

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
 Data File : BF096511.D
 Acq On : 6 Jul 2017 4:42
 Operator : SJ/MA
 Sample : I3975-03
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B7-4-6

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-BF070117.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	4.892	473	477	488	rBV	251121	296109	14.11%	1.560%
2	5.322	545	550	553	rBV	2206899	2043905	97.41%	10.767%
3	6.351	720	725	735	rVB	2176605	2098177	100.00%	11.053%
4	6.481	743	747	751	rBV	2204119	2029129	96.71%	10.689%
5	6.710	783	786	790	rBV	789354	704168	33.56%	3.709%
6	6.869	809	813	817	rBV	1760924	1509726	71.95%	7.953%
7	7.269	877	881	885	rBV	1201052	1173698	55.94%	6.183%
8	7.710	951	956	966	rBV	36155	48598	2.32%	0.256%
9	7.992	1000	1004	1008	rBV	1109490	966020	46.04%	5.089%
10	9.074	1183	1188	1191	rBV	2304372	1953671	93.11%	10.292%
11	9.169	1198	1204	1207	rVB3	31396	28229	1.35%	0.149%
12	9.469	1251	1255	1258	rBV	533499	480529	22.90%	2.531%
13	9.692	1291	1293	1298	rVB	38669	34446	1.64%	0.181%
14	9.745	1298	1302	1306	rBV	741279	712025	33.94%	3.751%
15	10.192	1375	1378	1381	rVB	52109	46449	2.21%	0.245%
16	10.416	1412	1416	1419	rBV2	15682	22127	1.05%	0.117%
17	10.533	1432	1436	1441	rBV	1067391	918116	43.76%	4.836%
18	10.668	1455	1459	1466	rVB	63930	81436	3.88%	0.429%
19	11.116	1531	1535	1538	rVB3	36191	33694	1.61%	0.177%
20	11.227	1550	1554	1557	rBV	760445	646965	30.83%	3.408%
21	11.251	1557	1558	1561	rVV	78007	43377	2.07%	0.229%
22	11.298	1562	1566	1570	rVV2	24263	24111	1.15%	0.127%
23	11.539	1604	1607	1609	rBV	25688	22577	1.08%	0.119%
24	11.839	1654	1658	1660	rBV4	26169	26355	1.26%	0.139%
