

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021116\
 Data File : BF085028.D
 Acq On : 11 Feb 2016 20:03
 Operator : SJ/IZ
 Sample : H1377-18
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB01-0-0.5

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-BF020116.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	1.667	6	7	11	rVB	137634	193971	5.58%	0.560%
2	1.735	11	13	29	rVB	1158921	1803916	51.94%	5.207%
3	4.730	273	275	283	rVB	577766	952431	27.42%	2.749%
4	5.199	313	316	318	rBV	2612947	3428008	98.70%	9.895%
5	6.262	406	409	412	rBV	2873197	3190655	91.86%	9.210%
6	6.376	417	419	421	rBV	3722870	3352883	96.53%	9.679%
7	6.604	437	439	442	rBV	1064252	915378	26.35%	2.642%
8	6.764	450	453	455	rBV	2839636	2553040	73.50%	7.370%
9	7.176	487	489	492	rBV	1760282	2102308	60.53%	6.069%
10	7.896	549	552	554	rBV	1570256	1329742	38.28%	3.838%
11	8.982	644	647	649	rBV	2741797	3473301	100.00%	10.026%
12	9.382	679	682	684	rBV	419383	489647	14.10%	1.413%
13	9.599	697	701	702	rBV	125522	122752	3.53%	0.354%
14	9.645	702	705	707	rVV	1666078	1431370	41.21%	4.132%
15	9.828	718	721	724	rBV2	22285	47509	1.37%	0.137%
16	10.090	742	744	746	rVB	142160	140549	4.05%	0.406%
17	10.308	760	763	767	rBV	46867	94416	2.72%	0.273%
18	10.433	772	774	776	rBV	2529145	2346584	67.56%	6.774%
19	10.571	784	786	789	rBV	115275	180812	5.21%	0.522%
20	10.753	800	802	807	rBV2	16696	37415	1.08%	0.108%
21	11.016	823	825	826	rBV	54811	62077	1.79%	0.179%
22	11.119	832	834	837	rBV	1336769	1312699	37.79%	3.789%
23	11.679	881	883	884	rBV	54306	50619	1.46%	0.146%
24	12.708	971	973	976	rBV	2691515	2648274	76.25%	7.645%
25	13.622	1050	1053	1062	rBV2	196767	311206	8.96%	0.898%
