

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
 Data File : BG025506.D
 Acq On : 13 Jan 2017 6:56
 Operator : UM/SJ
 Sample : I1138-01
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1

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_G\METHODS\8270-BG122116.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	5.263	404	413	422	rBV	201029	344220	4.25%	0.811%
2	5.739	488	494	507	rBV	580326	1039973	12.85%	2.450%
3	7.361	760	770	779	rBV2	365658	750256	9.27%	1.767%
4	7.731	825	833	845	rBV	1098107	2000294	24.72%	4.712%
5	8.201	905	913	921	rBV	233289	434725	5.37%	1.024%
6	8.524	961	968	979	rVB	1090218	1966643	24.30%	4.633%
7	9.382	1107	1114	1125	rBV	943405	1860942	23.00%	4.384%
8	11.027	1387	1394	1405	rBV	293879	587672	7.26%	1.384%
9	13.448	1797	1806	1818	rBV	2684374	4358078	53.85%	10.266%
10	14.829	2034	2041	2049	rVB	553812	918382	11.35%	2.163%
11	15.246	2100	2112	2127	rBV	3025715	6852599	84.68%	16.142%
12	16.315	2286	2294	2308	rBV	2517282	3896898	48.15%	9.180%
13	17.572	2499	2508	2516	rBV2	764022	1223921	15.12%	2.883%
14	18.413	2647	2651	2657	rBV4	92413	136383	1.69%	0.321%
15	19.976	2911	2917	2922	rBV4	61448	121441	1.50%	0.286%
16	20.152	2936	2947	2953	rBV	6047076	8092519	100.00%	19.063%
17	20.822	3056	3061	3068	rVB7	55738	106401	1.31%	0.251%
18	21.862	3231	3238	3246	rBV	977016	1722553	21.29%	4.058%
19	22.320	3311	3316	3330	rBV4	239954	562671	6.95%	1.325%
20	23.471	3507	3512	3517	rBV2	88726	160791	1.99%	0.379%
21	24.394	3661	3669	3685	rBV2	455591	1531806	18.93%	3.608%
22	25.258	3806	3816	3828	rBV2	557226	1704766	21.07%	4.016%
23	27.631	4209	4220	4245	rBV3	401929	2077793	25.68%	4.894%

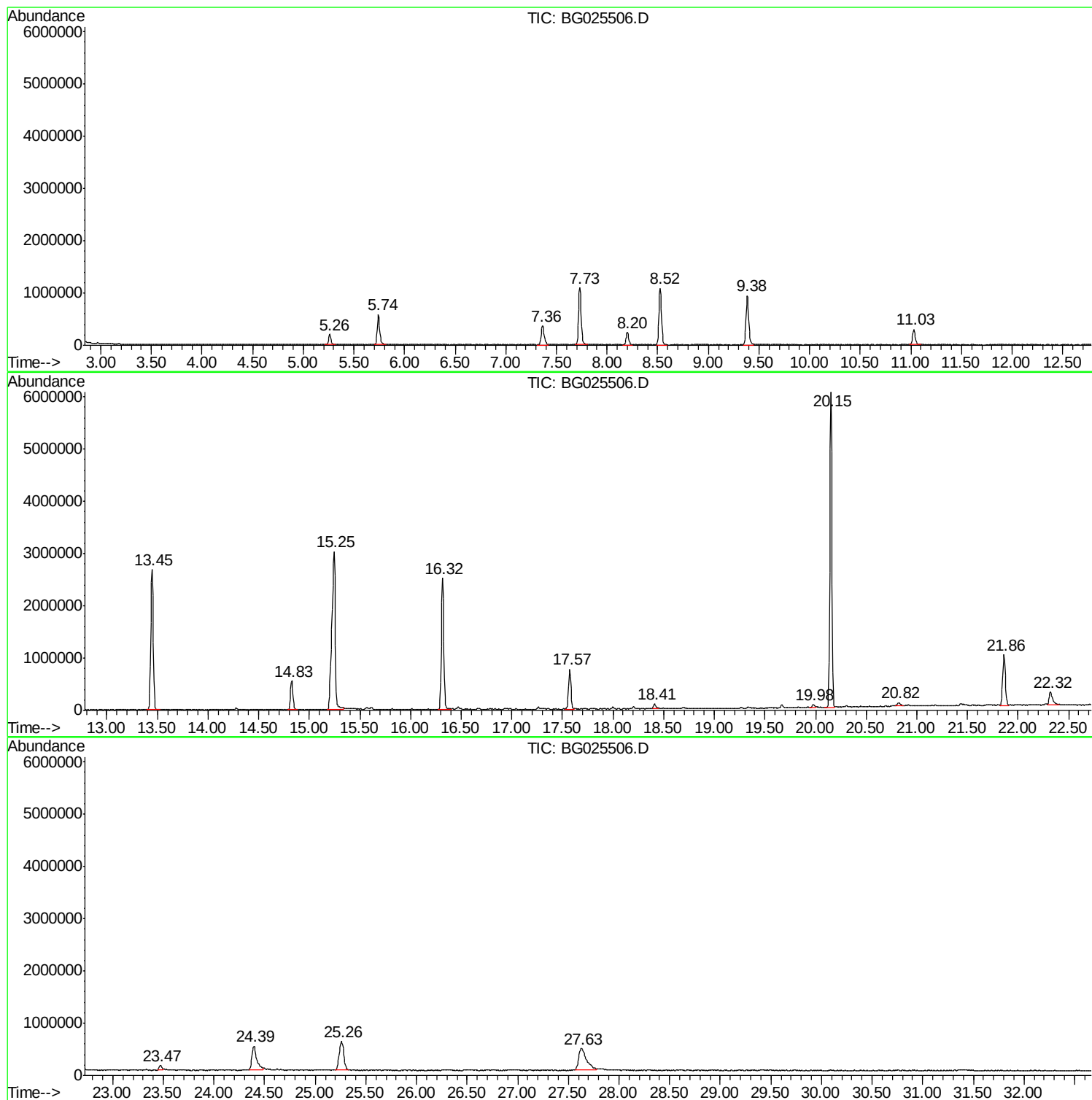
