852409	777883	24.04%	2.782%
7	7.039	838	842	846	rVB	2509656	2406195	74.36%	8.606%
8	7.445	905	911	914	rBV	1845625	1991676	61.55%	7.123%
9	8.163	1029	1033	1037	rVB	1198493	1003292	31.01%	3.588%
10	8.716	1123	1127	1130	rBV	170060	125595	3.88%	0.449%
11	9.239	1210	1216	1219	rBV	3361511	3235731	100.00%	11.572%
12	9.627	1278	1282	1285	rBV	316069	230904	7.14%	0.826%
13	9.922	1327	1332	1335	rBV	1093823	1011532	31.26%	3.618%
14	10.627	1449	1452	1456	rVB	327069	261671	8.09%	0.936%
15	10.710	1461	1466	1469	rBV	1531745	1528106	47.23%	5.465%
16	11.404	1580	1584	1587	rBV	1006216	802396	24.80%	2.870%
17	12.792	1815	1820	1826	rBV2	40702	42917	1.33%	0.153%
18	12.986	1849	1853	1856	rBV	2278991	2103314	65.00%	7.522%
19	13.457	1929	1933	1939	rBV	64951	76220	2.36%	0.273%
20	13.868	2000	2003	2007	rBV	64200	73952	2.29%	0.264%
21	14.039	2028	2032	2036	rBV	851149	730357	22.57%	2.612%
22	14.656	2134	2137	2141	rBV	73933	66765	2.06%	0.239%
23	14.798	2156	2161	2169	rBV	661281	804528	24.86%	2.877%
24	15.515	2278	2283	2293	rVB	582607	726314	22.45%	2.598%

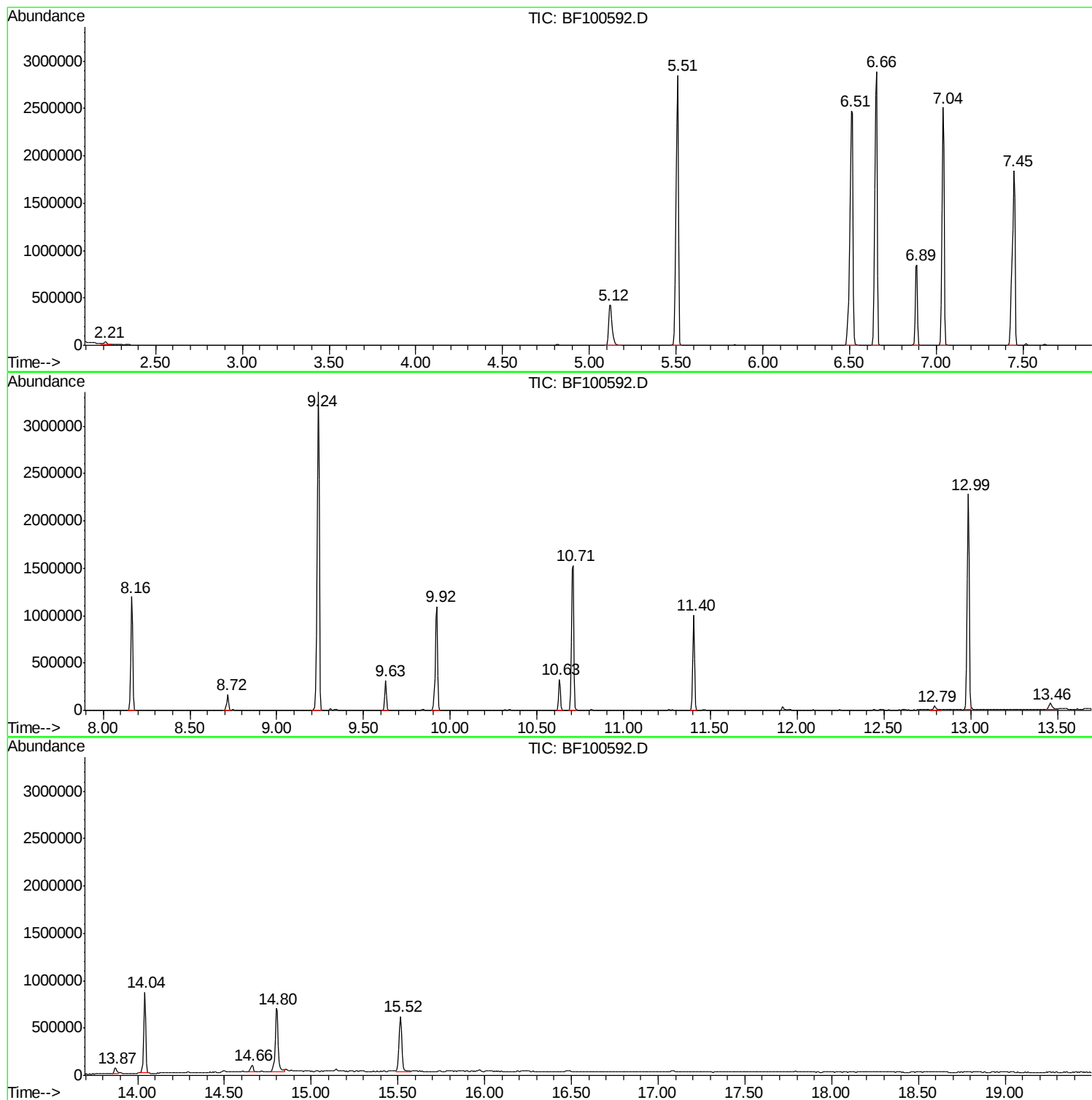
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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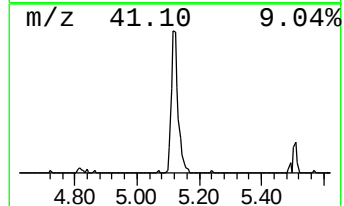
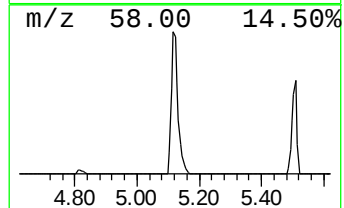
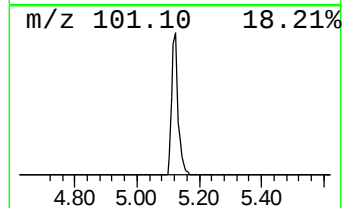
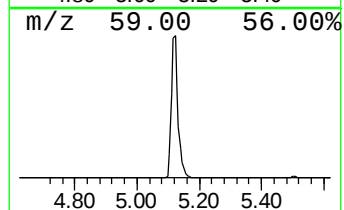
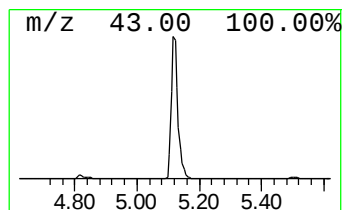
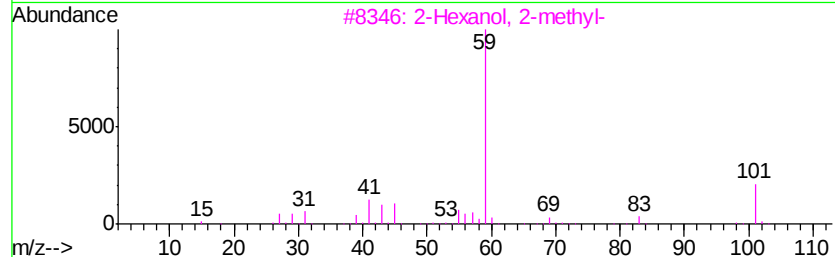
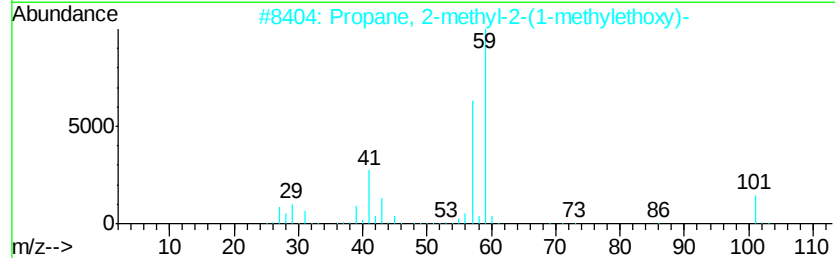
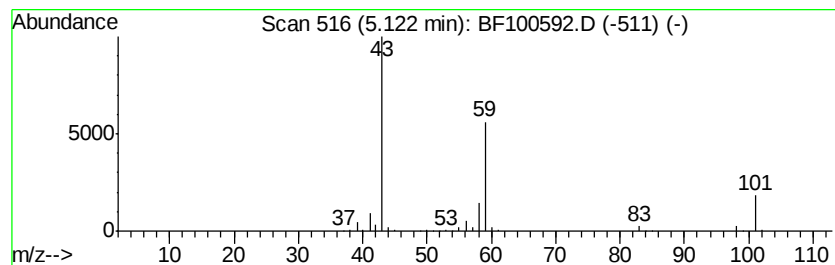
