

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
 Data File : BF091824.D
 Acq On : 20 Dec 2016 17:08
 Operator : UM/SJ
 Sample : H6165-03
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3-14-15

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-BF121716.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	4.944	247	250	259	rBV	1472296	2390212	34.65%	4.396%
2	5.379	285	288	290	rBV	5760399	6401128	92.81%	11.772%
3	6.419	375	379	381	rBV	5484648	6897331	100.00%	12.684%
4	6.533	386	389	392	rBV	5519078	5671305	82.22%	10.430%
5	6.762	407	409	411	rBV	1464284	1283706	18.61%	2.361%
6	6.922	420	423	425	rBV	4359391	4795807	69.53%	8.820%
7	7.333	455	459	461	rBV	2779520	3895785	56.48%	7.164%
8	8.042	519	521	524	rBV	1462520	1592870	23.09%	2.929%
9	9.048	606	609	613	rBV	167341	173014	2.51%	0.318%
10	9.128	613	616	618	rBV	5810352	5996807	86.94%	11.028%
11	9.516	648	650	653	rBV	719396	758350	10.99%	1.395%
12	9.802	672	675	677	rBV	1523310	1761606	25.54%	3.240%
13	10.236	712	713	715	rVB	127926	93073	1.35%	0.171%
14	10.591	741	744	746	rBV	2843038	3127502	45.34%	5.752%
15	10.705	752	754	759	rVB	130469	172911	2.51%	0.318%
16	11.151	791	793	795	rBV	89660	106742	1.55%	0.196%
17	11.276	802	804	807	rBV	1641827	1638499	23.76%	3.013%
18	12.865	940	943	946	rBV	4259911	4208228	61.01%	7.739%
19	13.105	959	964	966	rBV	122760	158952	2.30%	0.292%
20	13.768	1019	1022	1026	rBV	402884	514376	7.46%	0.946%
21	13.917	1032	1035	1037	rBV	1087699	1381882	20.04%	2.541%
22	14.020	1042	1044	1046	rVV	81447	75352	1.09%	0.139%
