

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102215\
 Data File : BF082463.D
 Acq On : 22 Oct 2015 23:53
 Operator : UM/IZ
 Sample : G4119-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-101915-2

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-BF101015.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	4.251	183	185	195	rBV	84646	119466	5.13%	0.547%
2	4.937	242	245	254	rVB	820084	1144750	49.14%	5.238%
3	5.371	281	283	287	rBV	1759604	1698396	72.91%	7.771%
4	5.760	315	317	320	rVB	25864	23766	1.02%	0.109%
5	6.412	372	374	377	rBV	1454186	1553818	66.71%	7.110%
6	6.537	382	385	387	rBV	1420171	1818718	78.08%	8.322%
7	6.754	402	404	407	rBV	527454	639622	27.46%	2.927%
8	6.915	415	418	420	rBV	1613489	1427932	61.30%	6.534%
9	7.326	452	454	457	rBV	755841	1057226	45.39%	4.837%
10	7.440	462	464	468	rVB2	30692	40370	1.73%	0.185%
11	7.806	494	496	506	rBV	15924	31058	1.33%	0.142%
12	8.046	515	517	520	rBV	837458	866275	37.19%	3.964%
13	9.132	609	612	614	rBV	2439566	2329342	100.00%	10.658%
14	9.532	644	647	649	rBV	640372	554749	23.82%	2.538%
15	9.806	668	671	674	rBV	1244715	1146547	49.22%	5.246%
16	10.241	707	709	710	rVB	38332	34594	1.49%	0.158%
17	10.606	738	741	743	rBV	968077	1375196	59.04%	6.292%
18	10.709	748	750	757	rVB2	74459	94856	4.07%	0.434%
19	11.155	788	789	794	rVB2	47521	72608	3.12%	0.332%
20	11.292	799	801	804	rBV	1132296	1126946	48.38%	5.156%
21	11.349	804	806	810	rVB	16047	24770	1.06%	0.113%
22	11.521	819	821	825	rVB	72605	78661	3.38%	0.360%
23	11.589	825	827	829	rBV	39757	36181	1.55%	0.166%
24	11.829	846	848	854	rBV	167084	169869	7.29%	0.777%