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	16.36 ng	636403	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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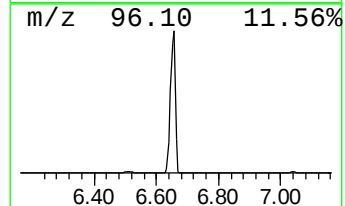
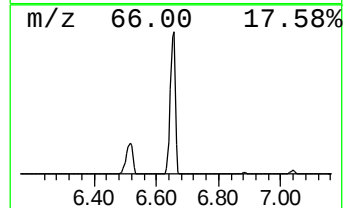
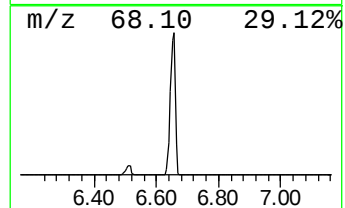
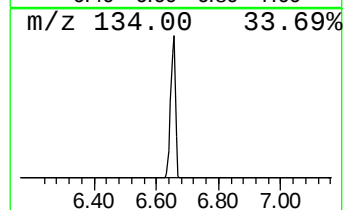
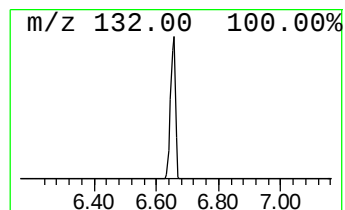
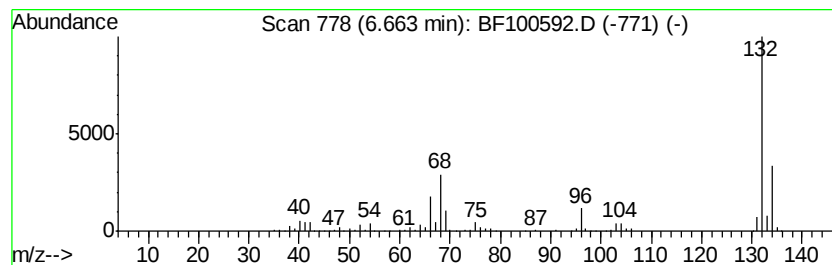
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	78.32 ng	3046210	1,4-Dichlorobenzene-d4	6.89

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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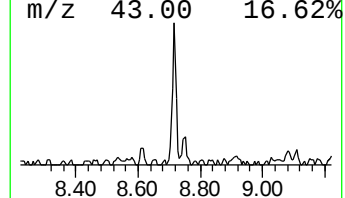
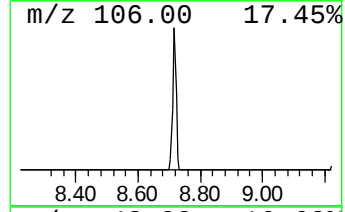
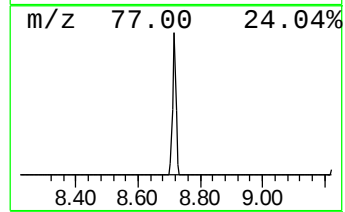
