

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051617\
 Data File : BF095161.D
 Acq On : 16 May 2017 17:49
 Operator : SJ/MA
 Sample : I3153-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DS-3-4

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-BF050217.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	5.137	540	544	567	rBV	186372	416472	12.90%	1.697%
2	5.742	643	647	683	rBV	1387603	2554491	79.13%	10.411%
3	7.319	910	915	931	rBV	1696212	2529492	78.36%	10.309%
4	7.442	931	936	954	rVB	2010965	2860280	88.61%	11.657%
5	7.778	989	993	1006	rVB	377228	469432	14.54%	1.913%
6	8.013	1028	1033	1047	rBV	1625772	1920707	59.50%	7.828%
7	8.672	1140	1145	1171	rBV	1121917	1632581	50.58%	6.654%
8	9.789	1331	1335	1357	rBV	504576	699332	21.66%	2.850%
9	11.560	1631	1636	1652	rBV	2465429	3228024	100.00%	13.156%
10	12.254	1750	1754	1765	rBV	200759	305255	9.46%	1.244%
11	12.619	1811	1816	1835	rBV2	595473	849709	26.32%	3.463%
12	13.454	1952	1958	1963	rBV	32711	36860	1.14%	0.150%
13	13.918	2032	2037	2052	rBV	1280555	1856827	57.52%	7.568%
14	14.230	2086	2090	2098	rBV	28542	41074	1.27%	0.167%
15	15.024	2220	2225	2241	rBV	580911	825156	25.56%	3.363%
16	15.683	2332	2337	2346	rVB	32085	51741	1.60%	0.211%
17	15.983	2382	2388	2400	rBV2	63352	121474	3.76%	0.495%
18	17.348	2614	2620	2630	rBV	2418866	2892019	89.59%	11.787%
19	18.600	2826	2833	2844	rBV5	36569	109793	3.40%	0.447%
20	18.695	2844	2849	2864	rVB	485918	696179	21.57%	2.837%
21	20.365	3129	3133	3144	rBV	247811	396765	12.29%	1.617%
22	20.894	3218	3223	3227	rBV6	24642	42803	1.33%	0.174%

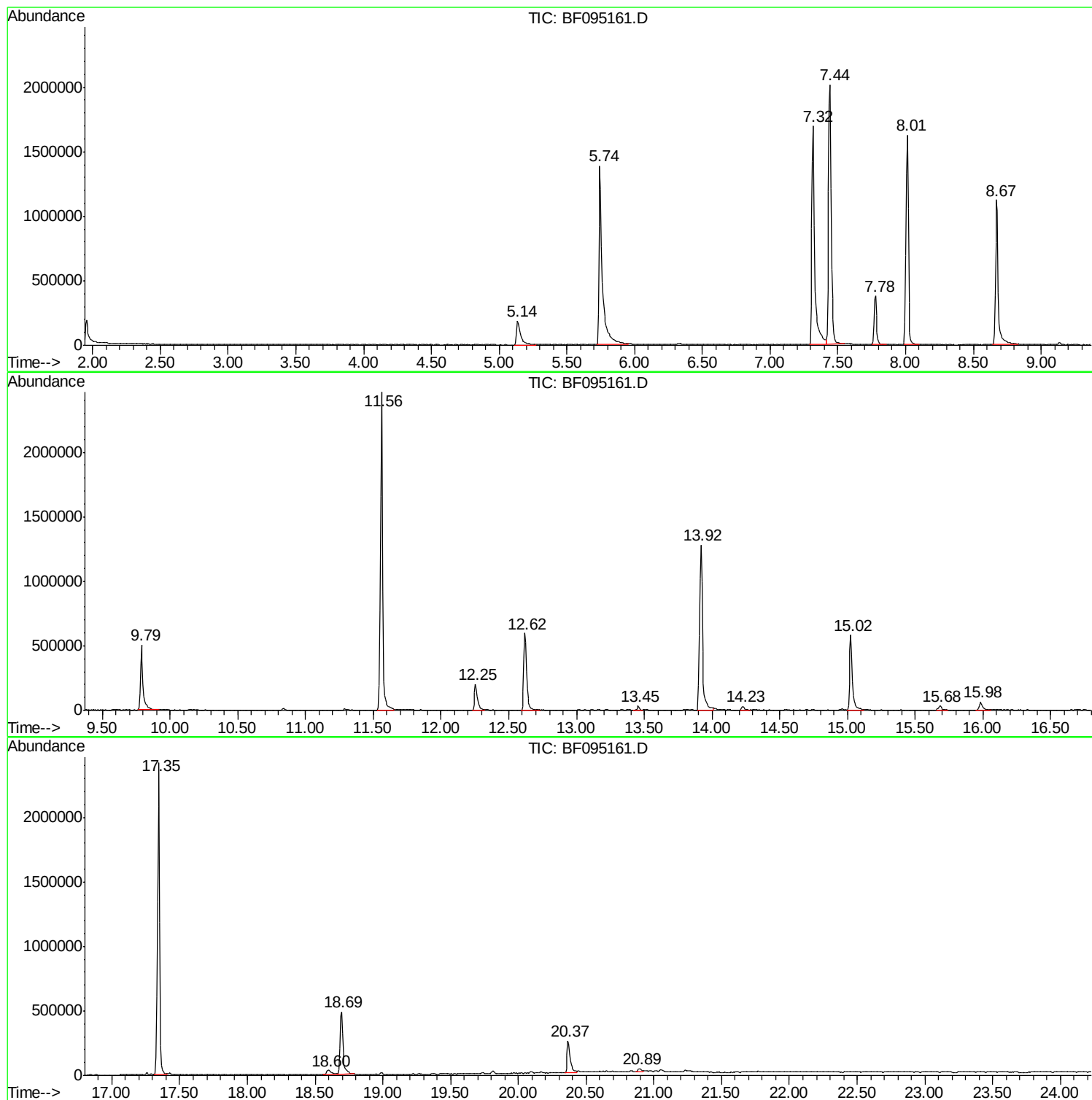