25	12.081	867	870	872	rBV	40114	47018	2.02%	0.215%
26	12.618	915	917	919	rBV	42875	56004	2.40%	0.256%
27	12.881	938	940	943	rBV	1543685	2154604	92.50%	9.859%
28	13.795	1017	1020	1027	rBV	103824	196113	8.42%	0.897%
29	13.955	1031	1034	1036	rBV	1022663	1044010	44.82%	4.777%
30	14.767	1101	1105	1108	rBV2	13806	35774	1.54%	0.164%
31	15.430	1160	1163	1168	rBV	543628	801170	34.39%	3.666%
32	15.910	1203	1205	1209	rBV4	9742	28293	1.21%	0.129%
33	16.333	1239	1242	1246	rVB2	12473	26510	1.14%	0.121%

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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

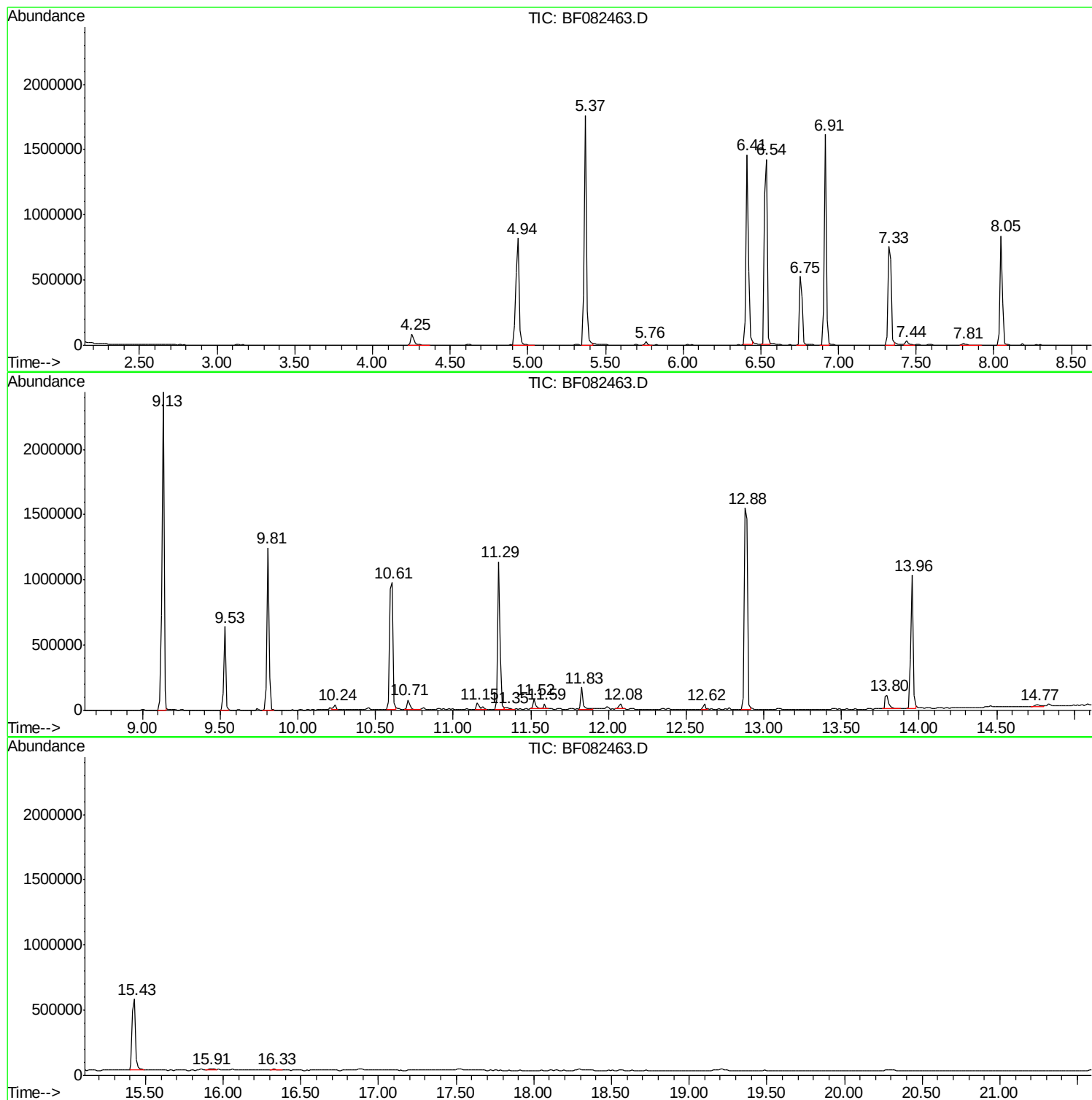
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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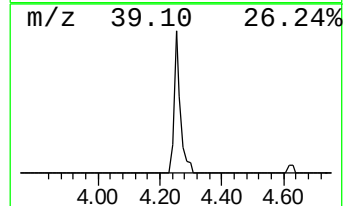