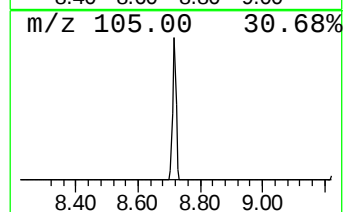
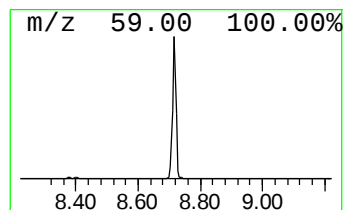
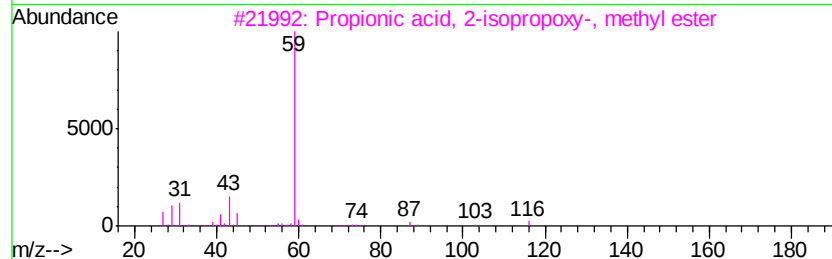
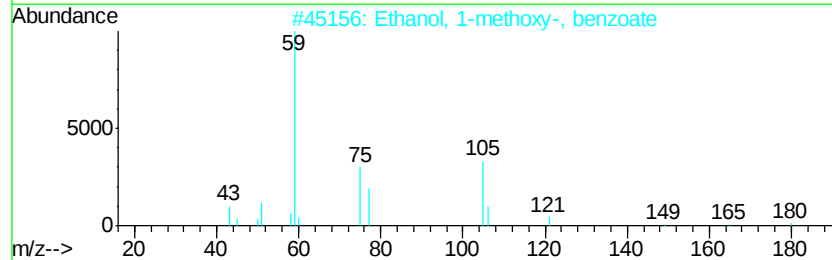
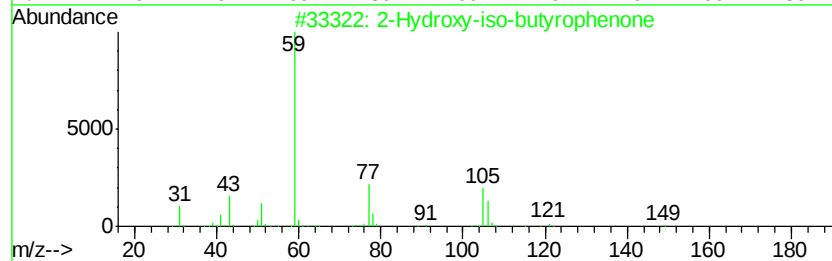
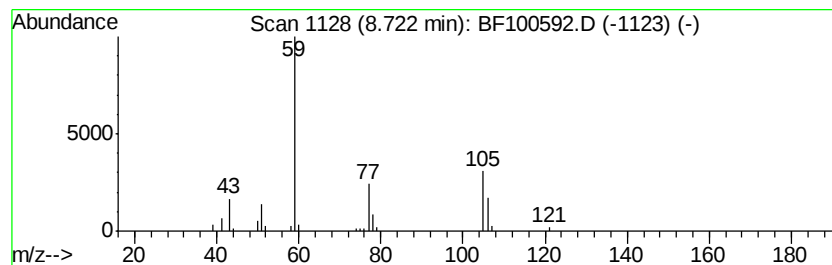
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.50 ng	125595	Napthalene-d8	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7



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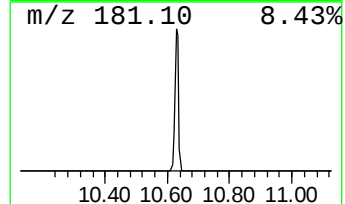
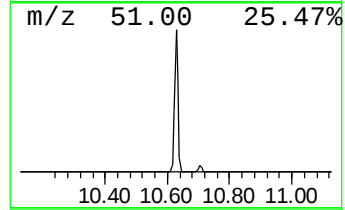
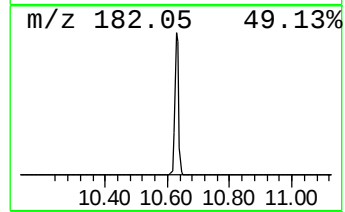
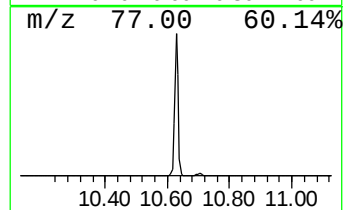
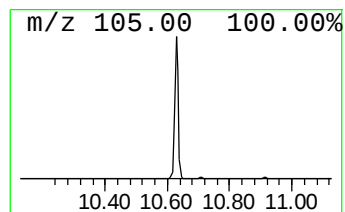
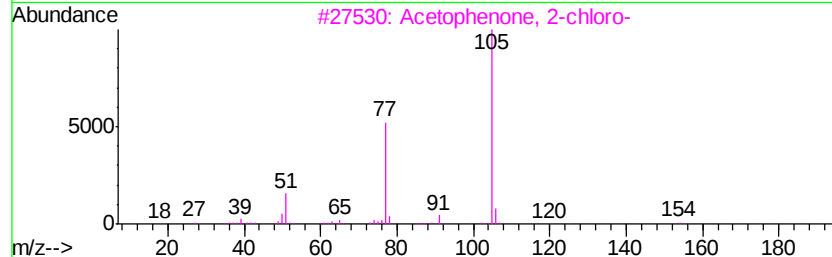
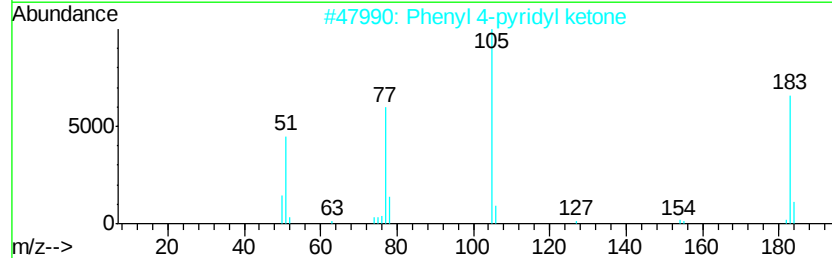
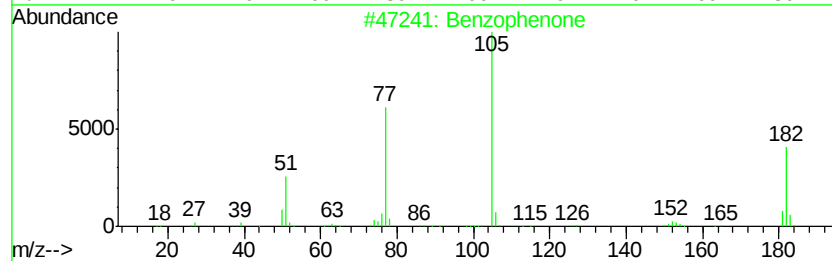