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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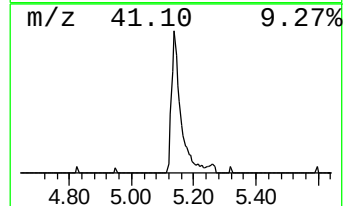
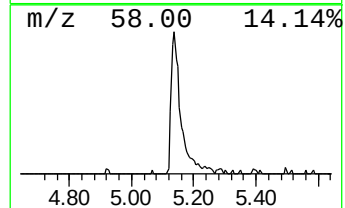
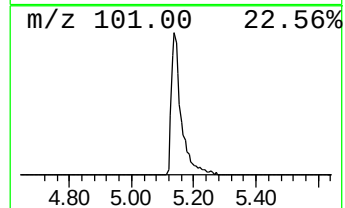
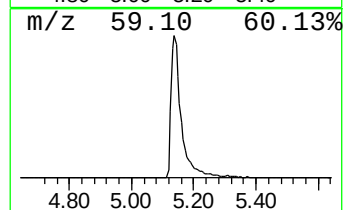
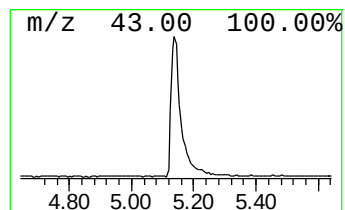
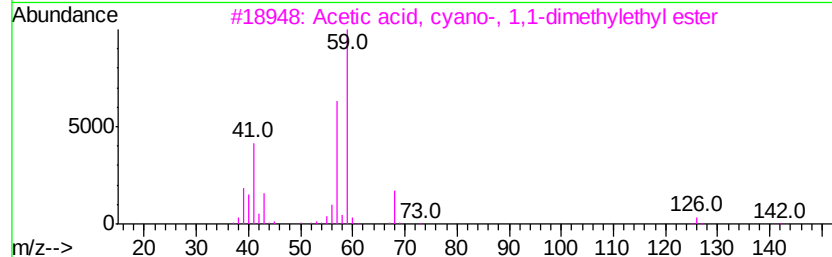
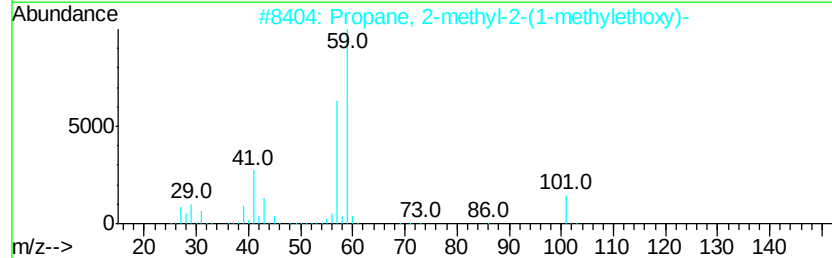
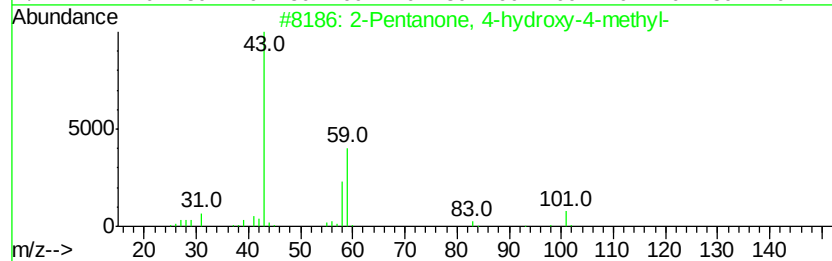
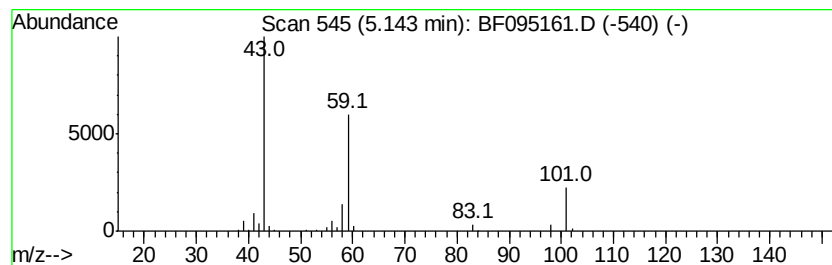
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	17.74 ng	416472	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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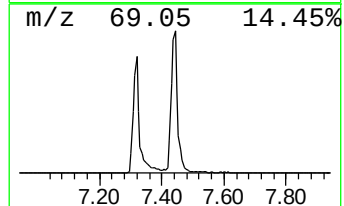
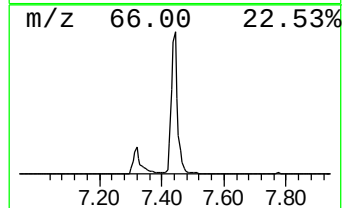
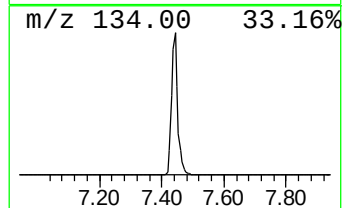
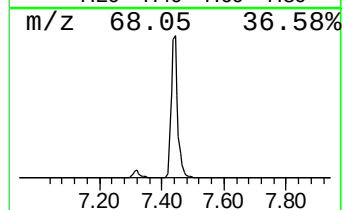
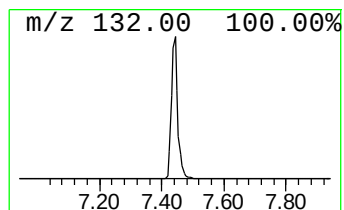
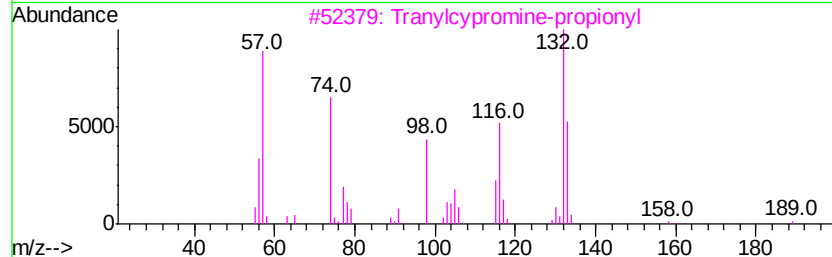