23	14.397	1075	1077	1079	rBV	114182	121996	1.77%	0.224%
24	15.002	1128	1130	1131	rBV	69781	72435	1.05%	0.133%
25	15.311	1155	1157	1160	rBV	725840	1086905	15.76%	1.999%

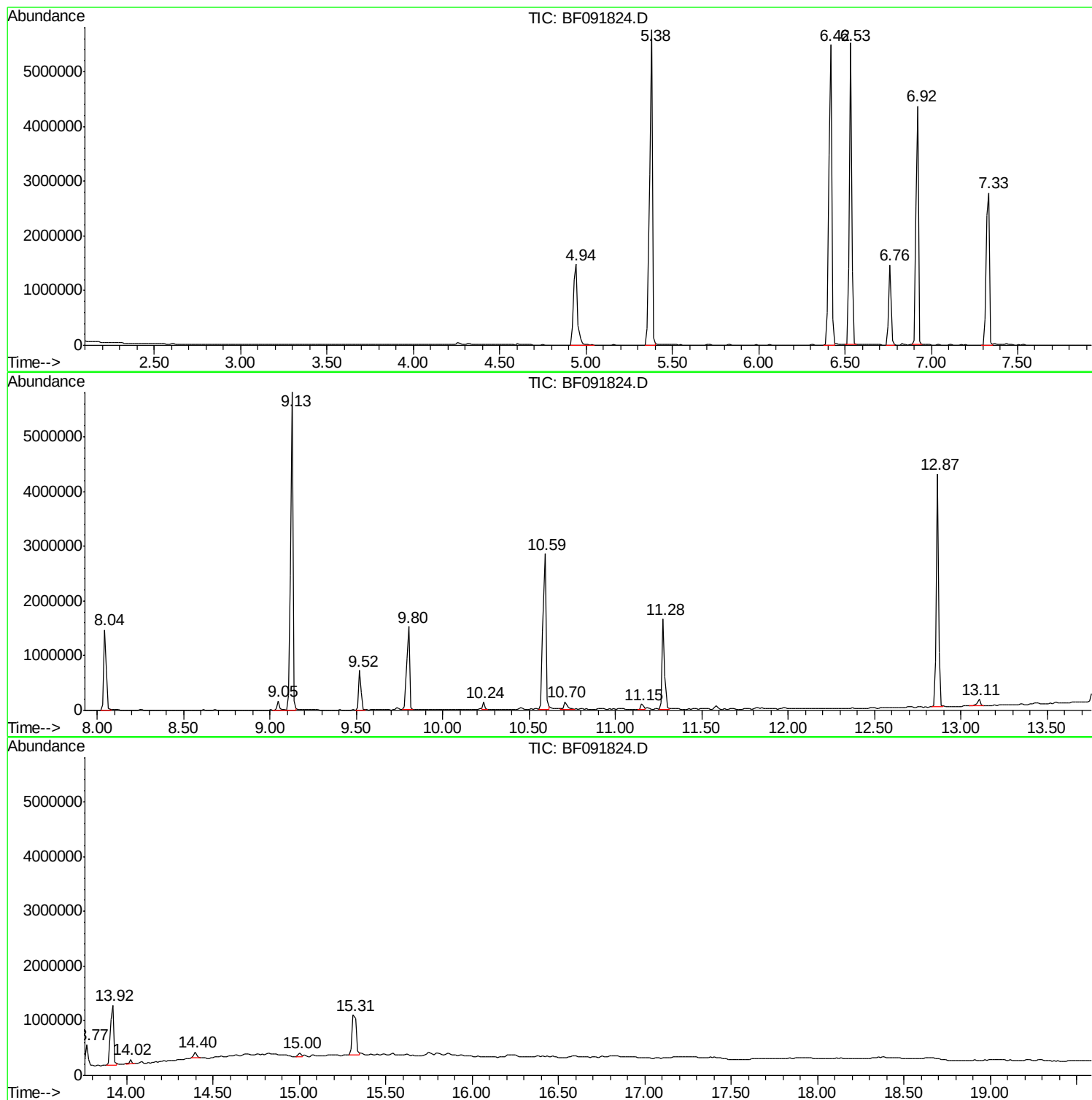
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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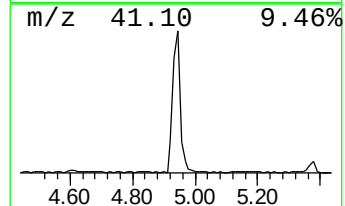
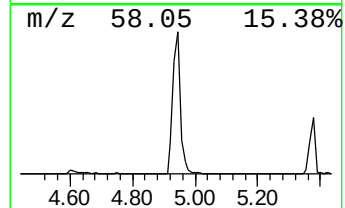
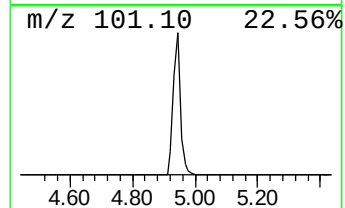
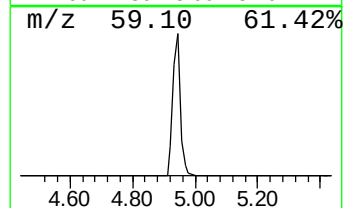
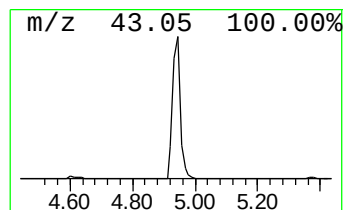
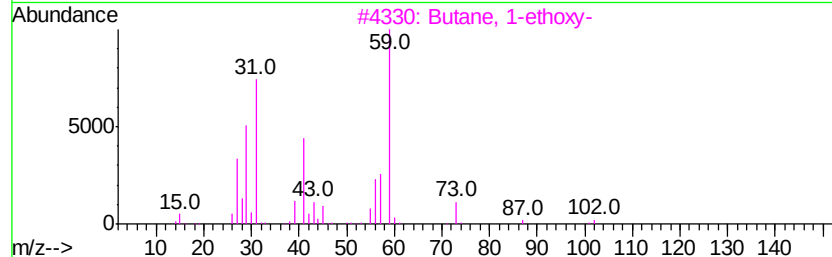
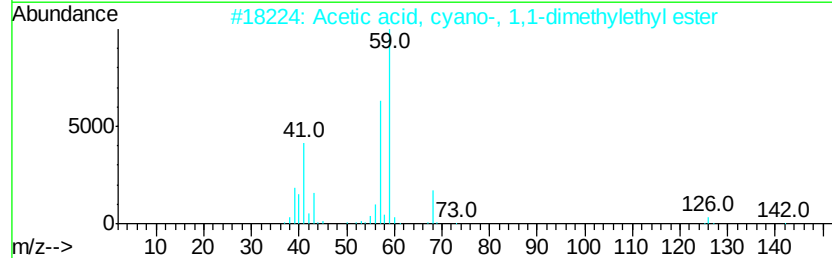
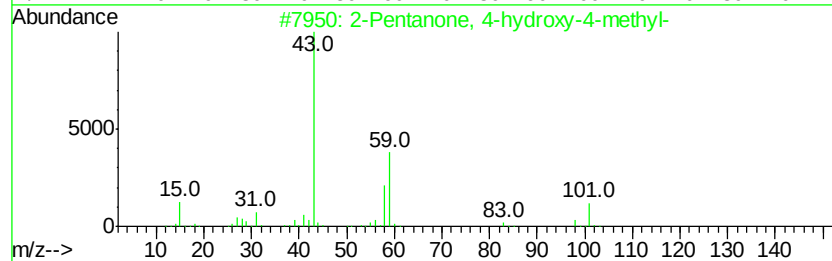
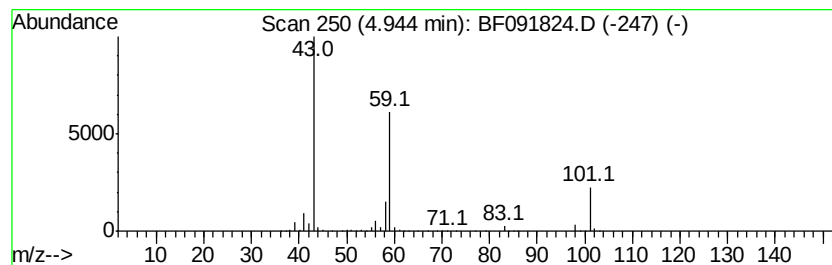