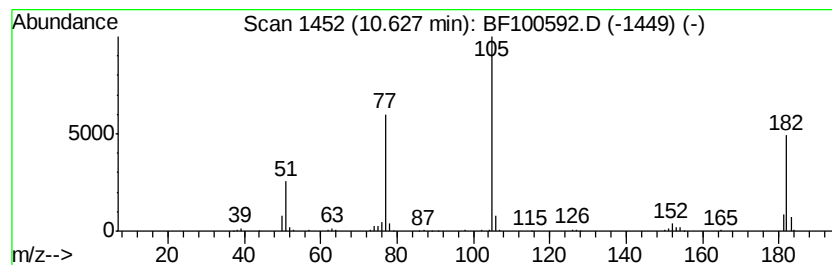
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Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.63	5.17 ng	261671	Acenaphthene-d10	9.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
3		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5		Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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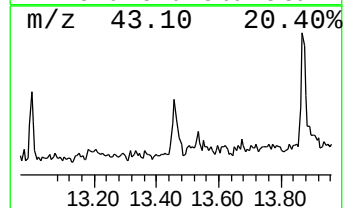
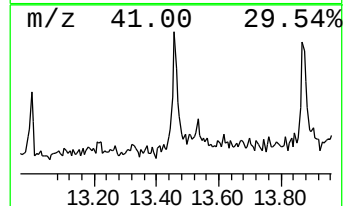
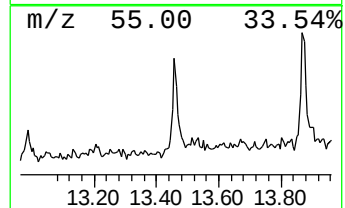
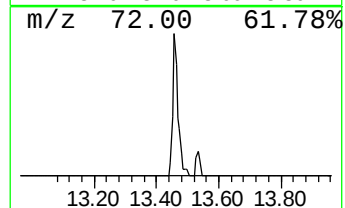
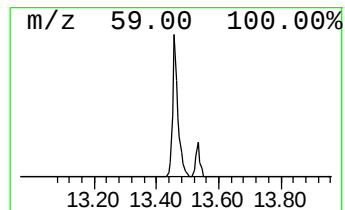
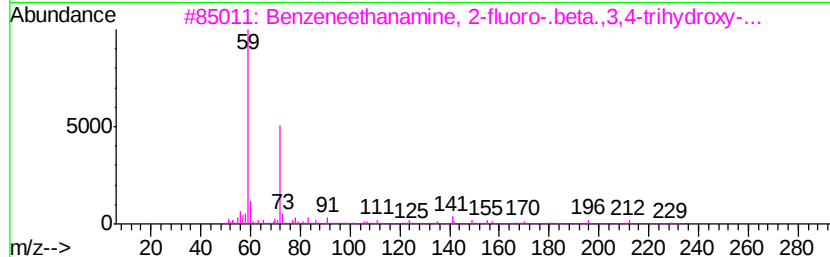
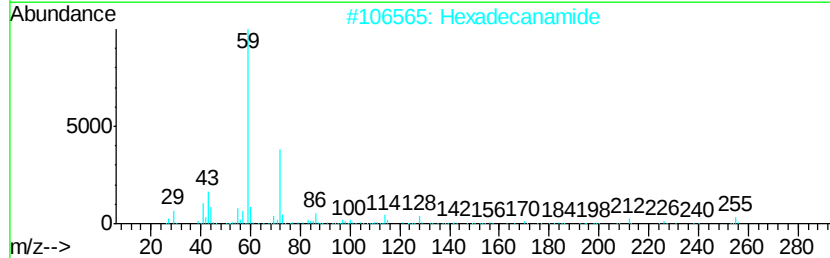
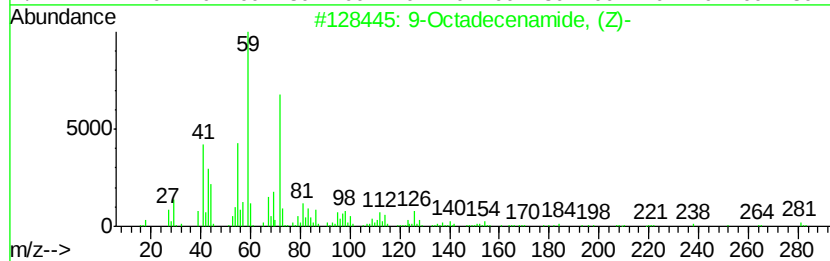
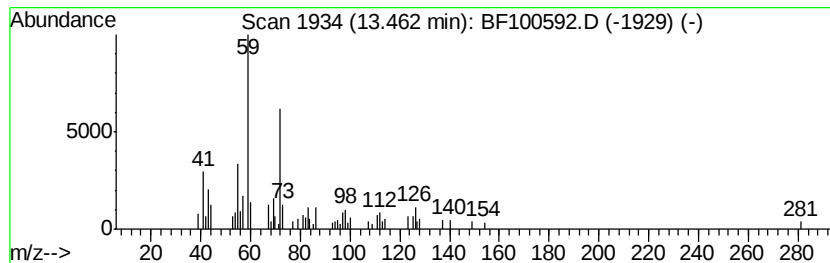