25	11.945	1671	1676	1681	rVB3	19093	29523	1.41%	0.156%
26	12.439	1756	1760	1763	rBV	94389	93807	4.47%	0.494%
27	12.662	1791	1798	1801	rBV	89580	106396	5.07%	0.560%
28	12.815	1820	1824	1827	rBV	1642633	1470240	70.07%	7.745%
29	13.298	1901	1906	1910	rVB2	144101	154832	7.38%	0.816%
30	13.721	1975	1978	1982	rVB2	86176	84820	4.04%	0.447%
31	13.862	1997	2002	2005	rBV	711661	728303	34.71%	3.837%
32	15.274	2238	2242	2245	rVB	323367	371766	17.72%	1.958%

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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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

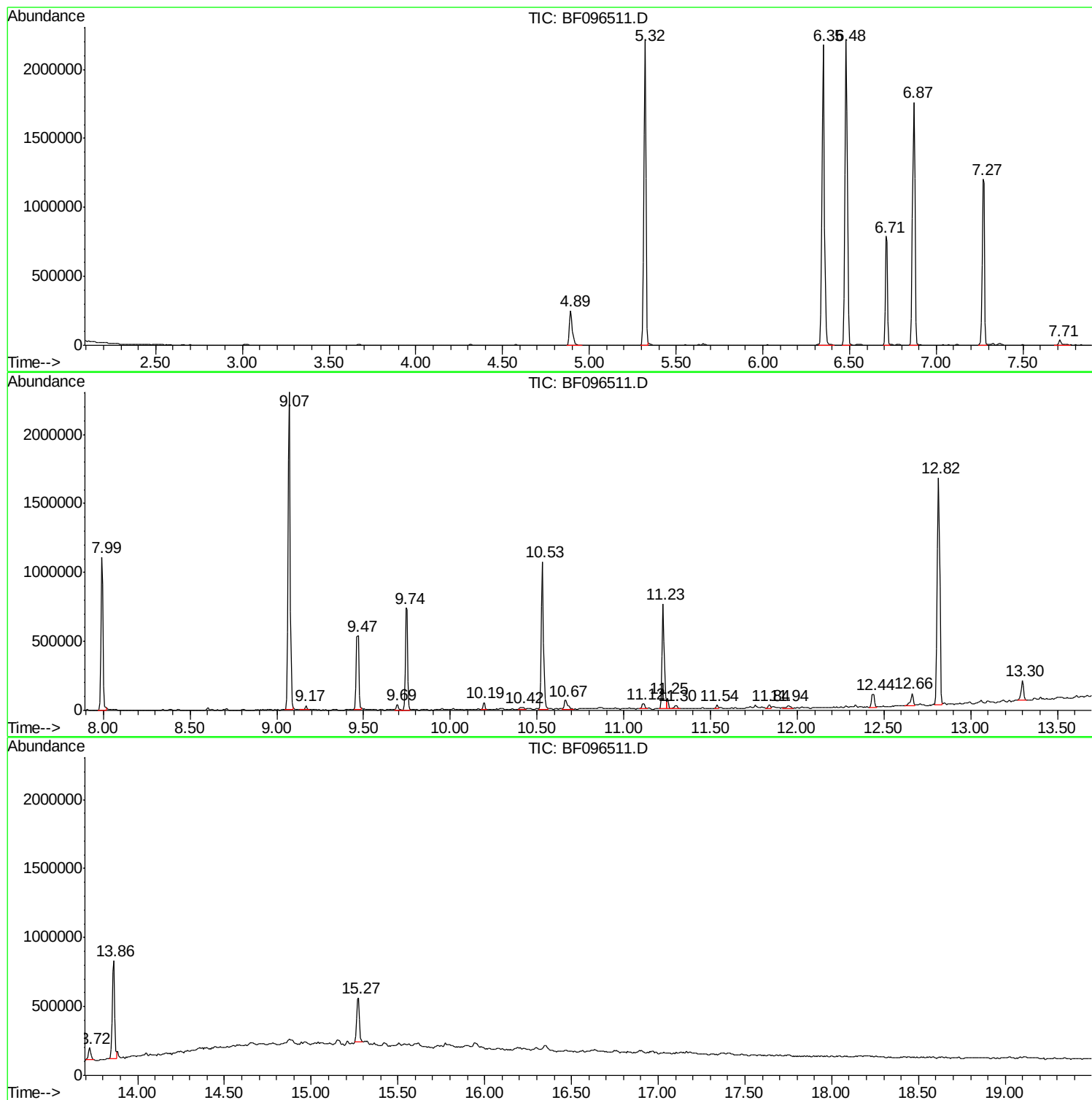
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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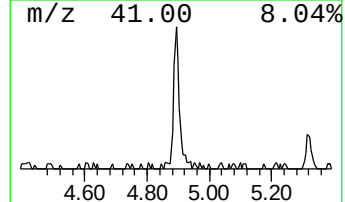
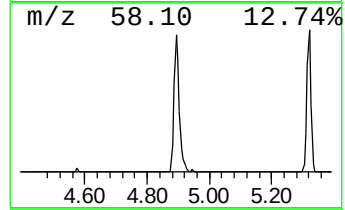