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.94	37.24 ng	2390210	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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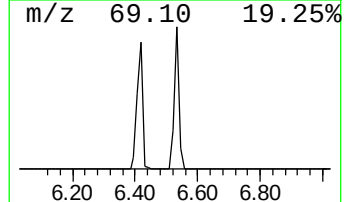
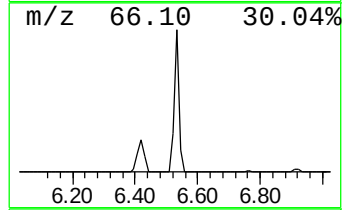
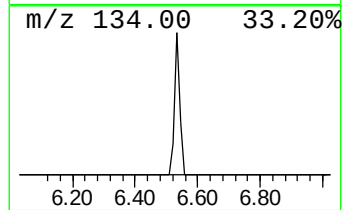
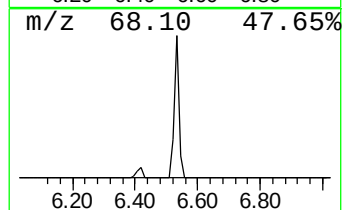
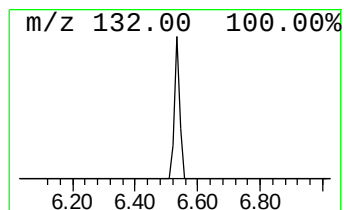
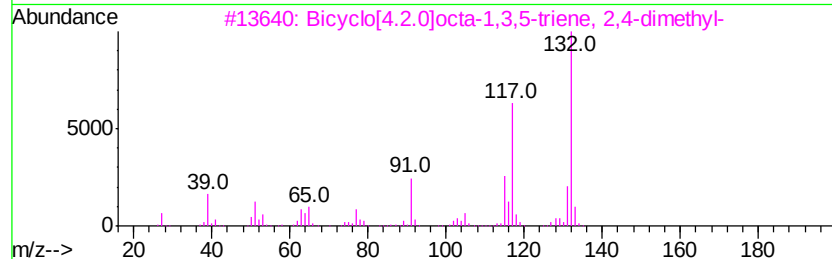
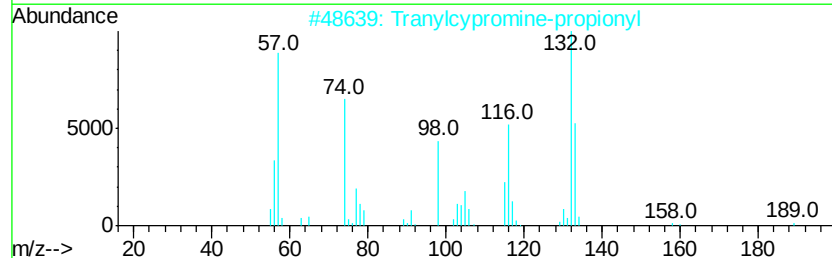
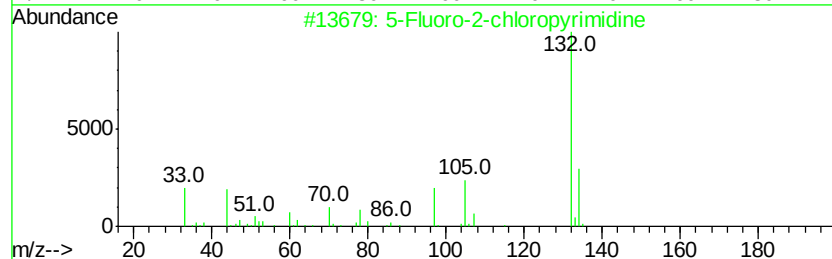
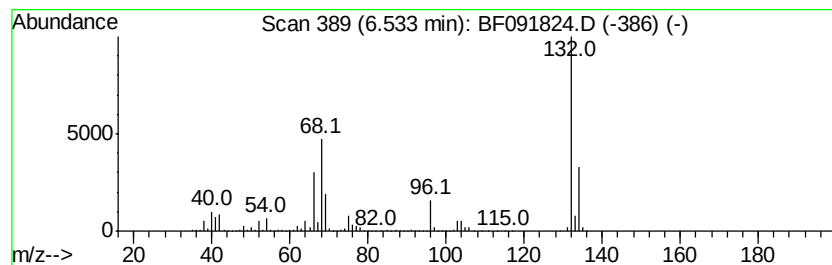
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	88.36 ng	5671310	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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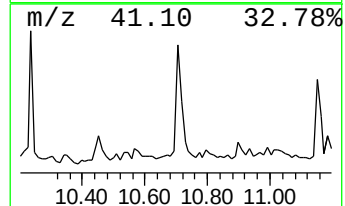
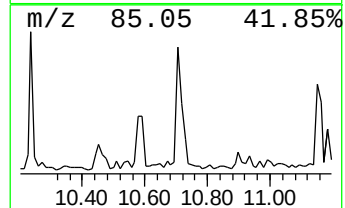