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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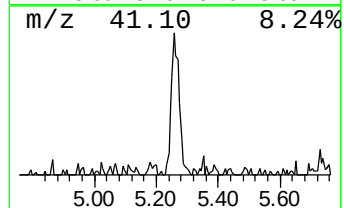
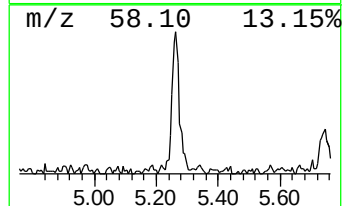
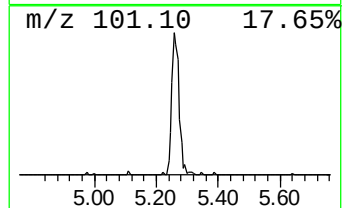
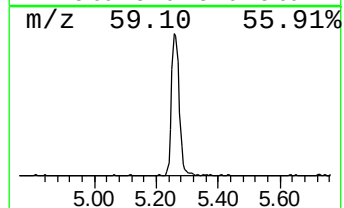
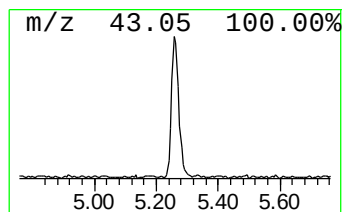
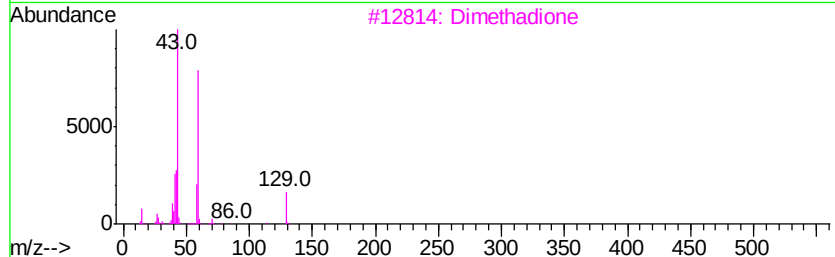
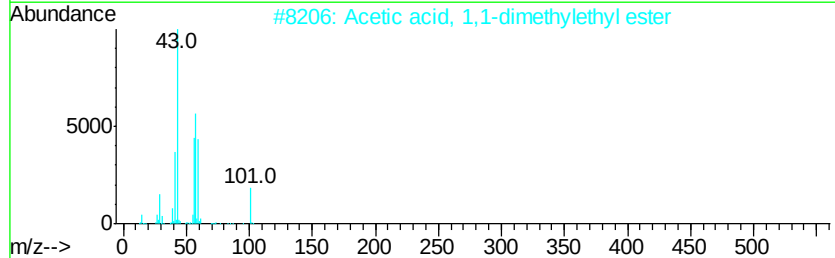
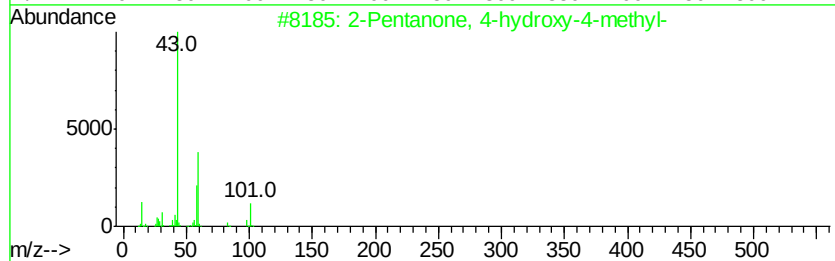
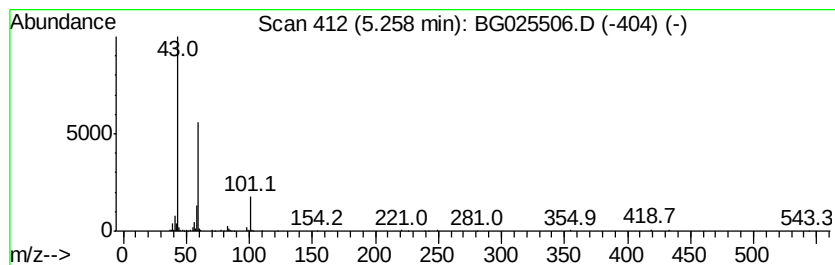
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	15.84 ng	344220	1,4-Dichlorobenzene-d4	8.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45	
3	Dimethadione	129	C5H7NO3	000695-53-4	42	
4	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	32	
5	3-Octanol	130	C8H18O	000589-98-0	25	



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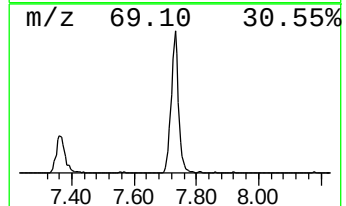
