

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
 Data File : BF098863.D
 Acq On : 27 Sep 2017 15:14
 Operator : SJ/JU
 Sample : I5434-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400536

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-BF092317.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	2.222	19	23	42	rVB	116030	233452	6.55%	0.729%
2	5.145	516	520	531	rVB	589077	756866	21.24%	2.363%
3	5.540	581	587	590	rBV	3106399	3363154	94.39%	10.501%
4	6.539	751	757	760	rBV	3169031	3508046	98.46%	10.953%
5	6.686	777	782	785	rBV	3403448	3505598	98.39%	10.946%
6	6.916	817	821	824	rBV	949742	815820	22.90%	2.547%
7	7.069	843	847	850	rBV	2798768	2435643	68.36%	7.605%
8	7.475	911	916	919	rBV	2262310	2192431	61.53%	6.846%
9	8.192	1034	1038	1042	rBV	1270543	1123708	31.54%	3.509%
10	9.269	1216	1221	1224	rBV	3844621	3563076	100.00%	11.125%
11	9.657	1283	1287	1290	rBV	620290	490964	13.78%	1.533%
12	9.951	1333	1337	1341	rVB	1485735	1229937	34.52%	3.840%
13	10.369	1406	1408	1411	rVB	60320	50606	1.42%	0.158%
14	10.739	1466	1471	1474	rBV	2181845	2002326	56.20%	6.252%
15	10.845	1486	1489	1493	rBV	77716	75390	2.12%	0.235%
16	11.439	1586	1590	1593	rBV	1393091	1207577	33.89%	3.771%
17	13.021	1854	1859	1862	rBV	3304907	3257147	91.41%	10.170%
18	13.904	2005	2009	2013	rBV	168023	166858	4.68%	0.521%
19	14.074	2034	2038	2042	rBV	978392	826257	23.19%	2.580%
20	14.539	2112	2117	2126	rBV3	35412	54362	1.53%	0.170%
21	14.827	2162	2166	2172	rBV	234628	248647	6.98%	0.776%
22	15.192	2224	2228	2230	rBV	30155	37751	1.06%	0.118%
23	15.562	2286	2291	2299	rBV	557595	746296	20.95%	2.330%