26	13.748	1062	1064	1067	rBV	978119	990556	28.52%	2.859%
27	14.068	1090	1092	1094	rBV	62365	63588	1.83%	0.184%
28	14.251	1106	1108	1112	rBV3	17907	38257	1.10%	0.110%
29	14.662	1142	1144	1147	rVB	39859	48387	1.39%	0.140%
30	15.108	1181	1183	1186	rBV	700952	816118	23.50%	2.356%
31	15.943	1253	1256	1262	rBV3	15865	40392	1.16%	0.117%
32	16.537	1305	1308	1314	rBV7	9904	35660	1.03%	0.103%
33	16.845	1331	1335	1340	rBV8	12948	37718	1.09%	0.109%

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB01-0-0.5

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-BF020116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

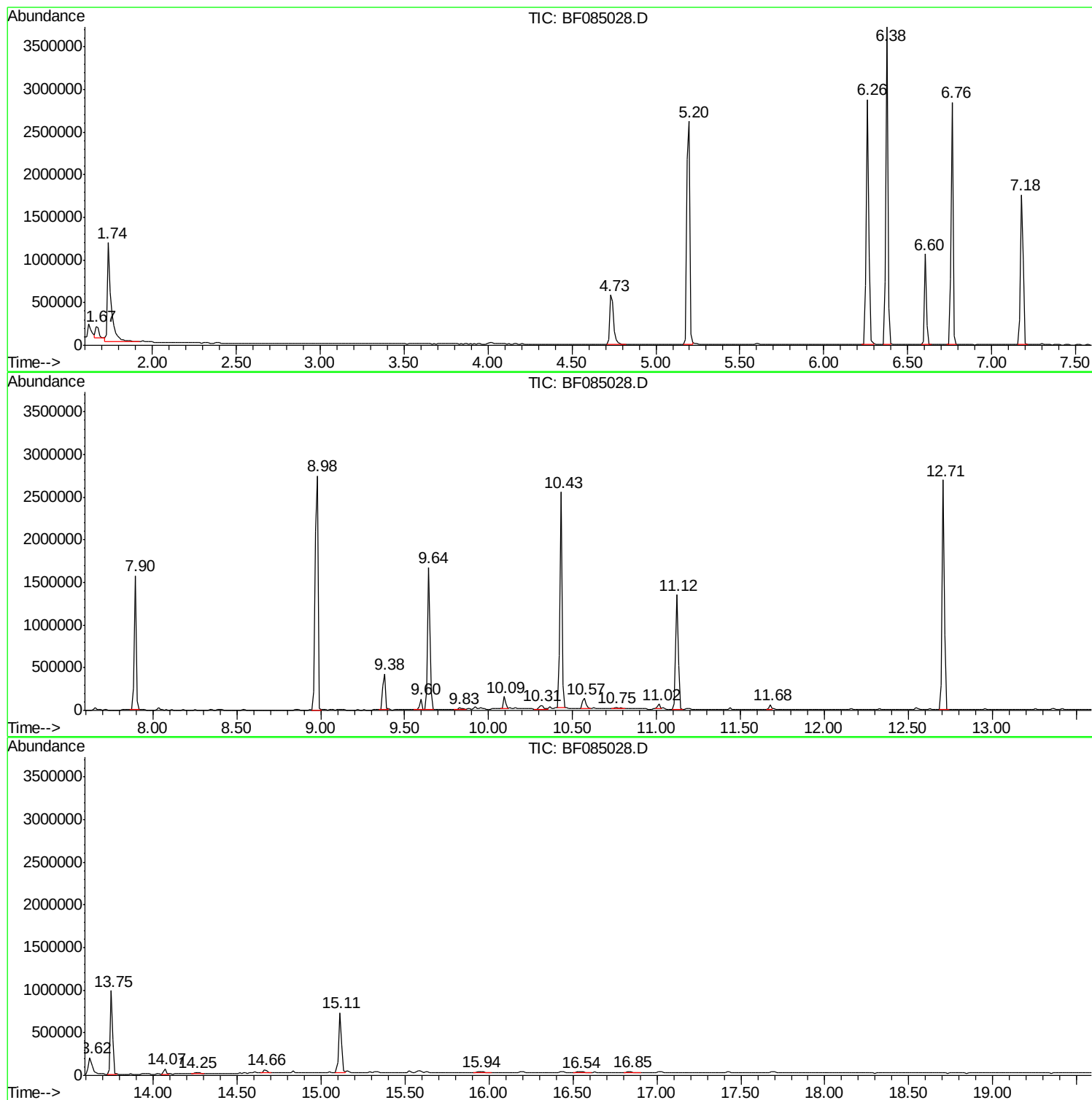
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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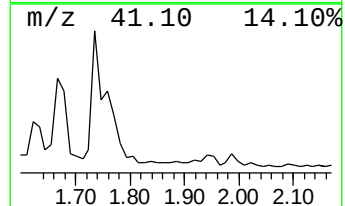
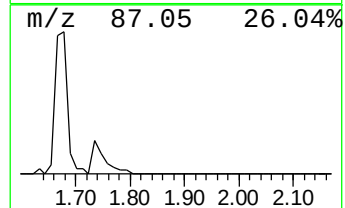