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.09 ng	76220	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2		Hexadecanamide	255	C16H33NO	000629-54-9	78
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		Nonanamide	157	C9H19NO	001120-07-6	59
5		Dodecanamide	199	C12H25NO	001120-16-7	59



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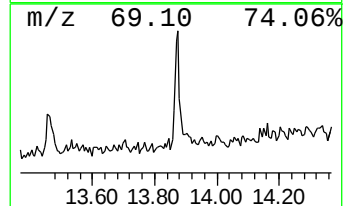
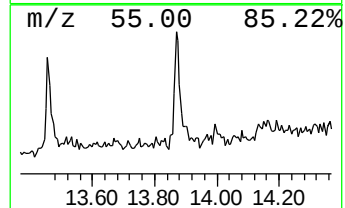
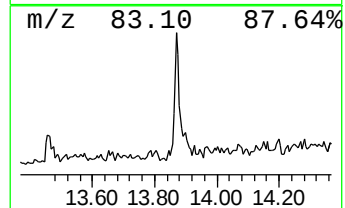
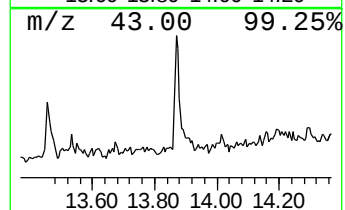
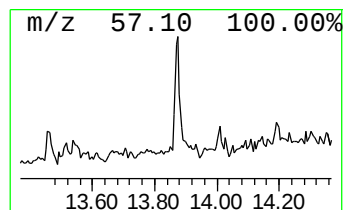
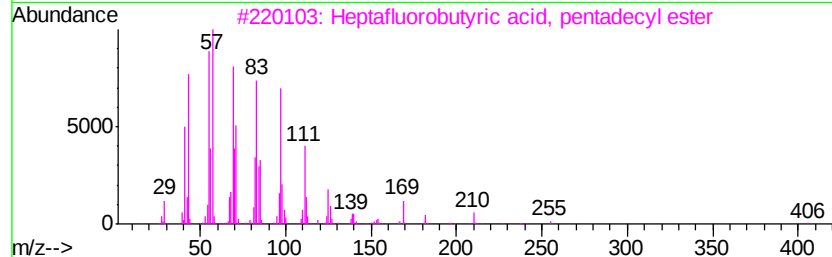
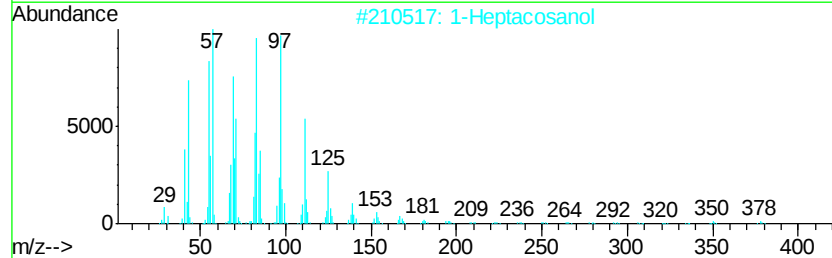
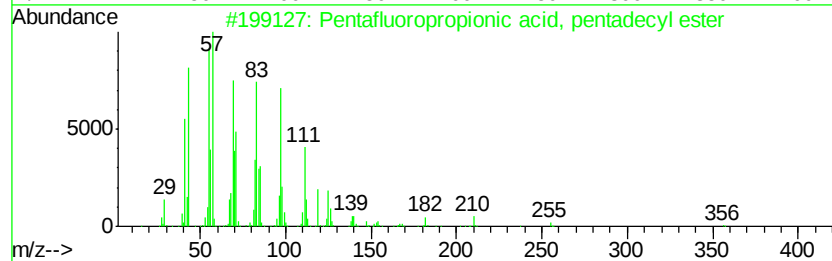
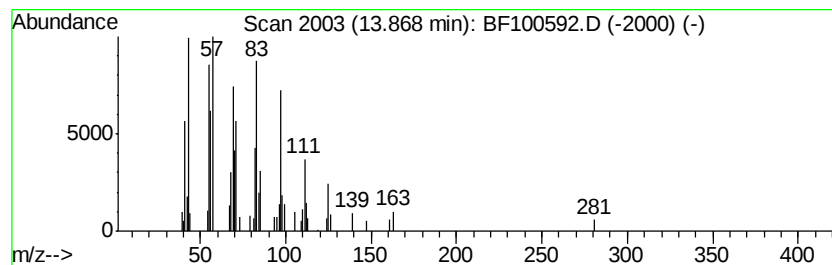