24	16.021	2365	2369	2375	rBV2	30501	46841	1.31%	0.146%
25	17.668	2642	2649	2656	rBV6	39031	88135	2.47%	0.275%

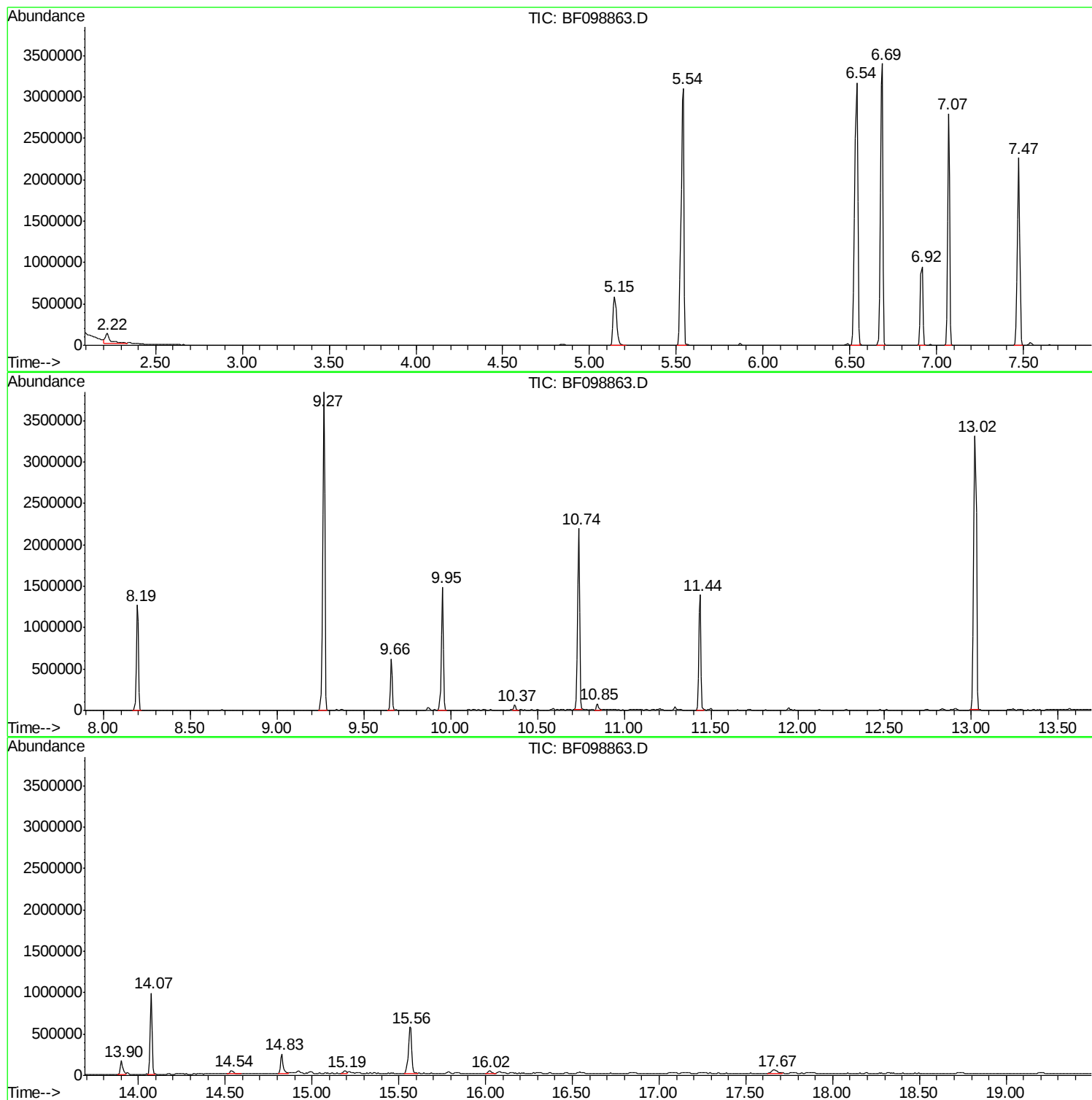
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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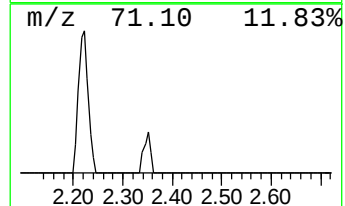
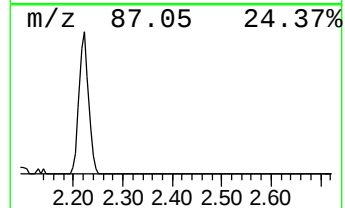
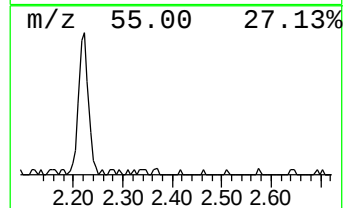
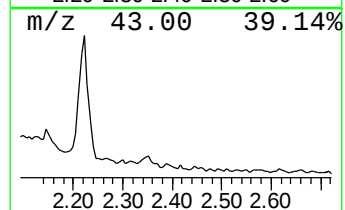
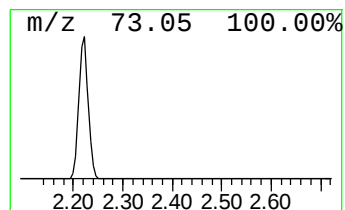
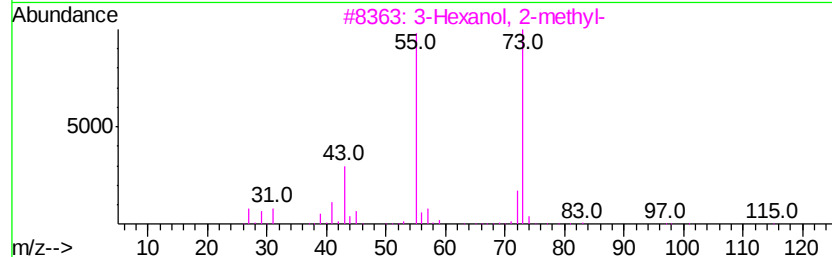
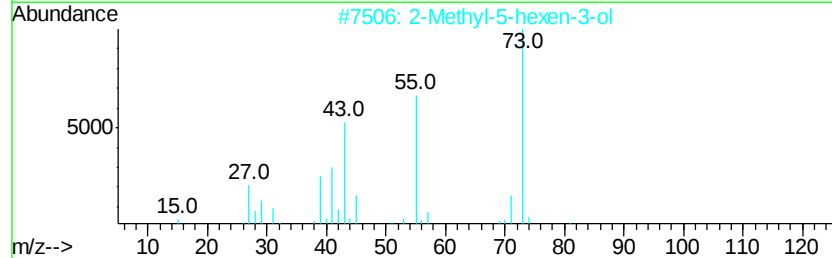
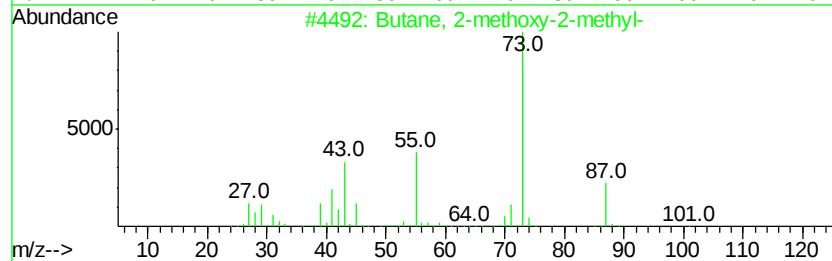
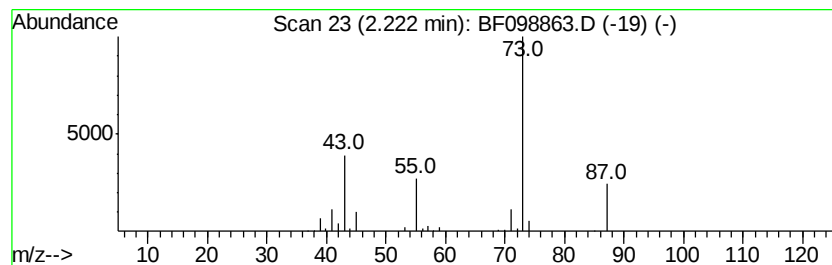
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	5.72 ng	233452	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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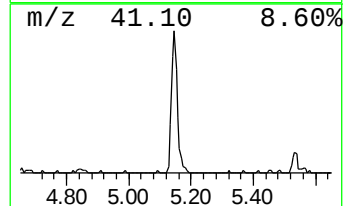