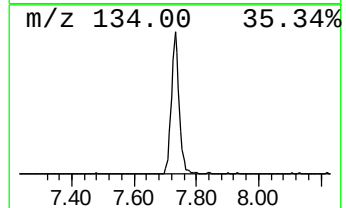
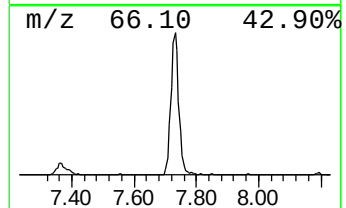
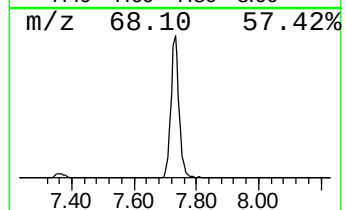
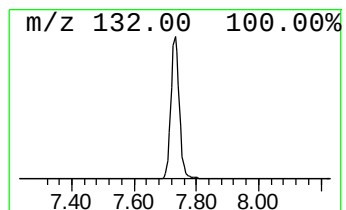
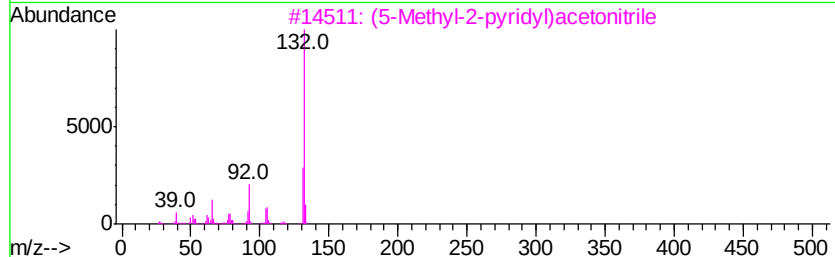
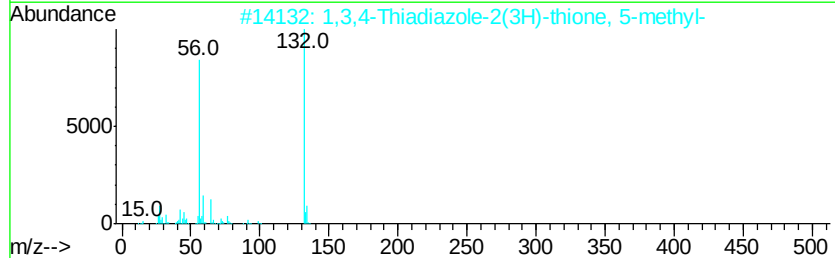
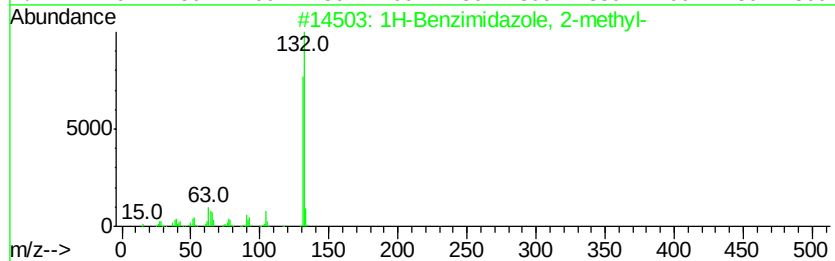
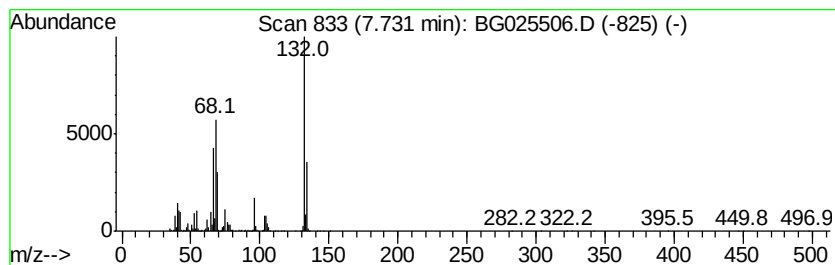
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	92.03 ng	2000290	1,4-Dichlorobenzene-d4	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
3		(5-Methyl-2-oxridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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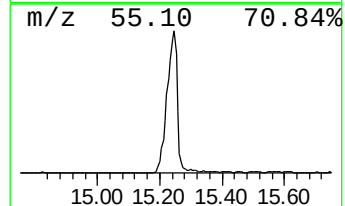
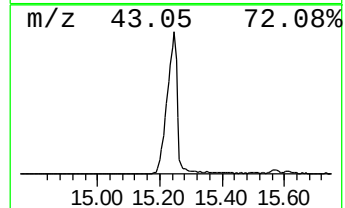
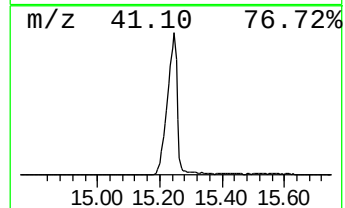
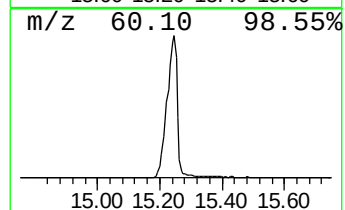
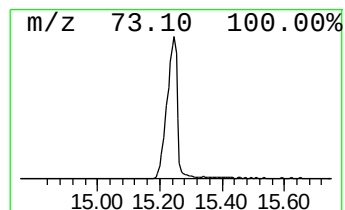