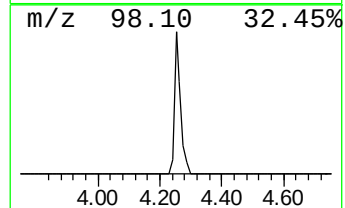
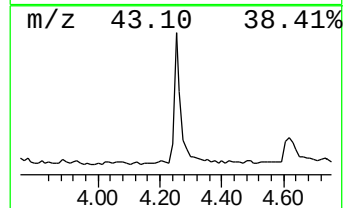
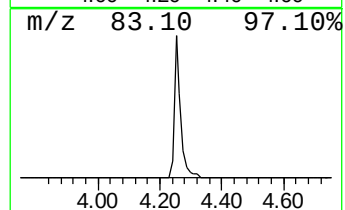
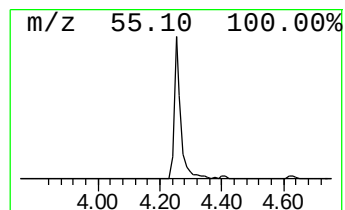
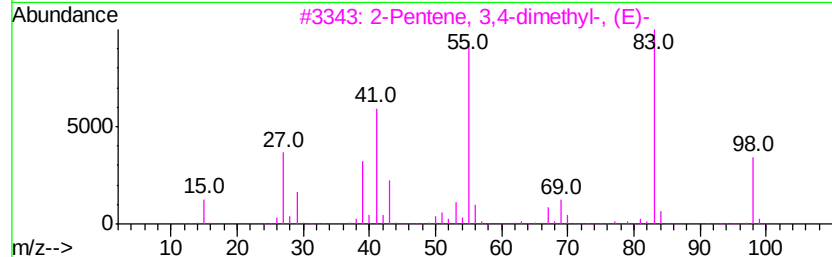
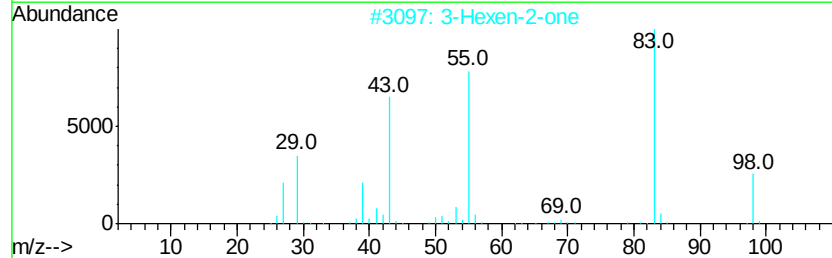
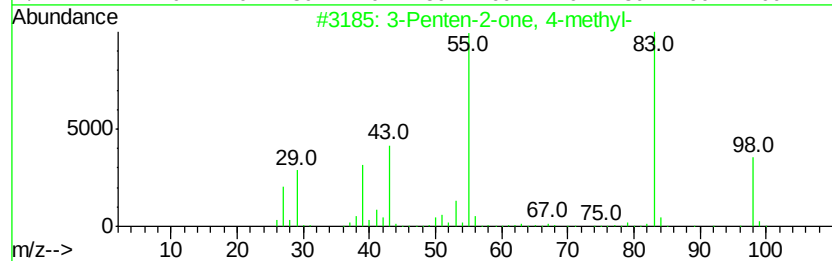
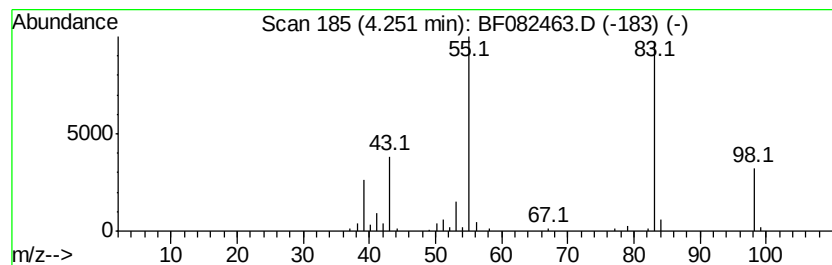
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	3.74 ng	119466	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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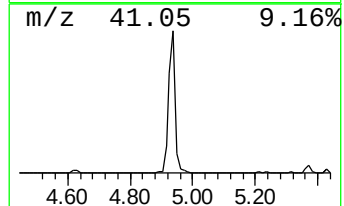
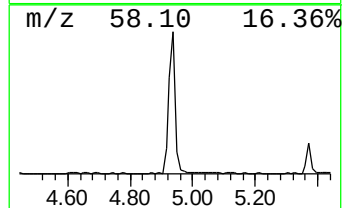
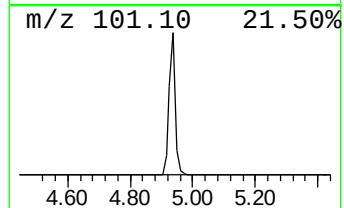
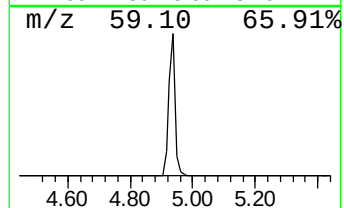
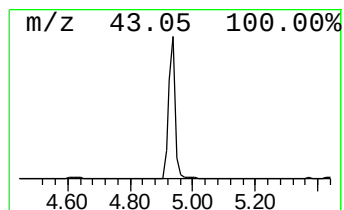
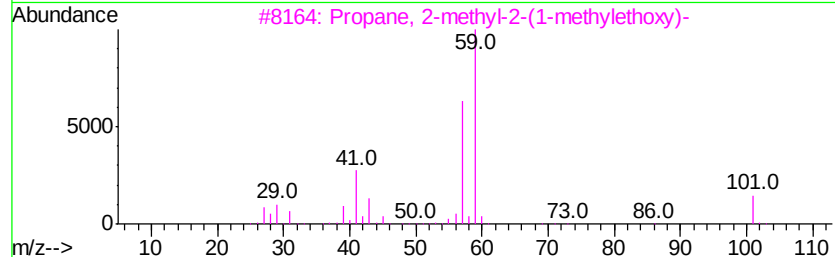
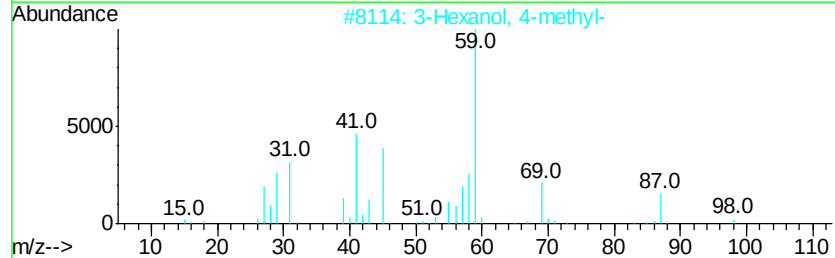