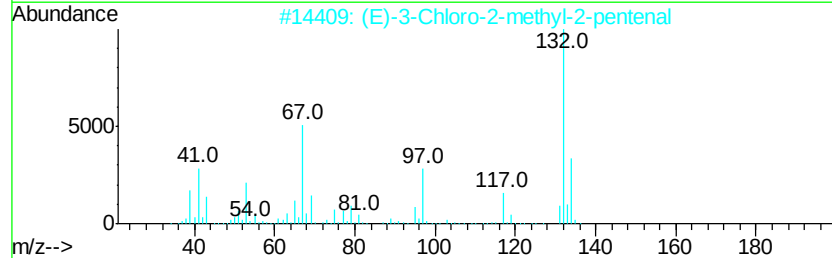
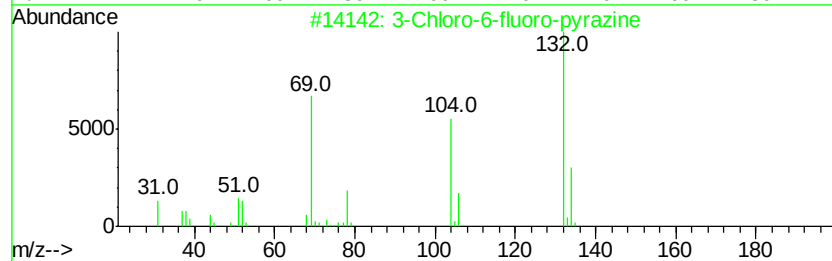
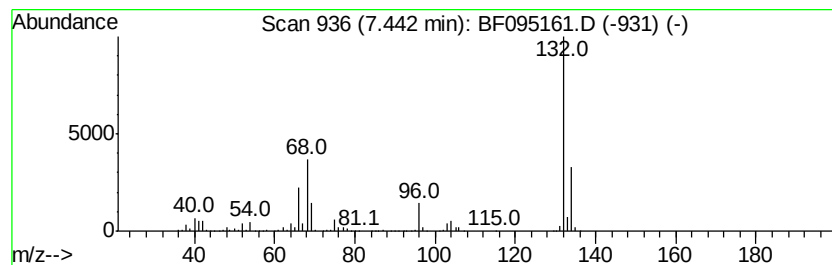
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Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	121.86 ng	2860280	1,4-Dichlorobenzene-d4	7.78

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	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Xenon	132	Xe	007440-63-3	9



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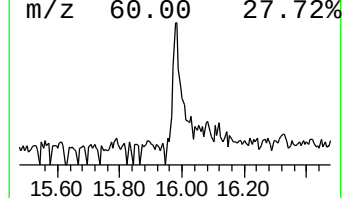
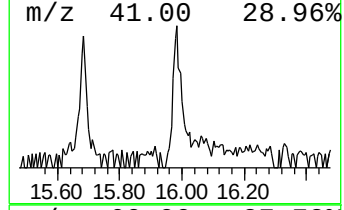
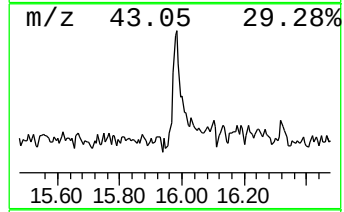
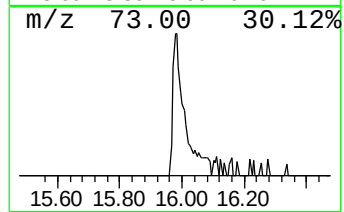
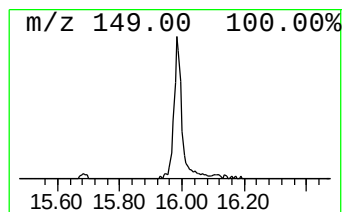
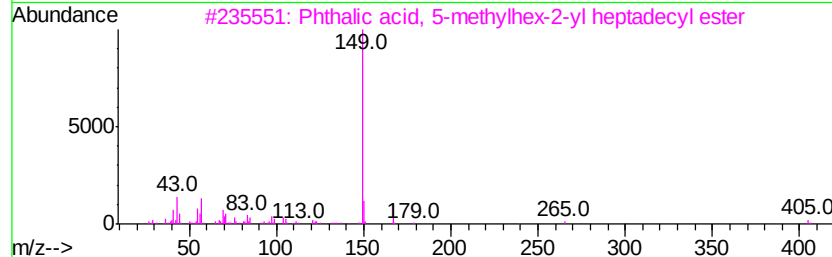
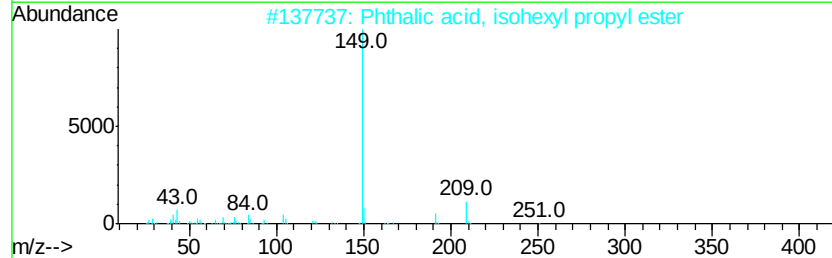
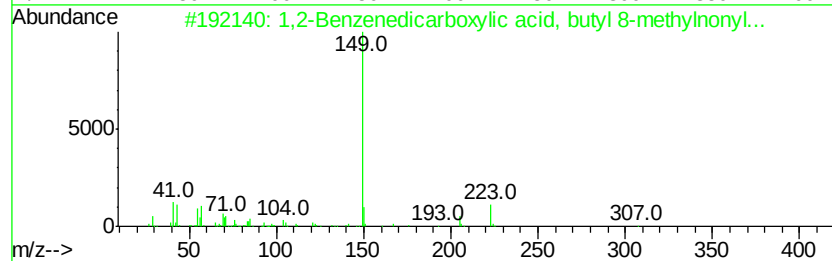
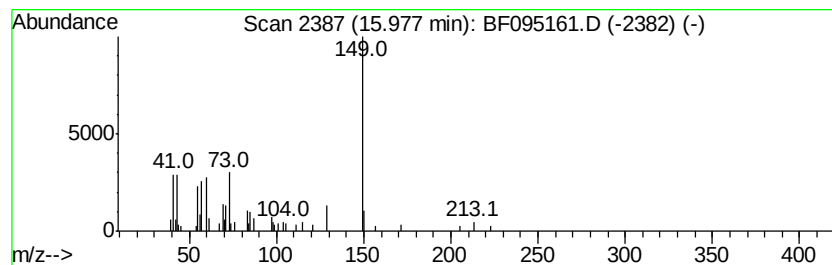