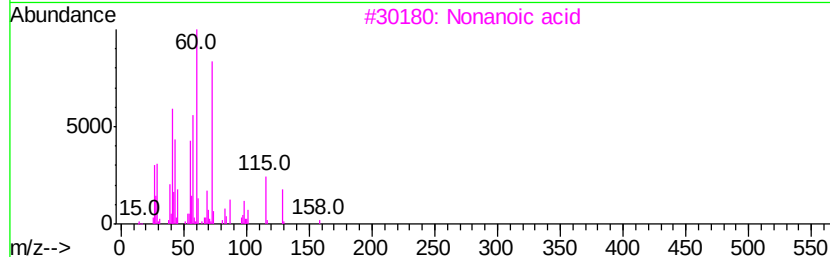
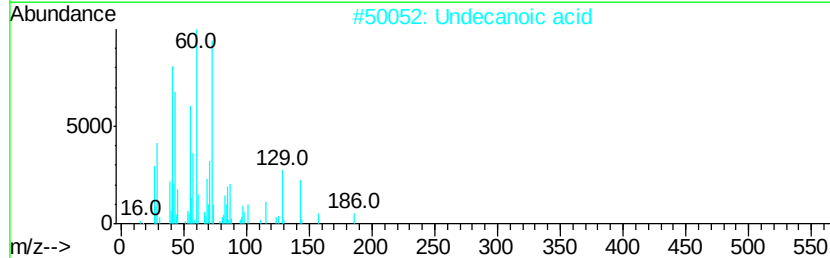
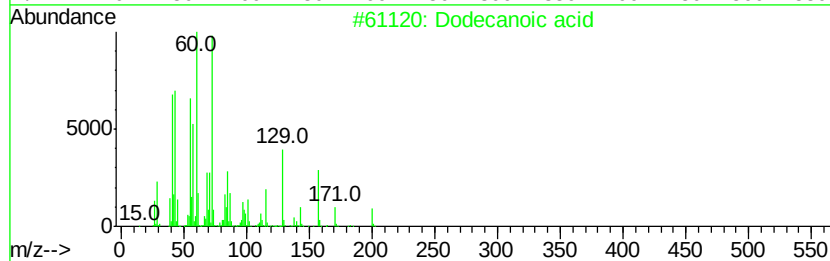
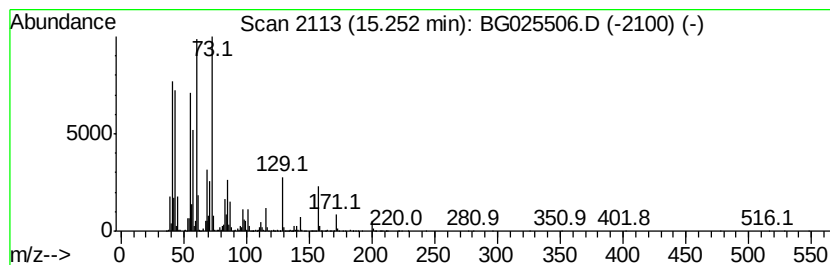
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.25	149.23 ng	6852600	Acenaphthene-d10		14.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	80
3			Nonanoic acid	158	C9H18O2	000112-05-0	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			Hexanoic acid	116	C6H12O2	000142-62-1	38



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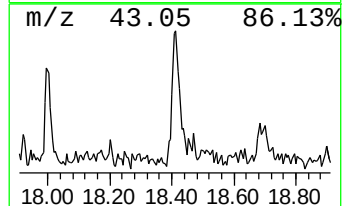
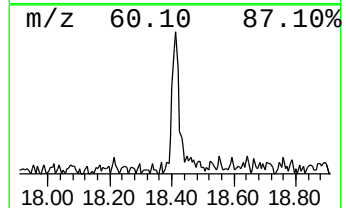
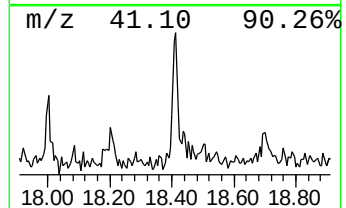
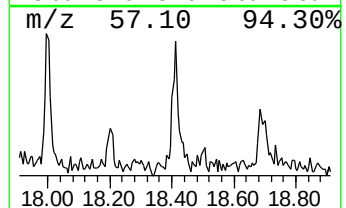
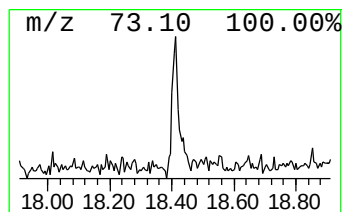
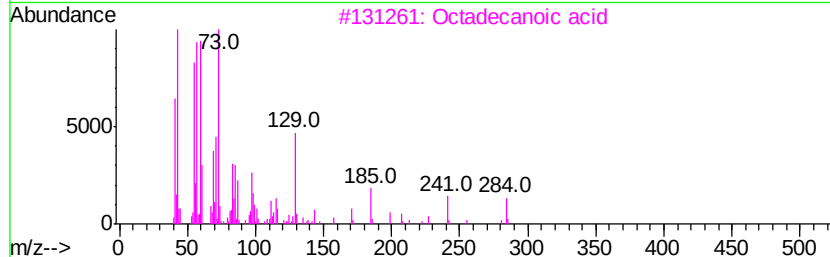
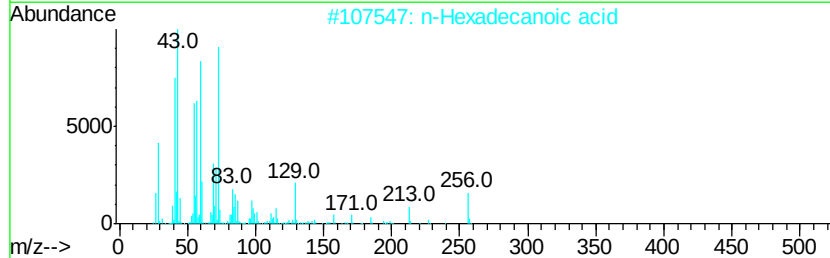
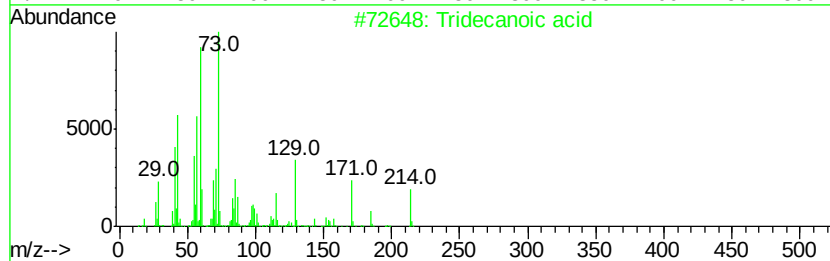