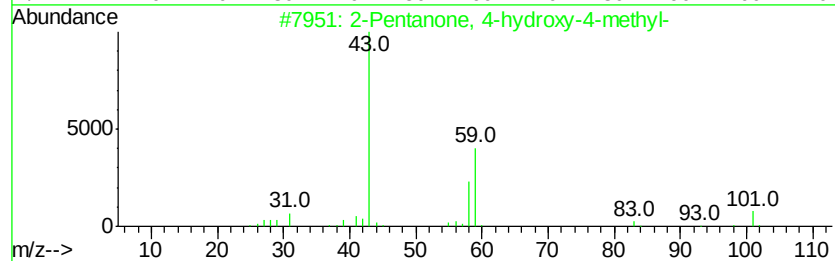
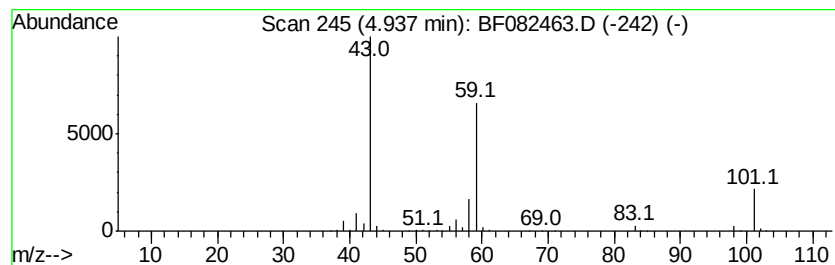
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	35.79 ng	1144750	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
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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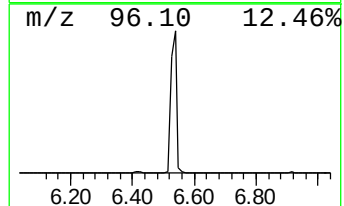
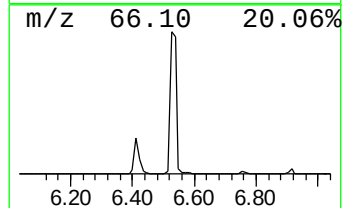
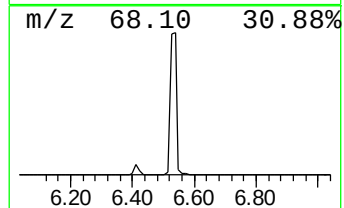
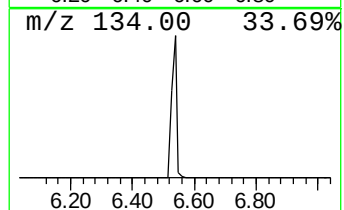
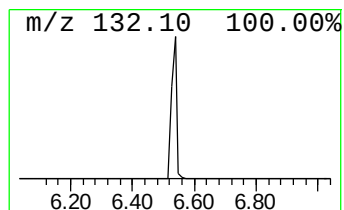
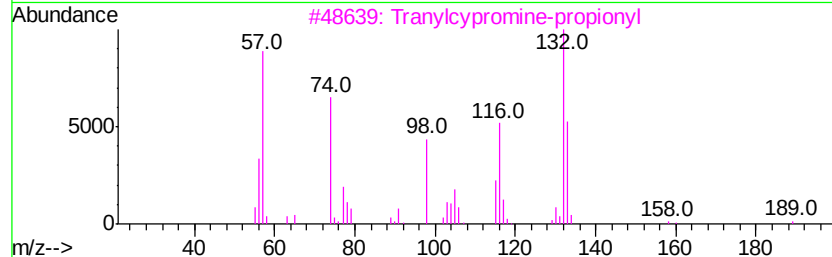
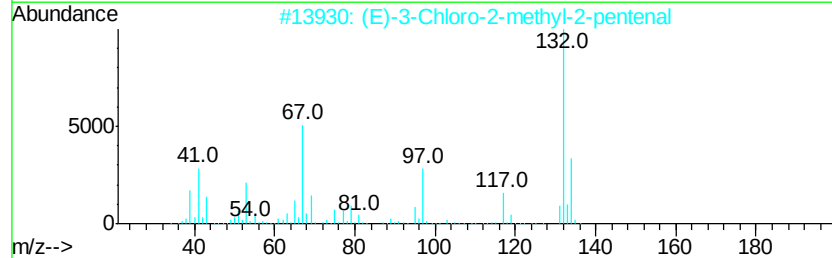
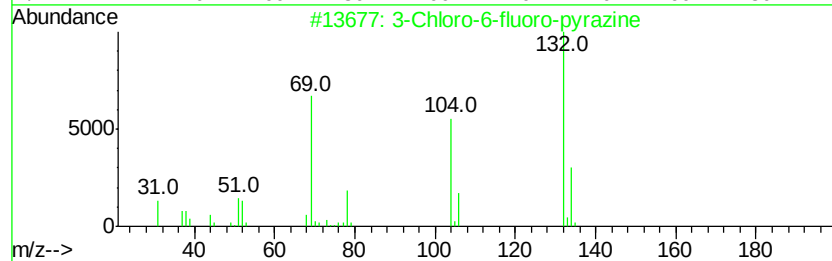
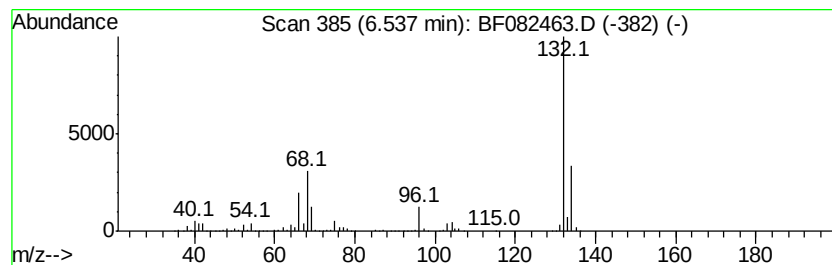
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	56.87 ng	1818720	1,4-Dichlorobenzene-d4	6.75