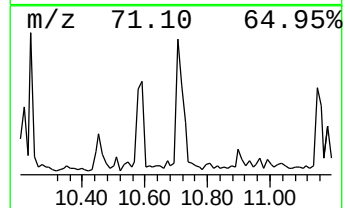
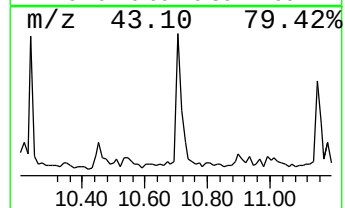
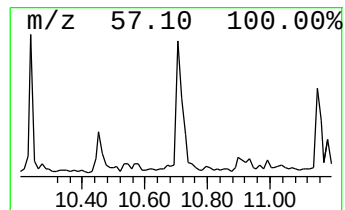
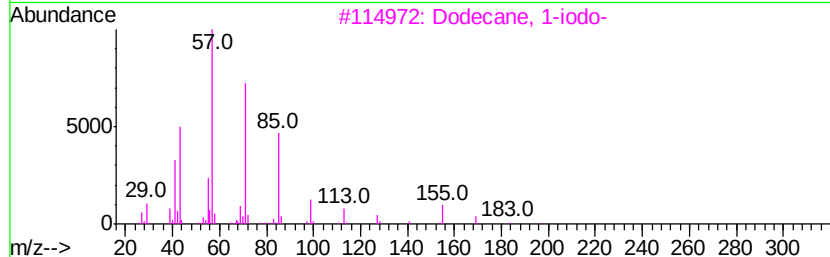
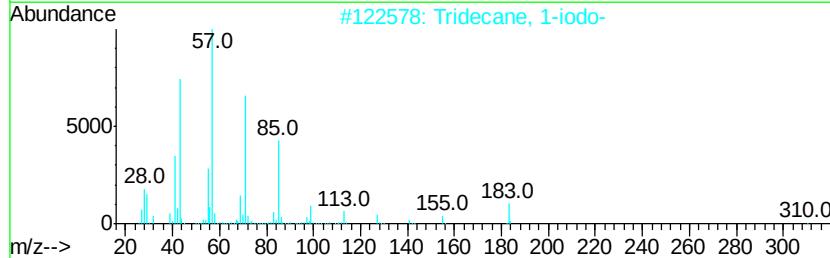
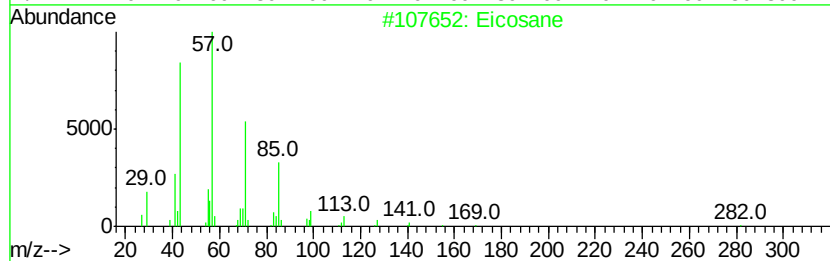
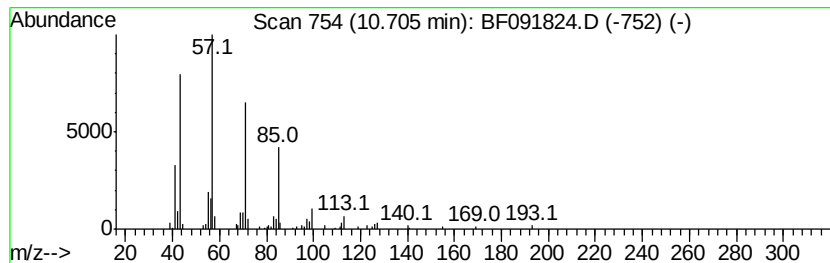
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.11 ng	172911	Phenanthrene-d10	11.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 91
2	Tridecane, 1-iodo-		310 C13H27I	035599-77-0 90
3	Dodecane, 1-iodo-		296 C12H25I	004292-19-7 86
4	Eicosane, 10-methyl-		296 C21H44	054833-23-7 78
5	Hexadecane		226 C16H34	000544-76-3 78



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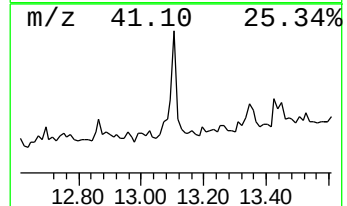
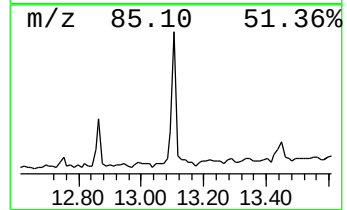