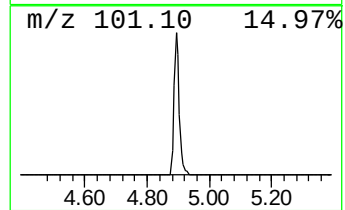
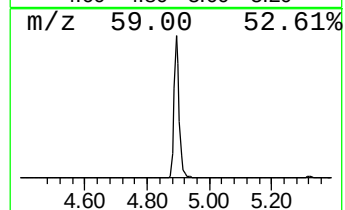
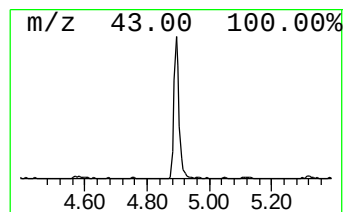
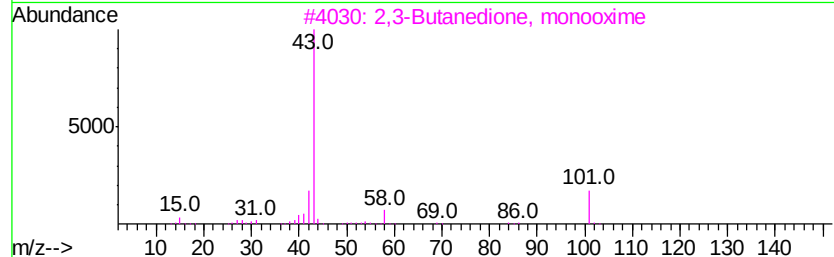
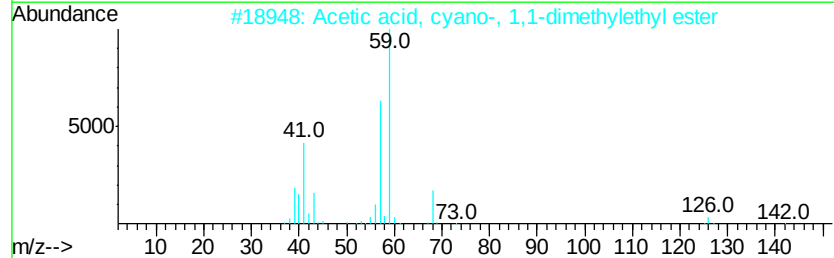
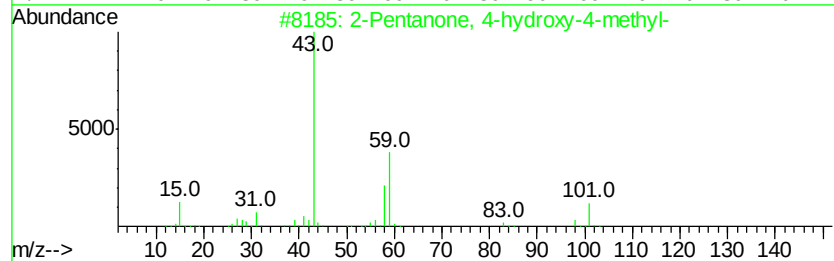
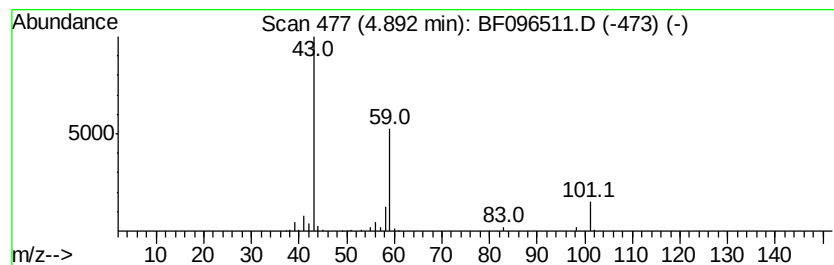
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	8.41 ng	296109	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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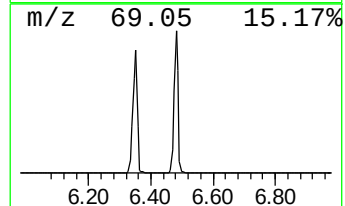
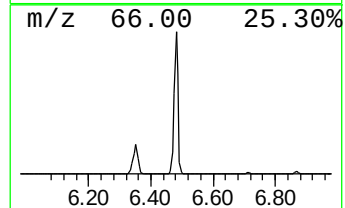
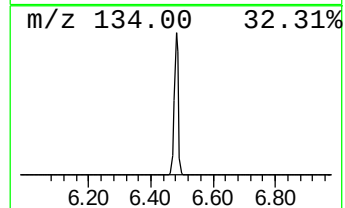
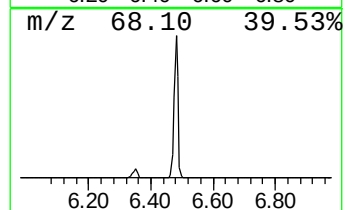
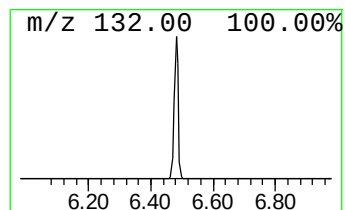
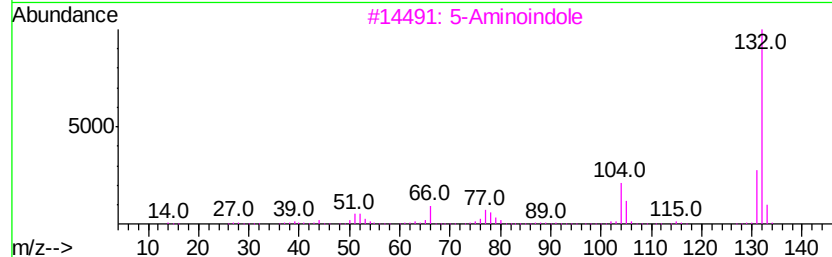
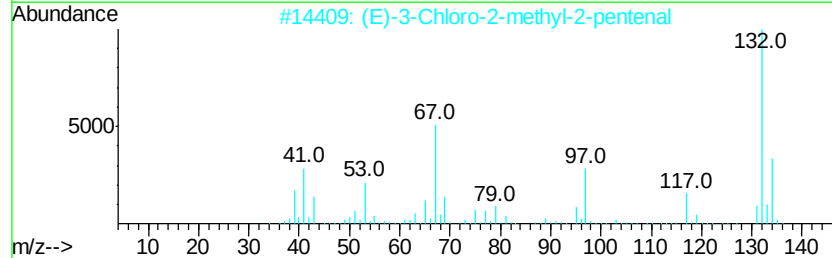
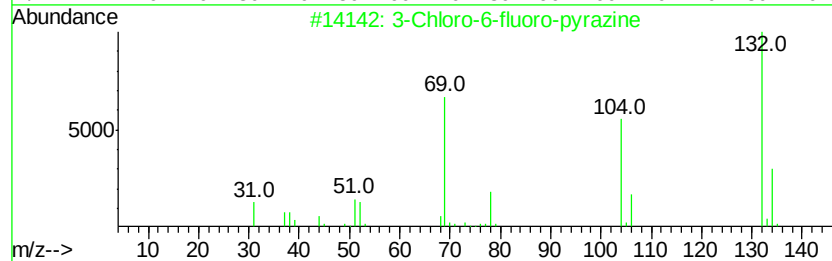
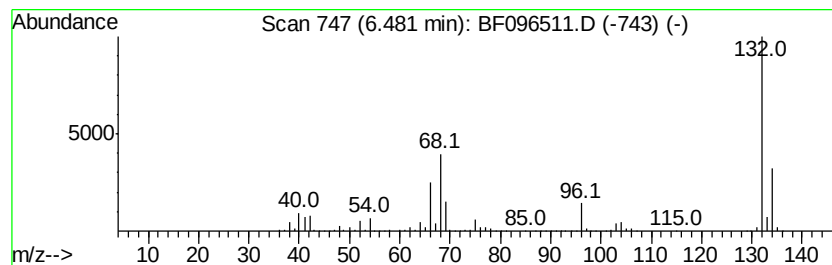