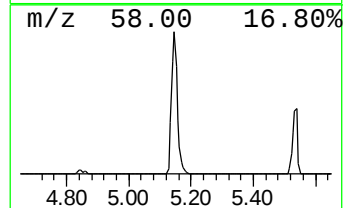
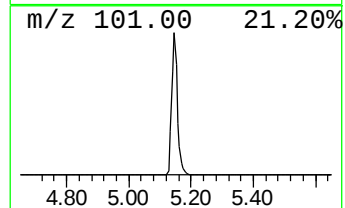
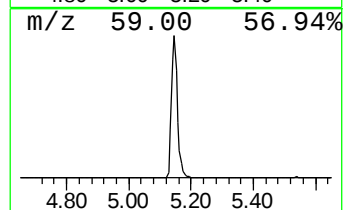
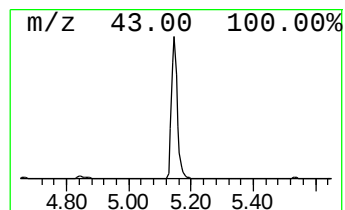
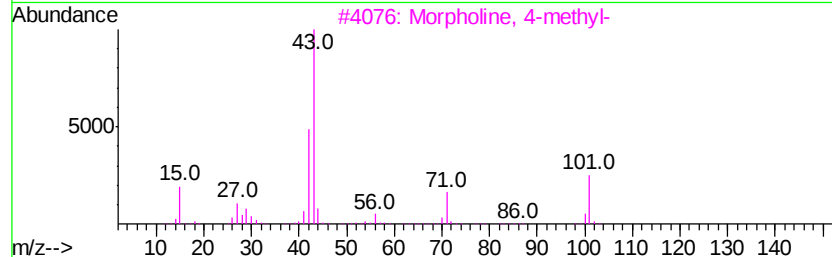
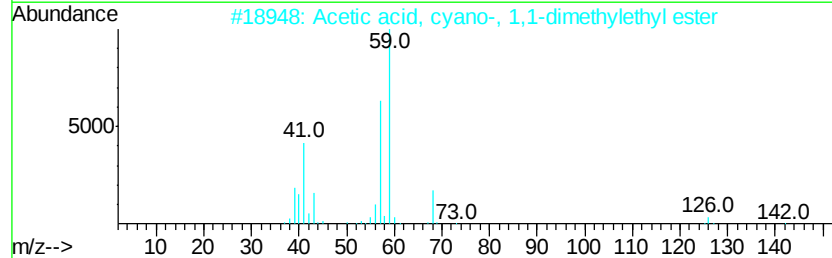
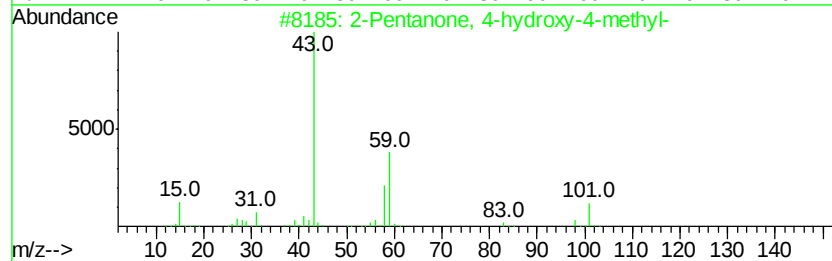
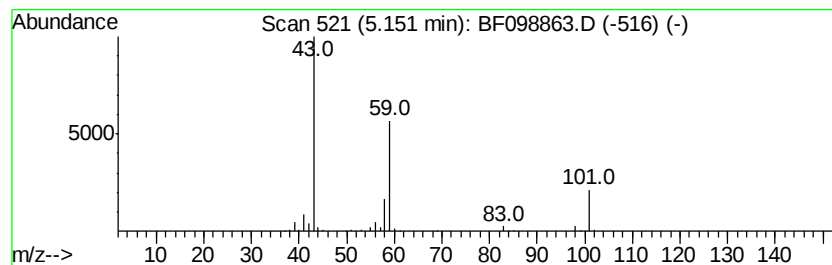
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	18.55 ng	756866	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9



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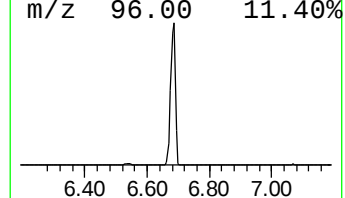
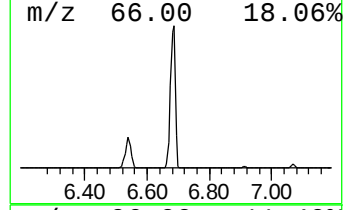
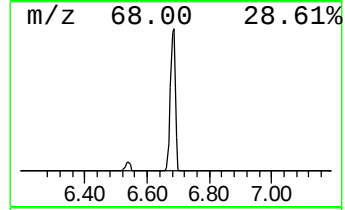
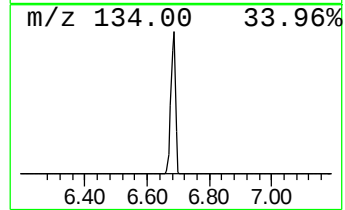
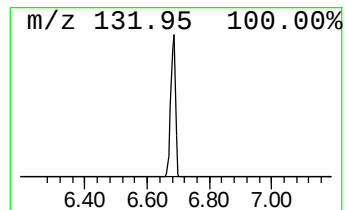