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Peak Number 4 1,2-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.94 ng	121474	Phenanthrene-d10	15.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,2-Benzenedicarboxylic acid, bu...	362 C22H34O4	000089-18-9	52
2	Phthalic acid, isohexyl propyl e...	292 C17H24O4	1000308-98-9	50
3	Phthalic acid, 5-methylhex-2-yl ...	502 C32H54O4	1000371-07-7	50
4	Phthalic acid, hex-2-yn-4-yl und...	400 C25H36O4	1000315-19-7	50
5	1,2-Benzenedicarboxylic acid, bu...	304 C18H24O4	000084-64-0	47



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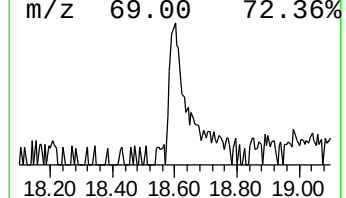
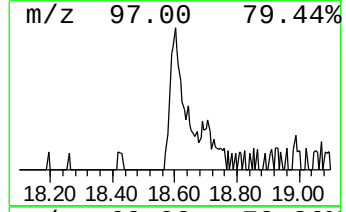
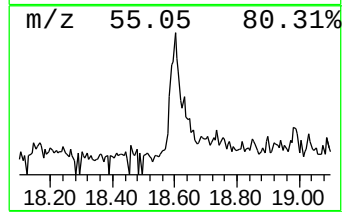
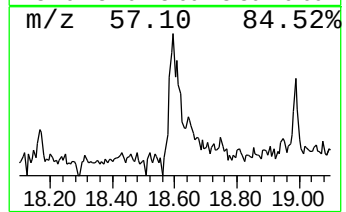
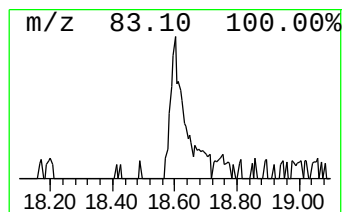
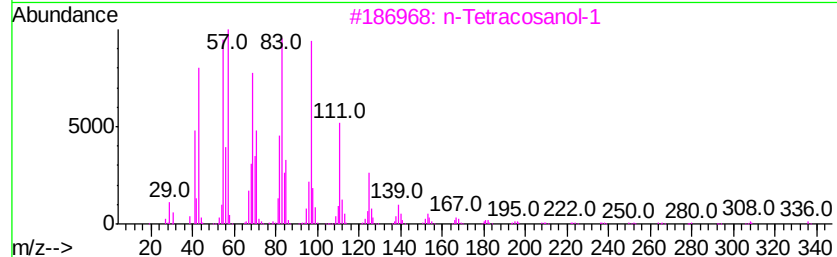