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	57.63 ng	2029130	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	10
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10



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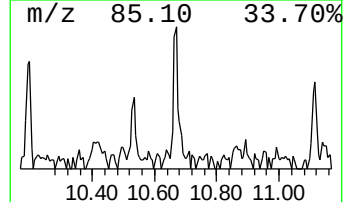
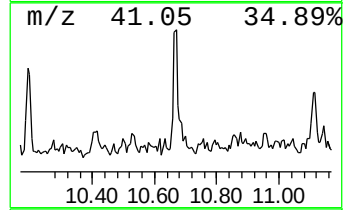
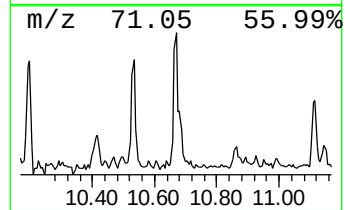
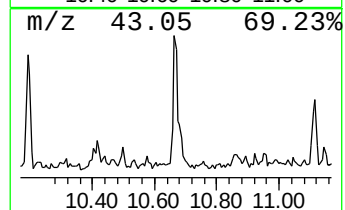
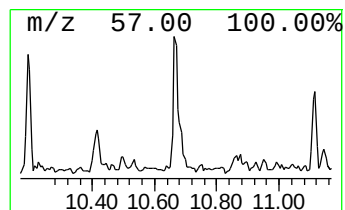
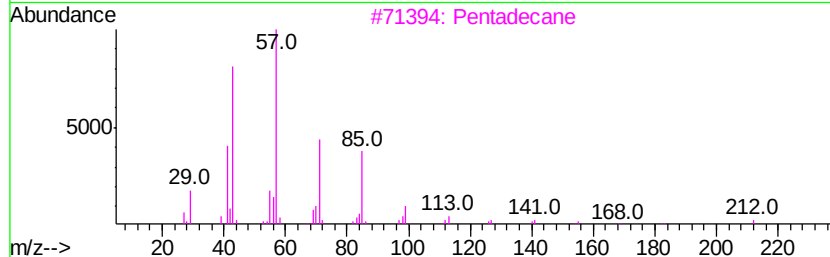
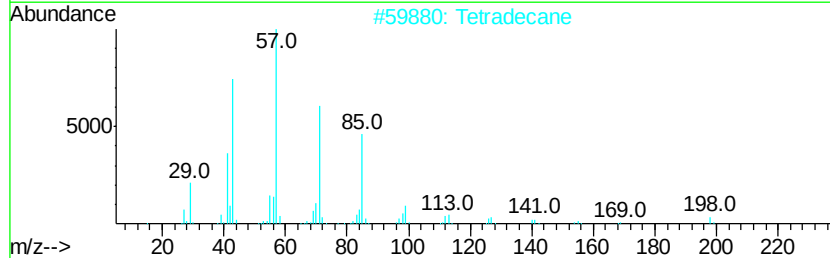
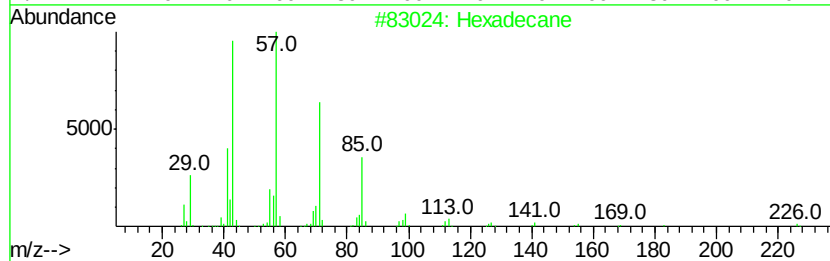
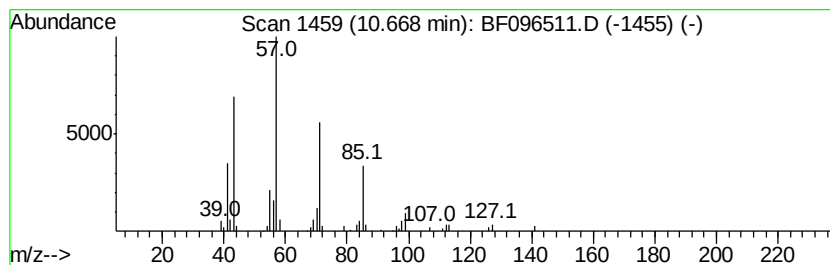
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.67	2.52 ng	81436	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Tetratetracontane	619	C44H90	007098-22-8	83