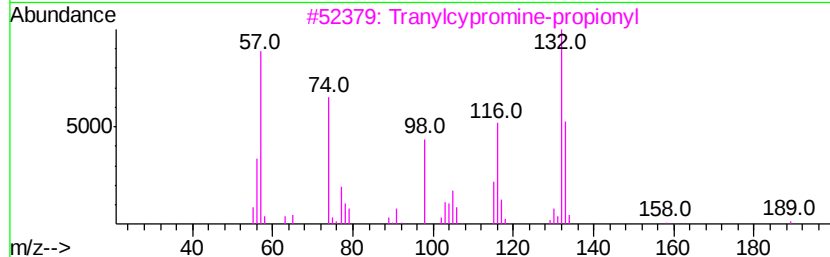
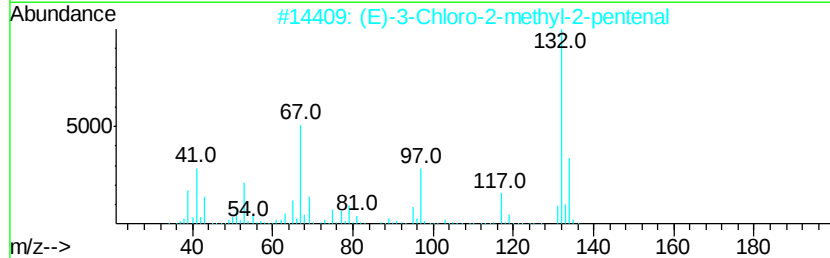
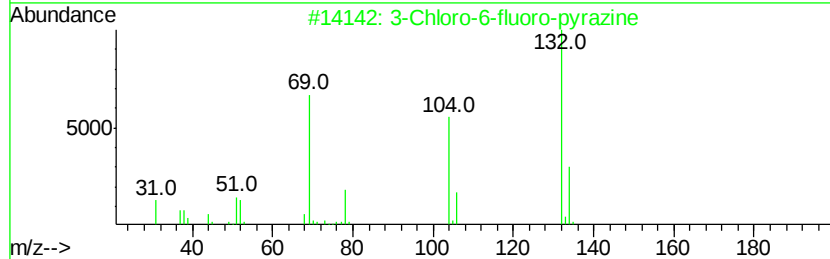
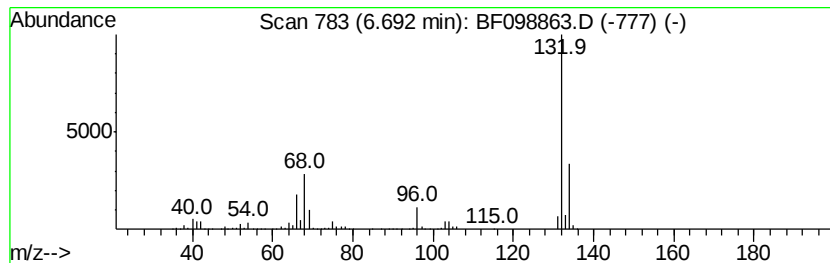
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.94 ng	3505600	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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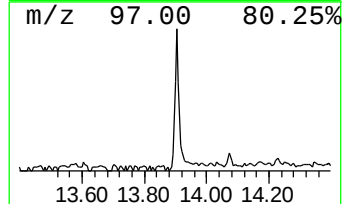
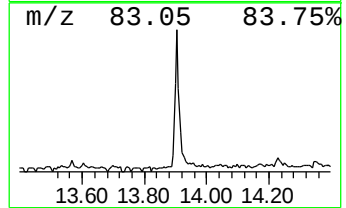
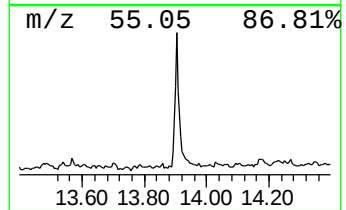
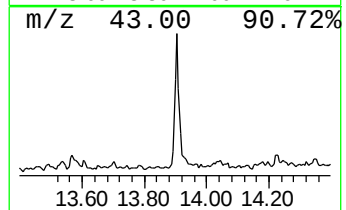
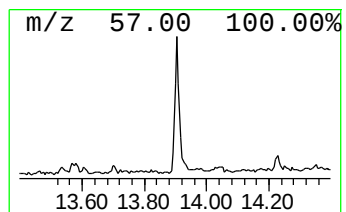
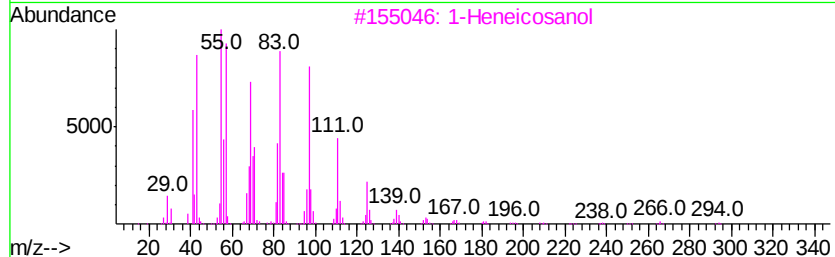
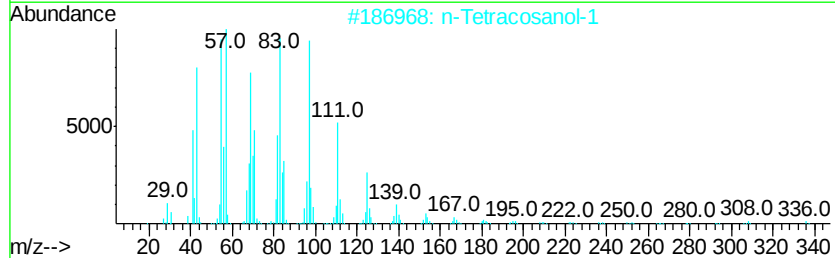
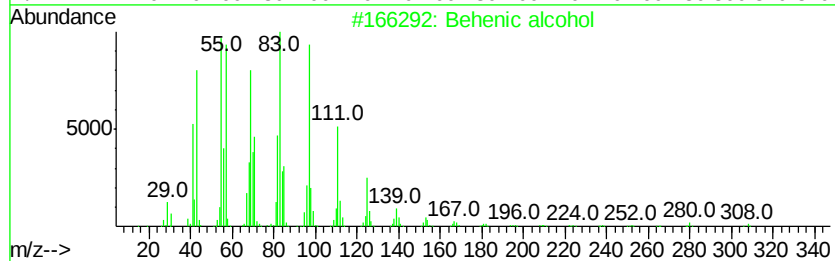
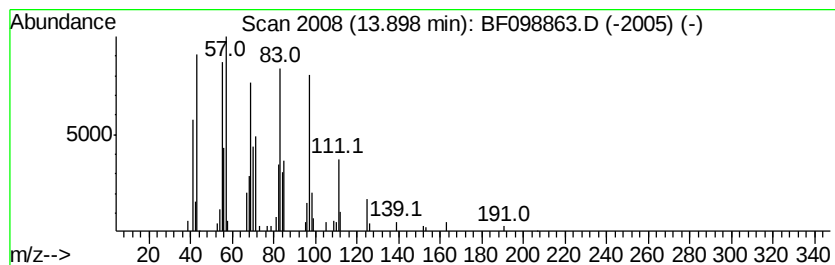