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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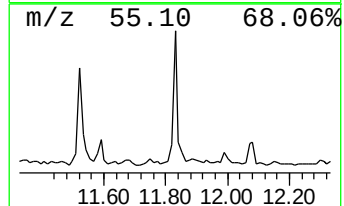
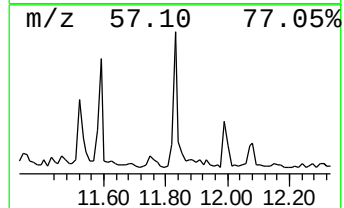
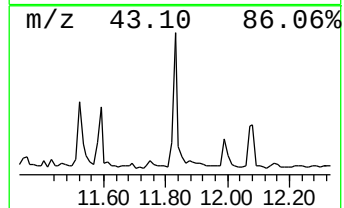
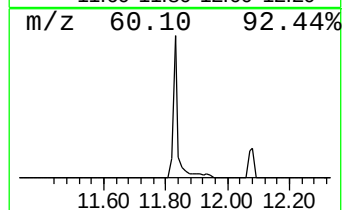
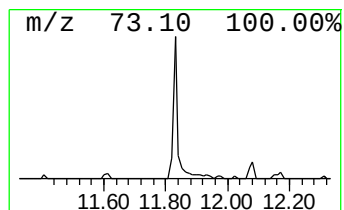
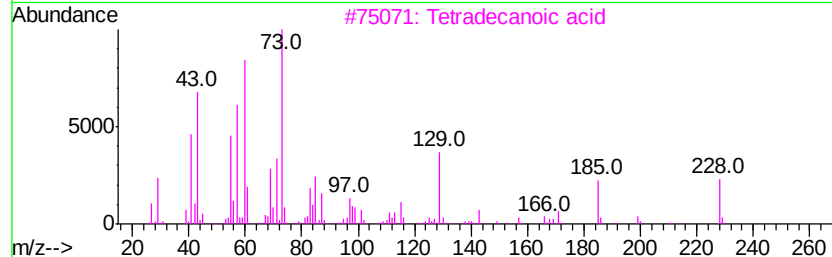
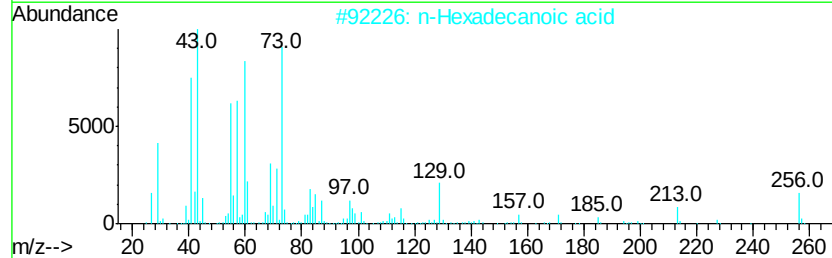
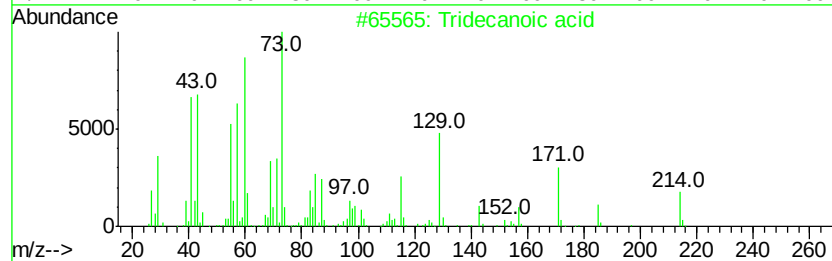
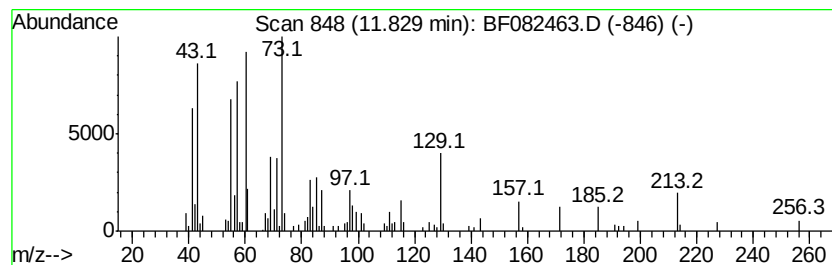
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	3.01 ng	169869	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Dodecanoic acid	200	C12H24O2	000143-07-7	72
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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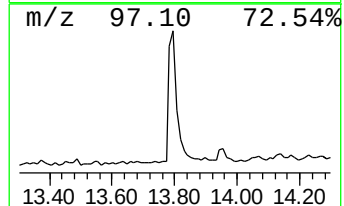
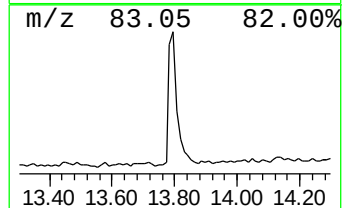