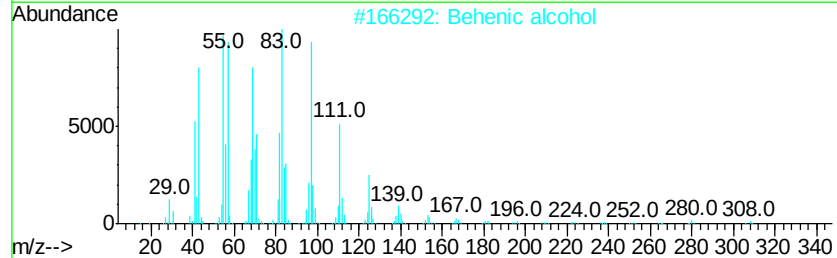
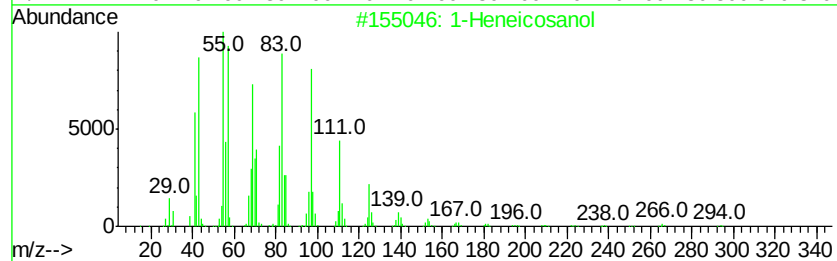
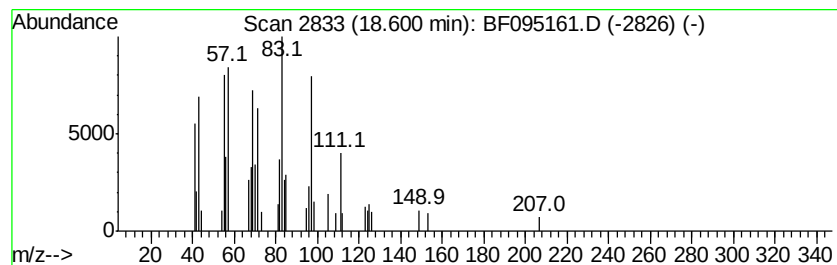
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.60	3.15 ng	109793	Chrysene-d12		18.69
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	87
2	Behenic alcohol	326	C22H46O	000661-19-8	87
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	83
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	74



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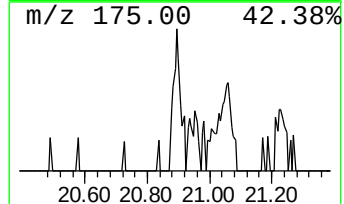
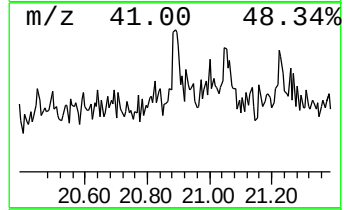
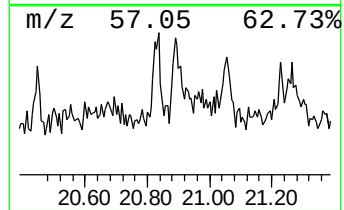
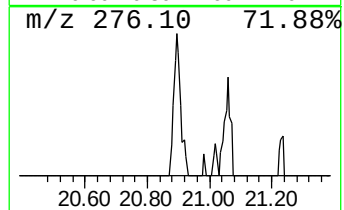
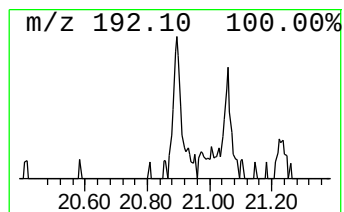
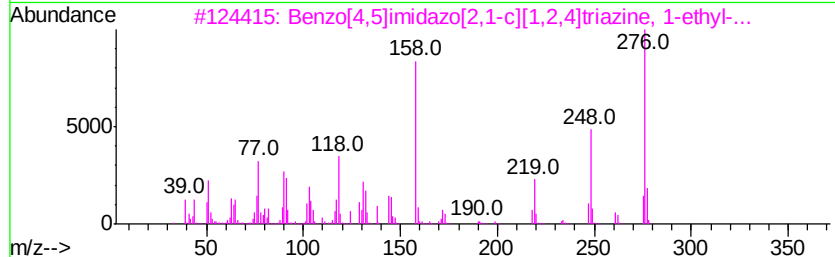
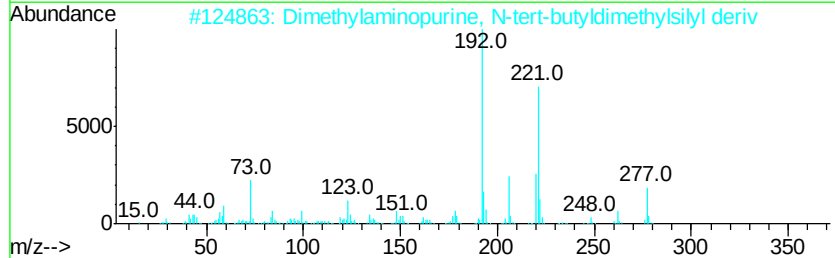
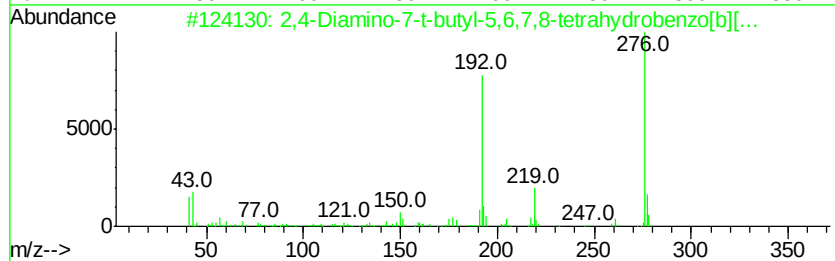