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Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	4.04 ng	166858	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Heptafluorobutvric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	93



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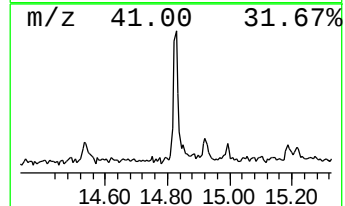
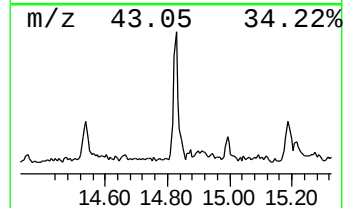
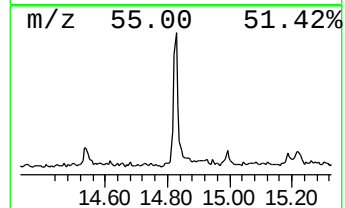
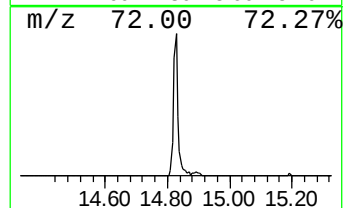
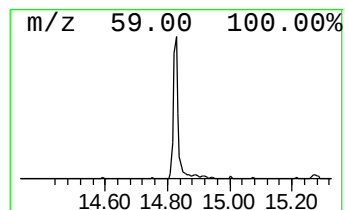
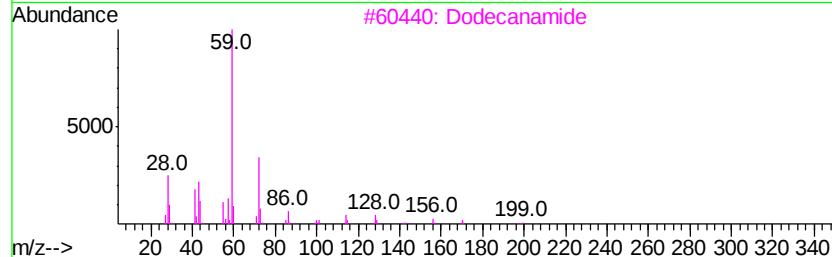
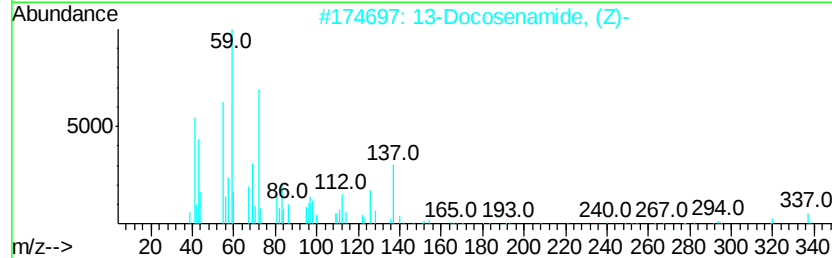
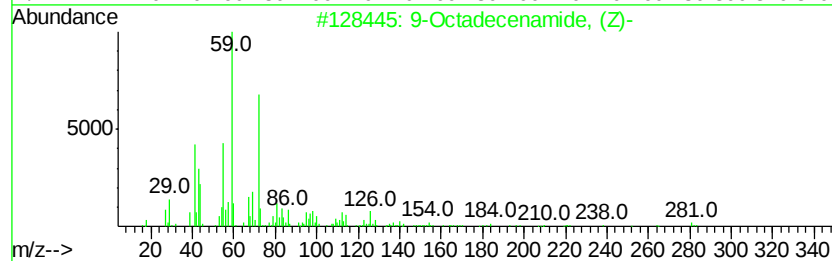
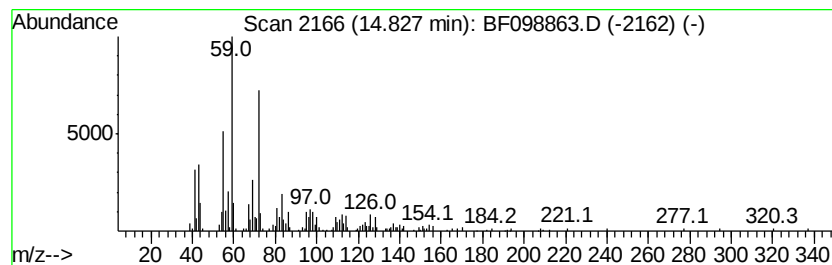
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	6.66 ng	248647	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
3	Dodecanamide	199	C12H25NO	001120-16-7	52
4	trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	43