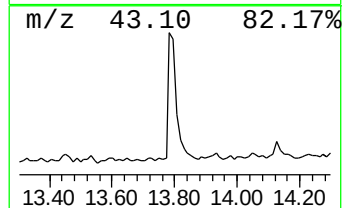
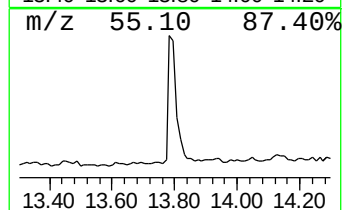
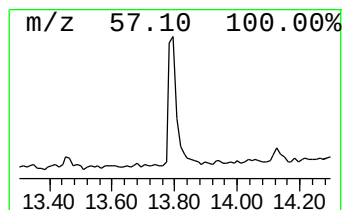
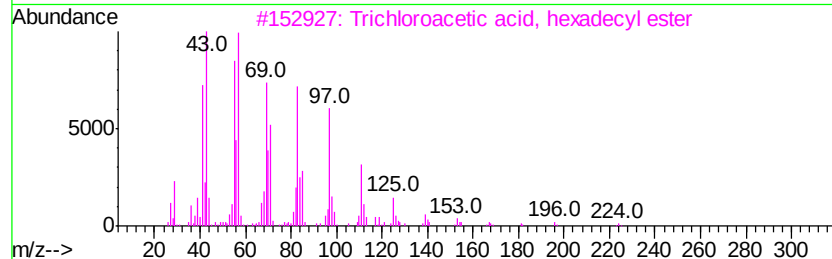
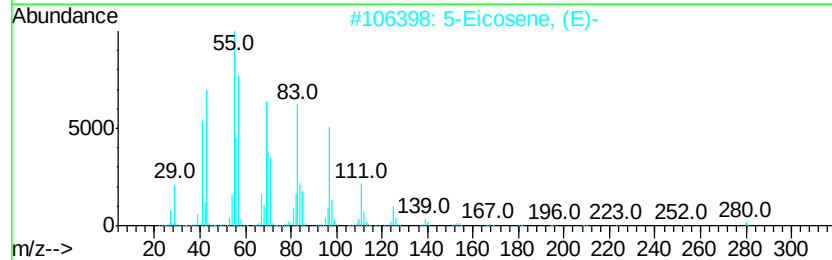
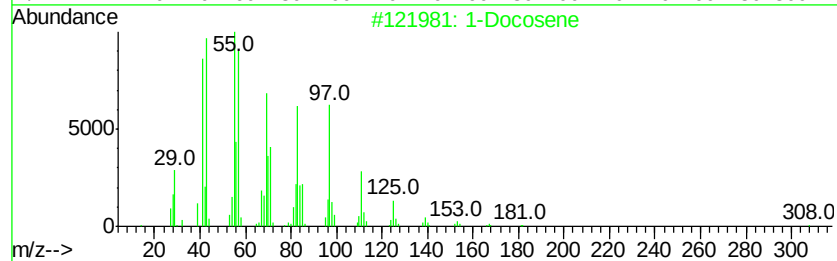
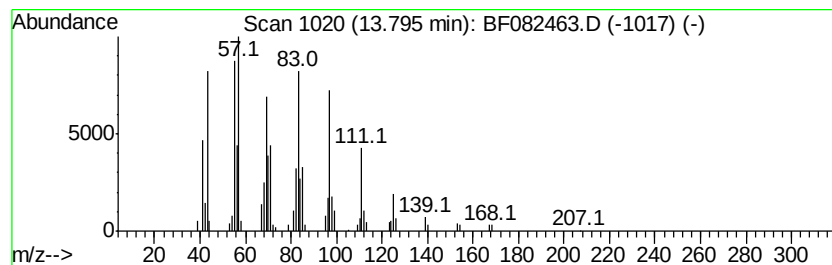
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.76 ng	196113	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90



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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.25	3.7	ng	119466	1	6.75	639622	20.0
2-Pentanone, 4-hy...	4.94	35.8	ng	1144750	1	6.75	639622	20.0
unknown6.54	6.54	56.9	ng	1818720	1	6.75	639622	20.0
Tridecanoic acid	11.83	3.0	ng	169869	4	11.29	1126950	20.0
1-Docosene	13.80	3.8	ng	196113	5	13.96	1044010	20.0