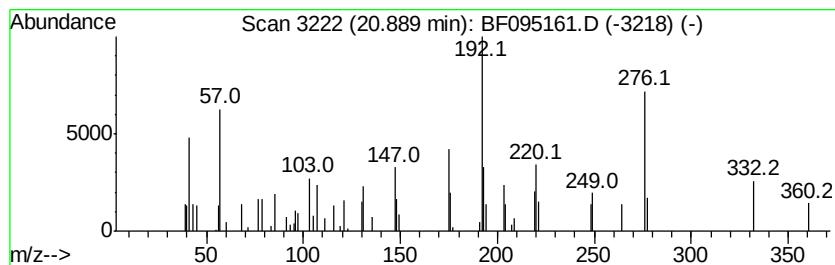
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown20.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.89	2.16 ng	42803	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Diamino-7-t-butyl-5,6,7,8-te...	276	C14H20N4S	049620-43-1	38
2		Dimethylaminopurine, N-tert-buty...	277	C13H23N5Si	1000364-71-6	27
3		Benzo[4,5]imidazo[2,1-c][1,2,4]t...	276	C17H16N4	1000302-82-6	25
4		Thiazole, 2-(phenylthio)-	193	C9H7NS2	033342-67-5	18
5		4-(4-Methoxybenzylidene)-1-pheny...	276	C19H16O2	339289-77-9	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	17.7	ng	416472	1	7.78	469432	20.0
unknown7.44	7.44	121.9	ng	2860280	1	7.78	469432	20.0
1,2-Benzenedicarb...	15.98	2.9	ng	121474	4	15.02	825156	20.0
1-Heneicosanol	18.60	3.1	ng	109793	5	18.69	696179	20.0
unknown20.89	20.89	2.2	ng	42803	6	20.37	396765	20.0