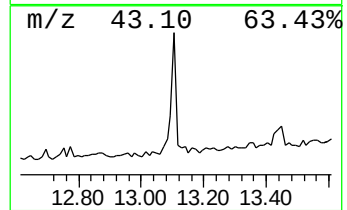
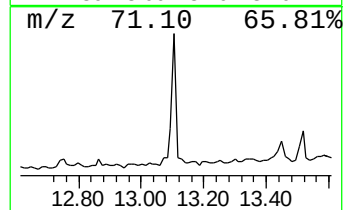
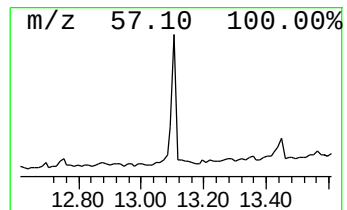
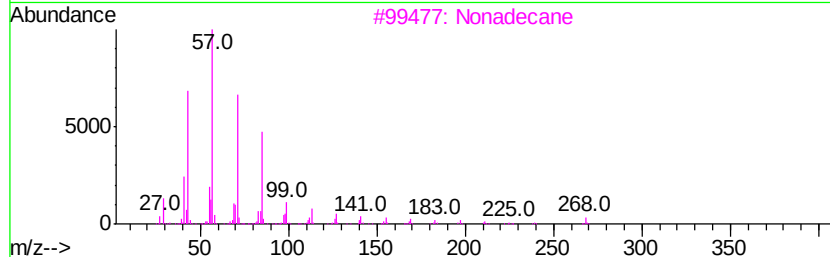
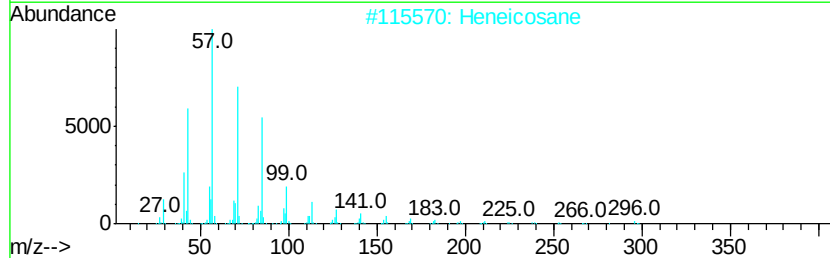
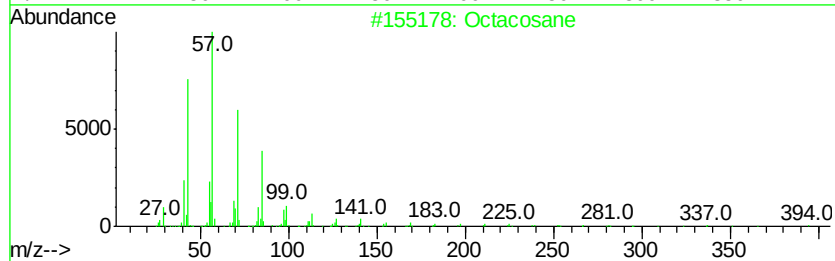
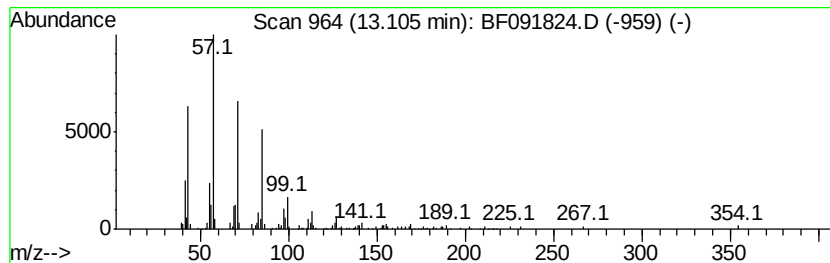
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.11	2.30 ng	158952	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Nonadecane	268	C19H40	000629-92-5	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Heptadecane	240	C17H36	000629-78-7	83



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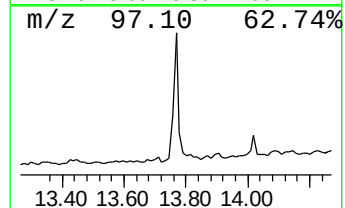
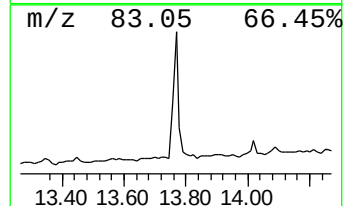
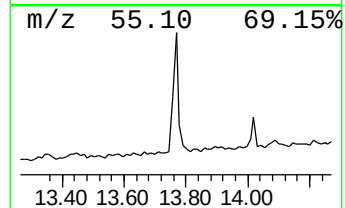
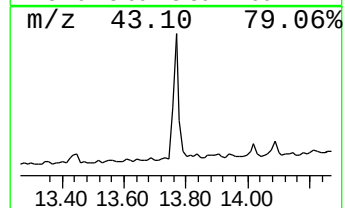