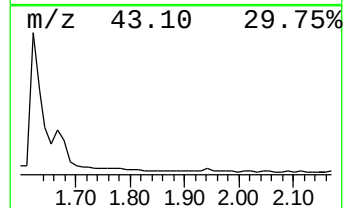
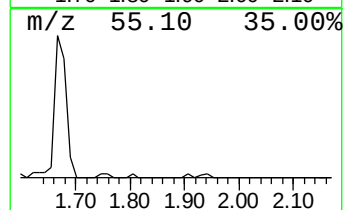
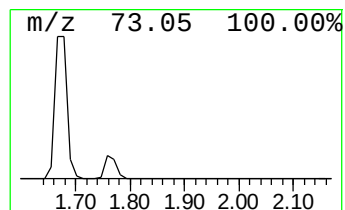
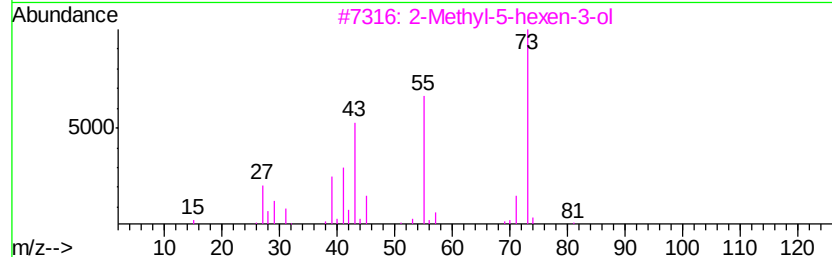
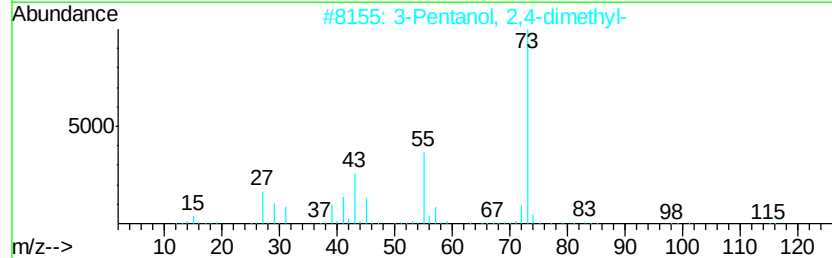
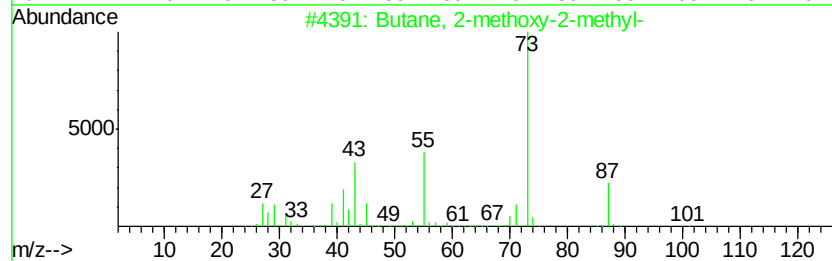
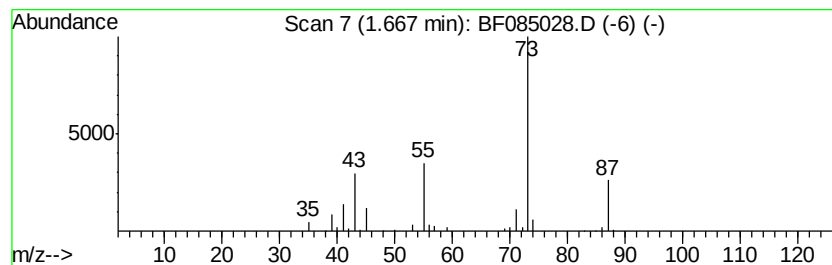
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	4.24 ng	193971	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4		1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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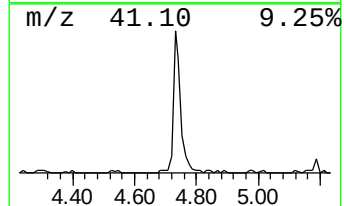
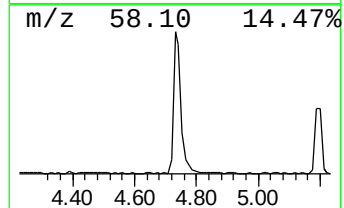
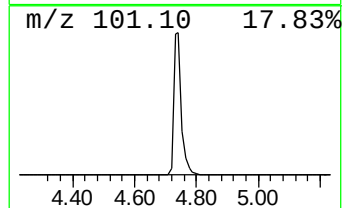
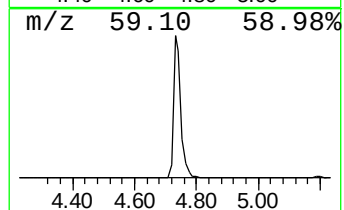
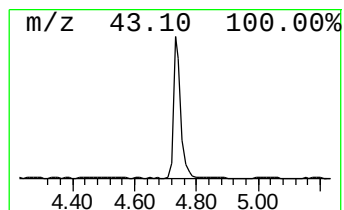
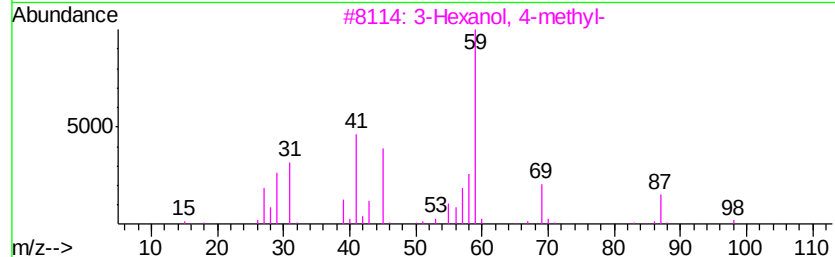
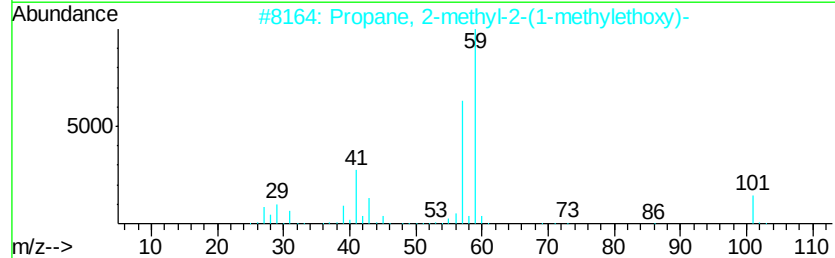