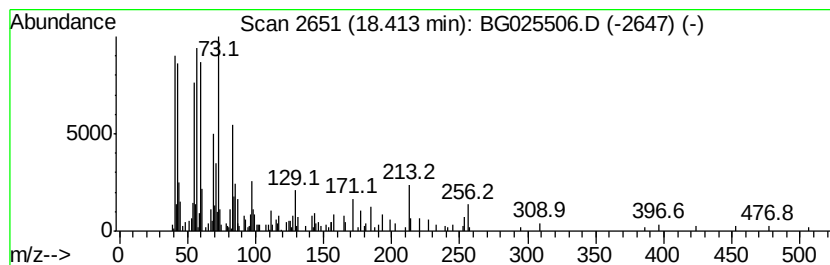
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	2.23 ng	136383	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	78
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Octadecanoic acid	284	C18H36O2	000057-11-4	62
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	50



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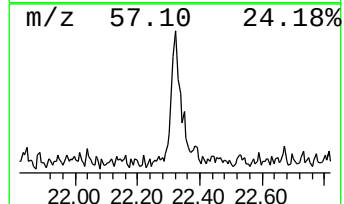
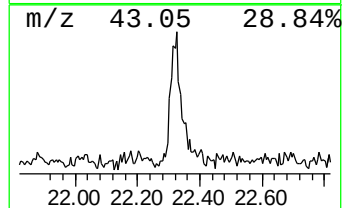
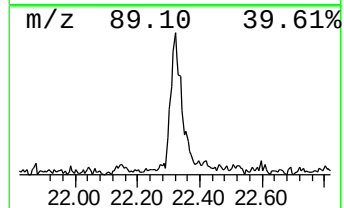
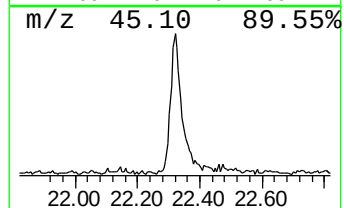
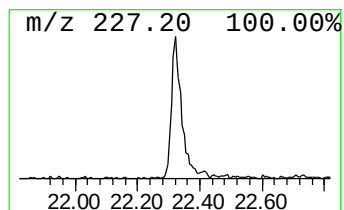
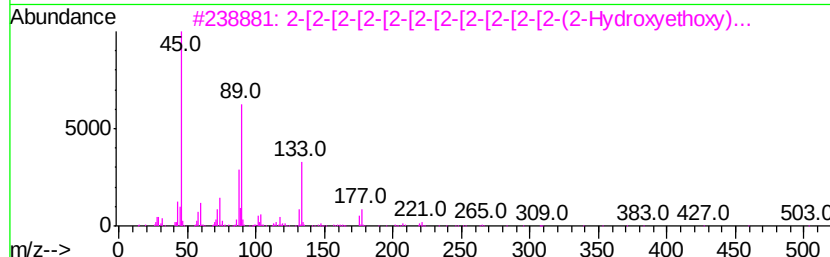
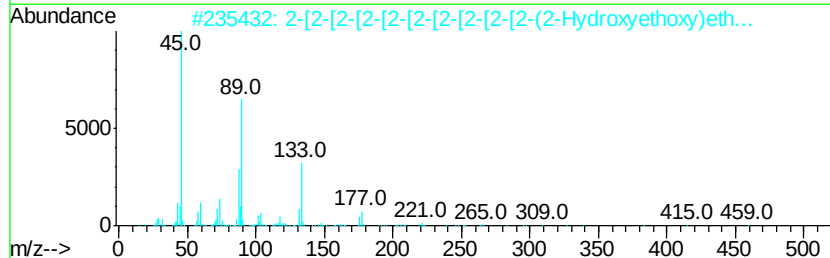
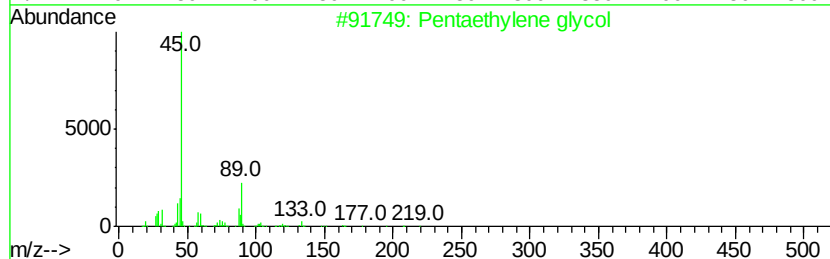
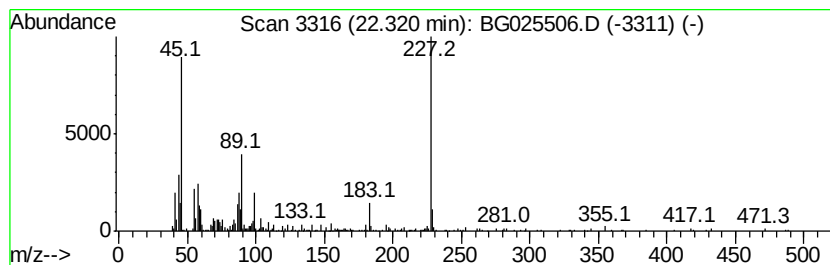
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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Peak Number 6  Pentaethylene glycol                      Concentration Rank 7

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R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.32	6.53 ng	562671	Chrysene-d12		21.86	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentaethylene glycol	238	C10H22O6	004792-15-8	38
2		2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	38
3		2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	38
4		Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	35
5		Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.26	15.8	ng	344220	1	8.20	434725	20.0
unknown7.73	7.73	92.0	ng	2000290	1	8.20	434725	20.0
Dodecanoic acid	15.25	149.2	ng	6852600	3	14.83	918382	20.0
Tridecanoic acid	18.41	2.2	ng	136383	4	17.57	1223920	20.0
Pentaethylene glycol	22.32	6.5	ng	562671	5	21.86	1722550	20.0