5	6,8-Dichlorooctanamide	211	C8H15Cl2NO	003579-00-8	43



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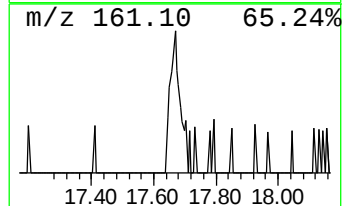
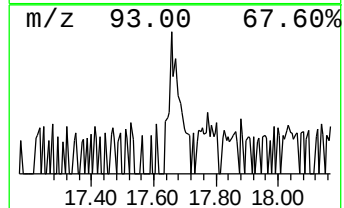
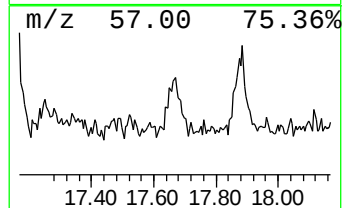
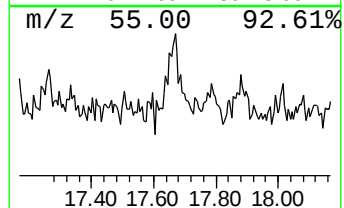
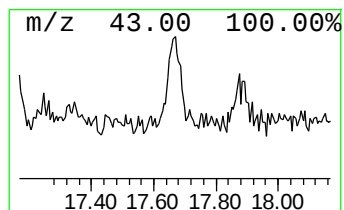
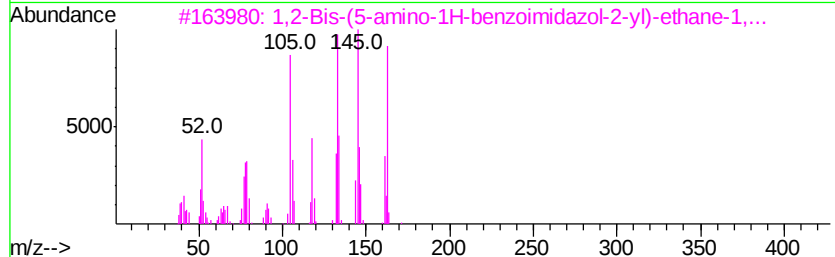
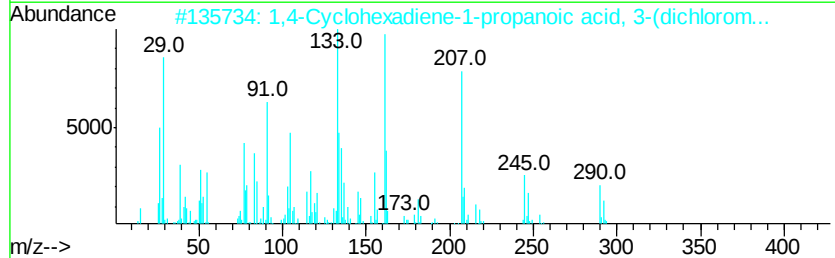
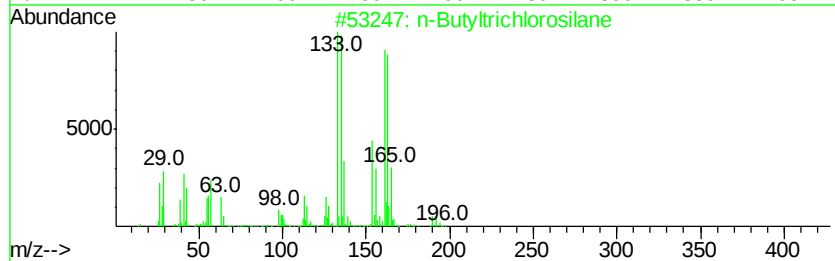
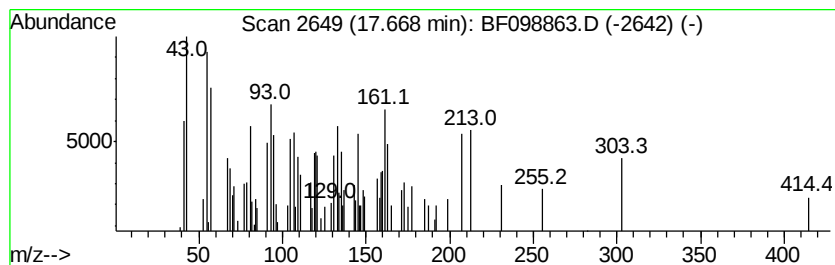
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.67 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	2.36 ng	88135	Perylene-d12	15.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Butyltrichlorosilane	190	C4H9Cl3Si	007521-80-4	25
2			1,4-Cyclohexadiene-1-propanoic a...	290	C13H16Cl2O3	056700-86-8	22
3			1,2-Bis-(5-amino-1H-benzoimidazo...	324	C16H16N6O2	031545-09-2	22
4			2H-Cyclopenta[c]pyridine-4-carbo...	207	C11H13N03	349498-68-6	22
5			[1,2,4]Triazolo[1,5-a]pyrimidine...	207	C8H9N5O2	1000351-62-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098863.D
Acq On : 27 Sep 2017 15:14
Operator : SJ/JU
Sample : I5434-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400536

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.22	5.7	ng	233452	1	6.92	815820	20.0
2-Pentanone, 4-hy...	5.15	18.6	ng	756866	1	6.92	815820	20.0
unknown6.69	6.69	85.9	ng	3505600	1	6.92	815820	20.0
Behenic alcohol	13.90	4.0	ng	166858	5	14.07	826257	20.0
9-Octadecenamide, ...	14.83	6.7	ng	248647	6	15.56	746296	20.0
unknown17.67	17.67	2.4	ng	88135	6	15.56	746296	20.0