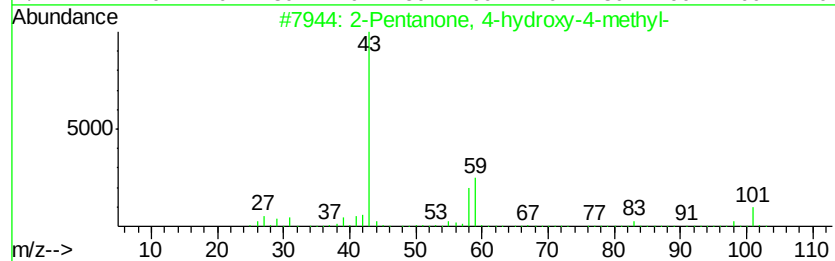
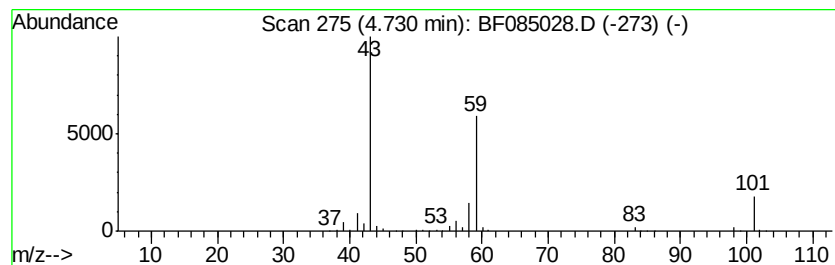
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	20.81 ng	952431	1,4-Dichlorobenzene-d4	6.60

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	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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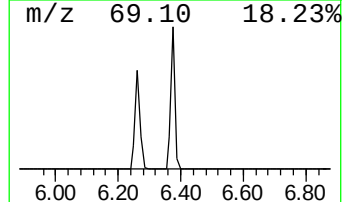
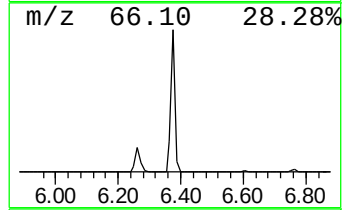
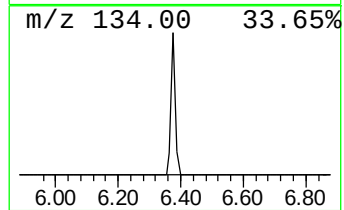
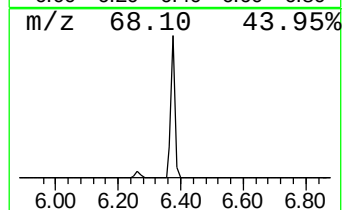
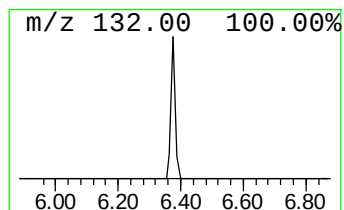
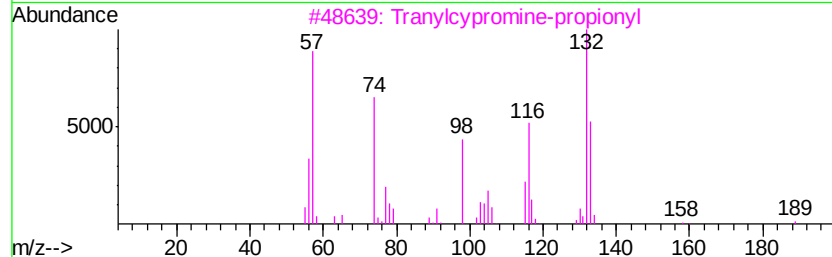
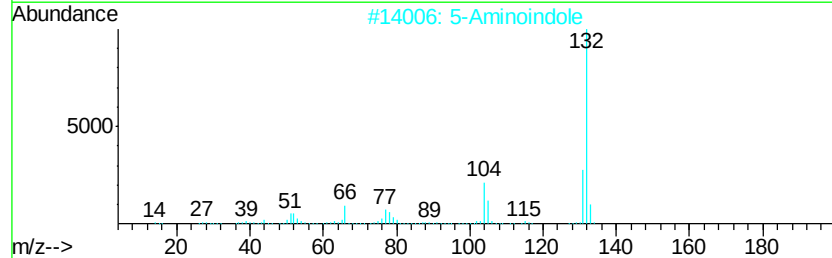
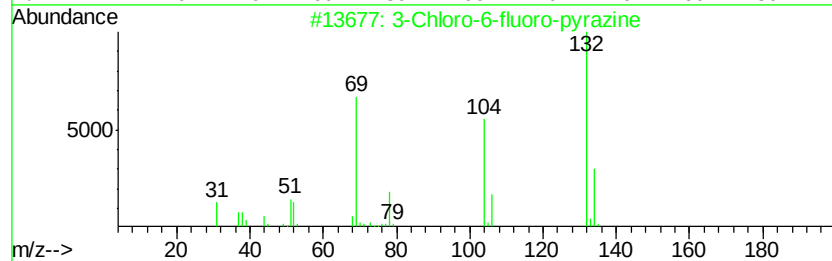
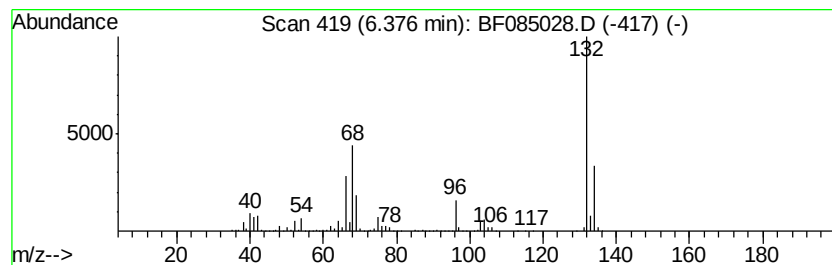
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	73.26 ng	3352880	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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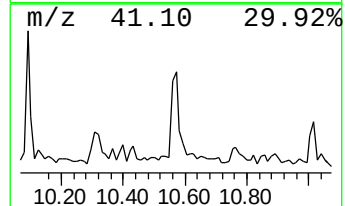