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TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.03 ng	73952	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5		1-Heneicosanol	312	C21H44O	015594-90-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100592.D
Acq On : 15 Nov 2017 17:05
Operator : SJ/JU
Sample : I6448-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EPE-120-2(10-12)

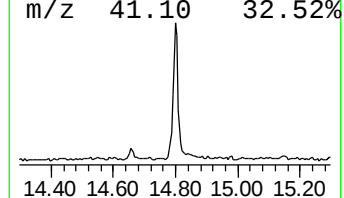
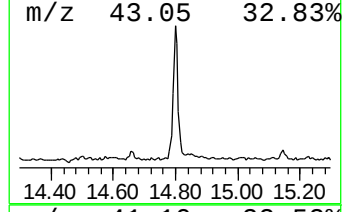
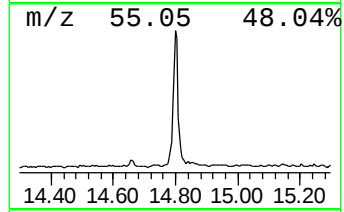
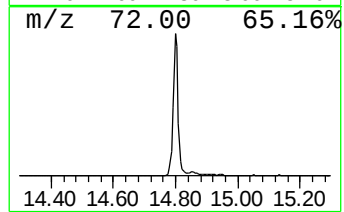
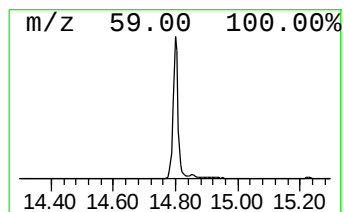
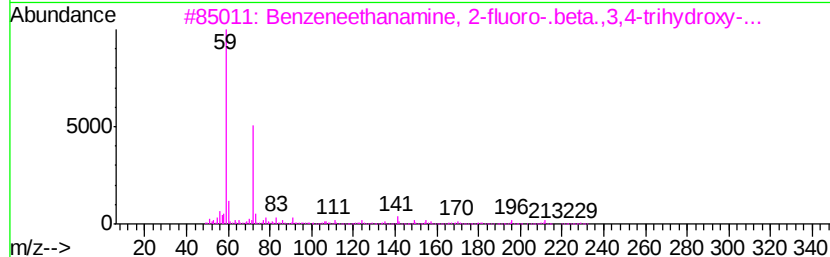
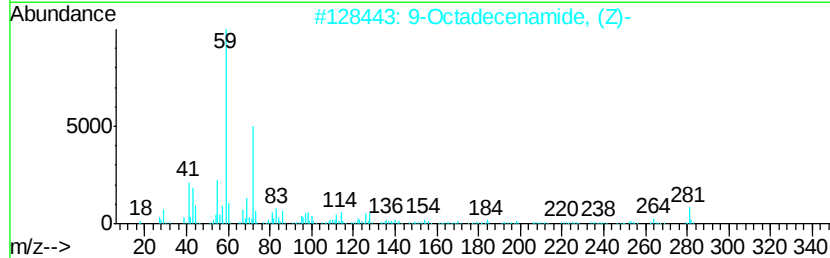
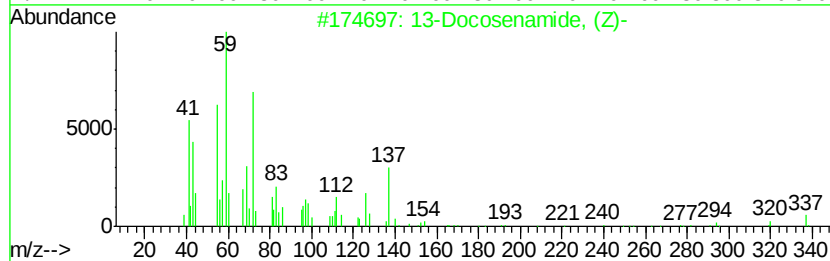
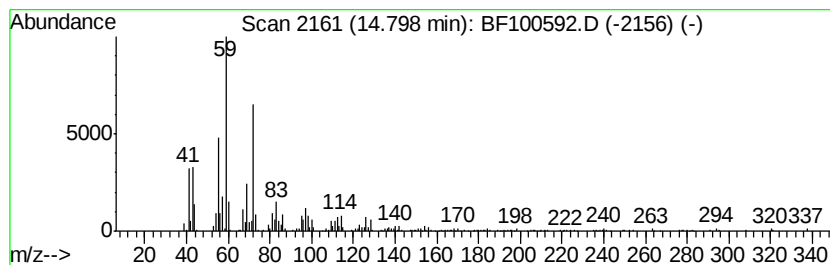
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	22.15 ng	804528	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5		Octanamide	143	C8H17NO	000629-01-6	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100592.D
Acq On : 15 Nov 2017 17:05
Operator : SJ/JU
Sample : I6448-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EPE-120-2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.12	16.4	ng	636403	1	6.89	777883	20.0
unknown6.66	6.66	78.3	ng	3046210	1	6.89	777883	20.0
2-Hydroxy-iso-but...	8.72	2.5	ng	125595	2	8.16	1003290	20.0
Benzophenone	10.63	5.2	ng	261671	3	9.92	1011530	20.0
9-Octadecenamide,...	13.46	2.1	ng	76220	5	14.04	730357	20.0
Pentafluoropropio...	13.87	2.0	ng	73952	5	14.04	730357	20.0
13-Docosenamide, ...	14.80	22.1	ng	804528	6	15.52	726314	20.0