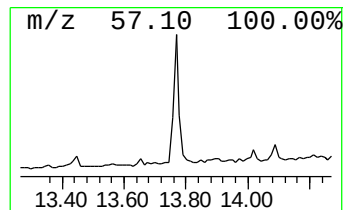
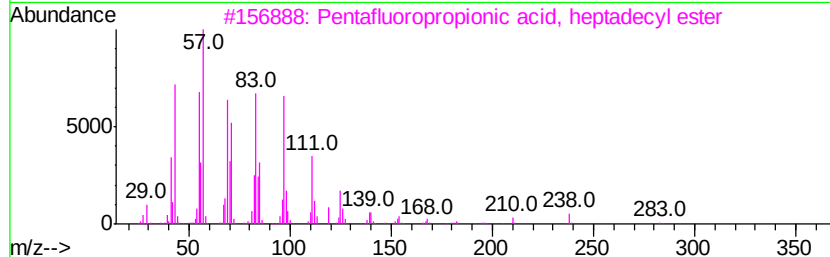
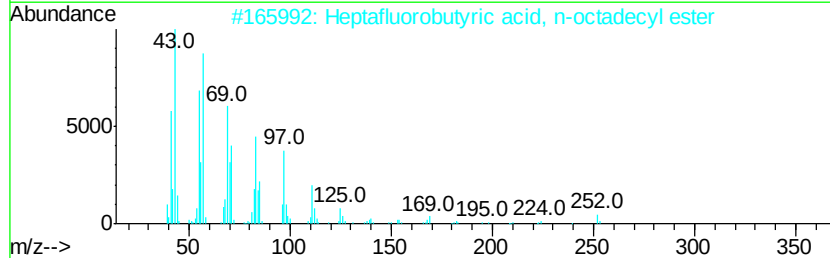
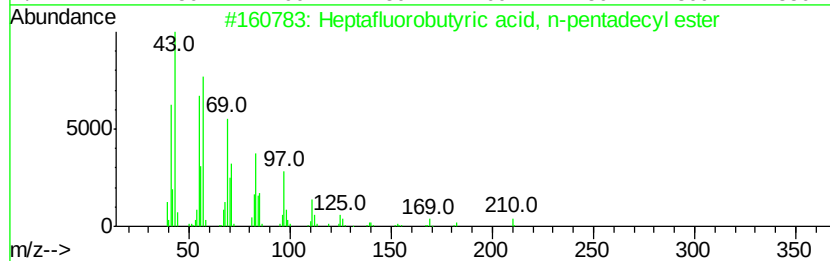
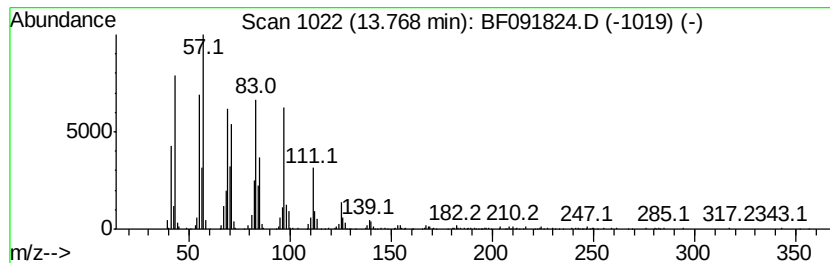
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	7.44 ng	514376	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
2		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4		Cyclotetradecane	196	C14H28	000295-17-0	91
5		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	37.2	ng	2390210	1	6.76	1283710	20.0
unknown6.53	6.53	88.4	ng	5671310	1	6.76	1283710	20.0
Eicosane	10.70	2.1	ng	172911	4	11.28	1638500	20.0
Octacosane	13.11	2.3	ng	158952	5	13.92	1381880	20.0
Heptafluorobutyri...	13.77	7.4	ng	514376	5	13.92	1381880	20.0