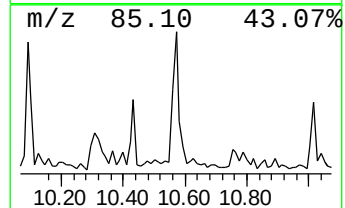
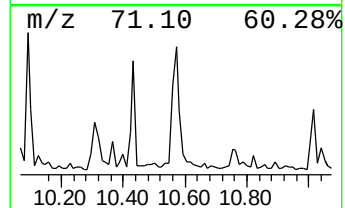
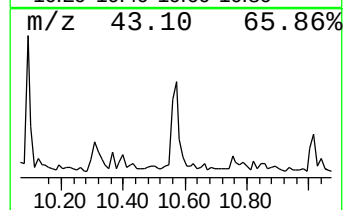
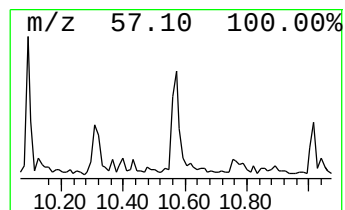
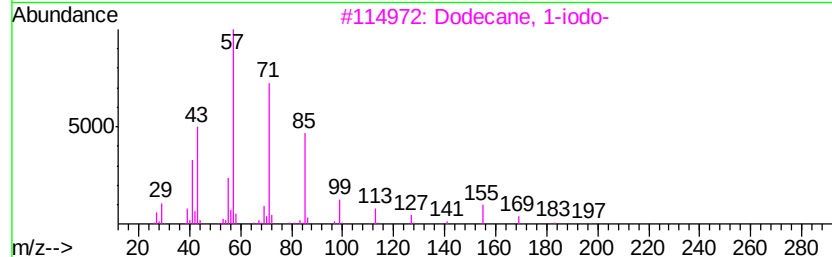
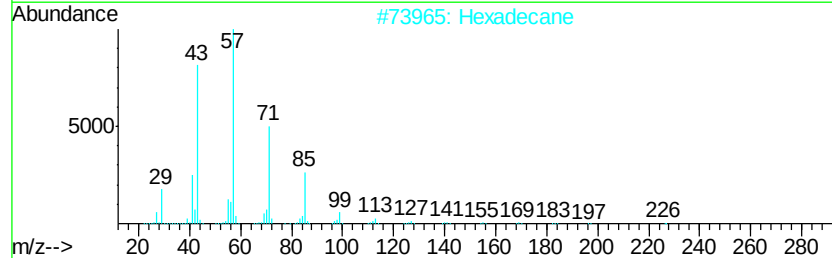
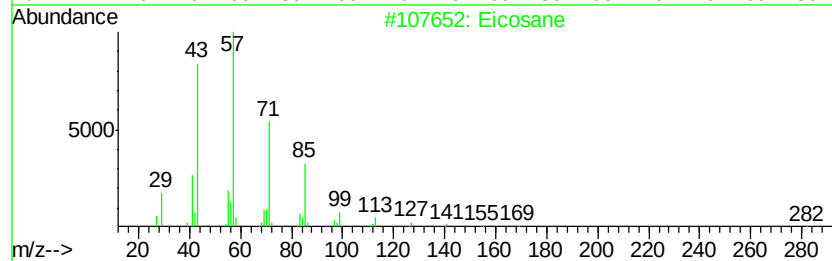
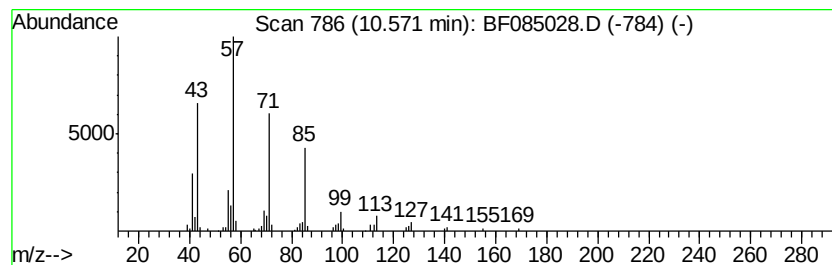
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	2.75 ng	180812	Phenanthrene-d10	11.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	Hexadecane	226 C16H34	000544-76-3	90
3	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	80
4	Undecane, 3,8-dimethyl-	184 C13H28	017301-30-3	78
5	Octacosane	394 C28H58	000630-02-4	78



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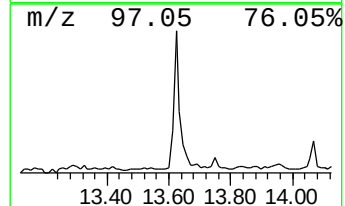
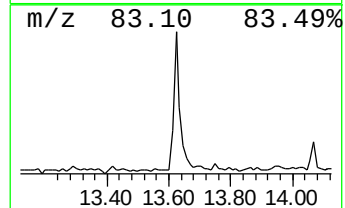
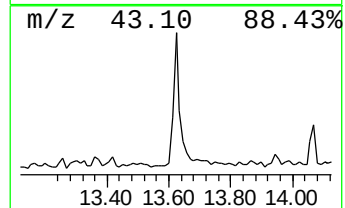
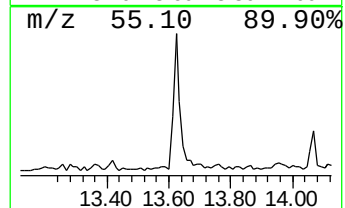
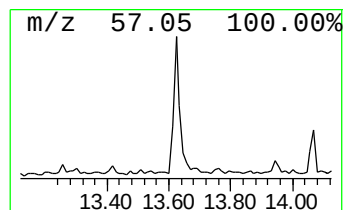
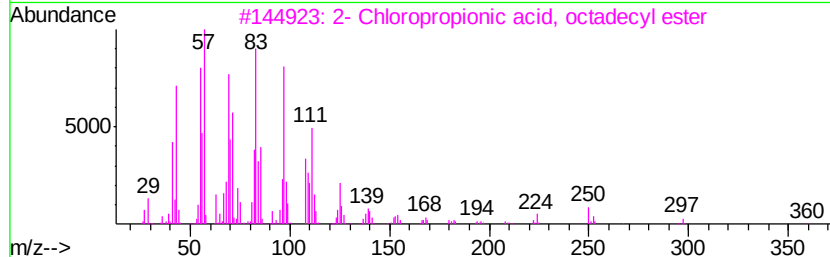
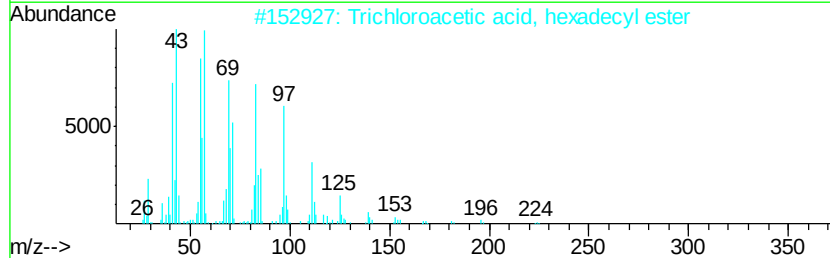
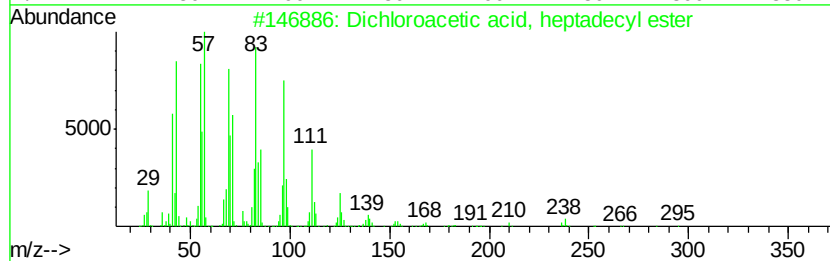
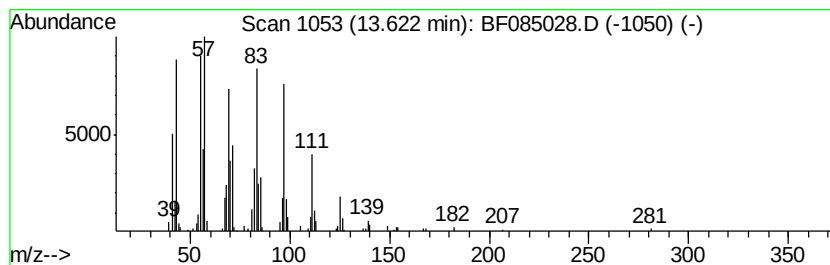
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	6.28 ng	311206	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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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
Butane, 2-methoxy...	1.67	4.2	ng	193971	1	6.60	915378	20.0
2-Pentanone, 4-hy...	4.73	20.8	ng	952431	1	6.60	915378	20.0
unknown6.38	6.38	73.3	ng	3352880	1	6.60	915378	20.0
Eicosane	10.57	2.8	ng	180812	4	11.12	1312700	20.0
Dichloroacetic ac...	13.62	6.3	ng	311206	5	13.75	990556	20.0