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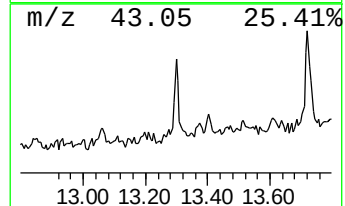
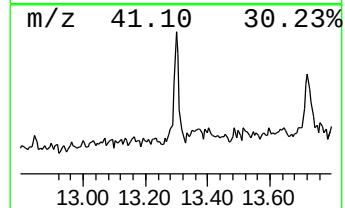
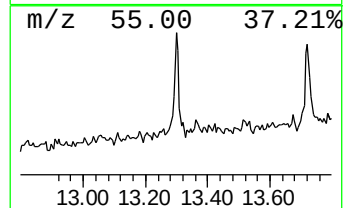
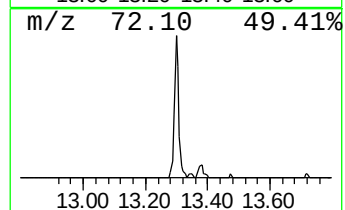
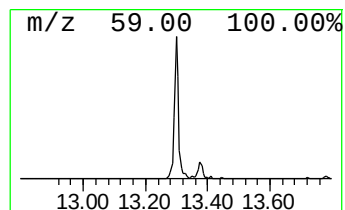
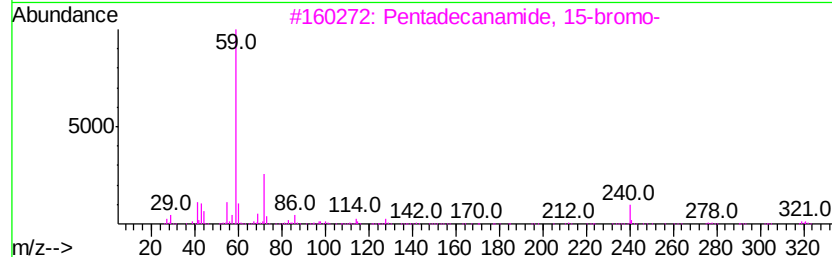
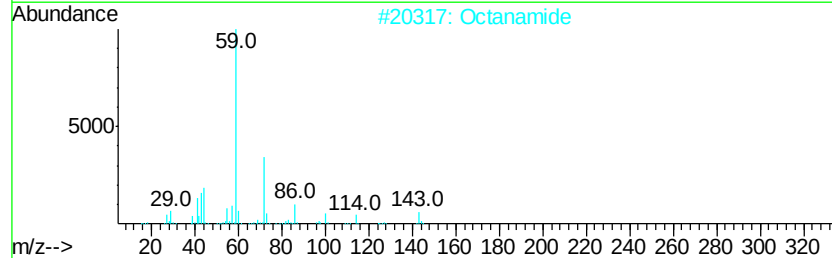
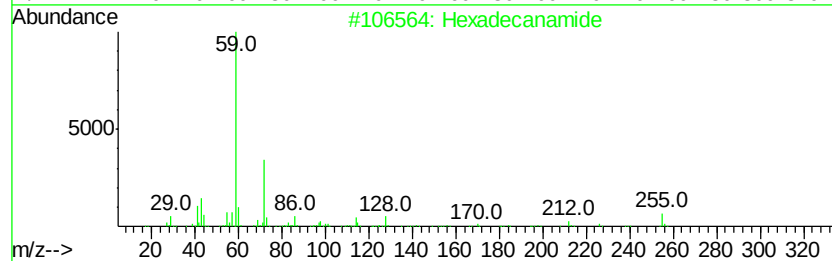
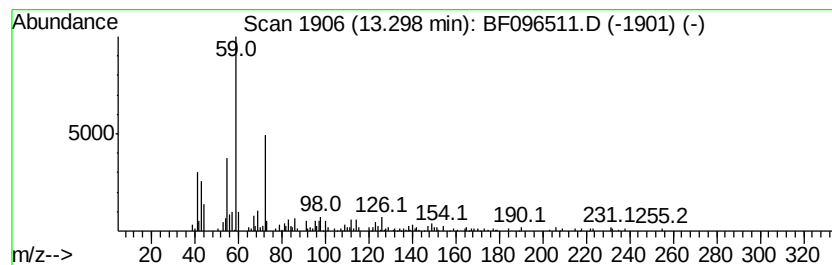
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.30	4.25 ng	154832	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	64
2	Octanamide	143	C8H17NO	000629-01-6	64
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
4	Tetradecanamide	227	C14H29NO	000638-58-4	59
5	Nonanamide	157	C9H19NO	001120-07-6	59



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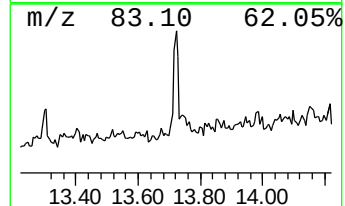
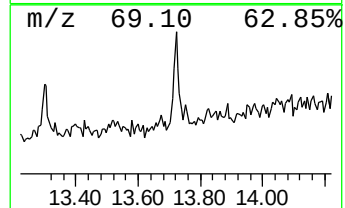
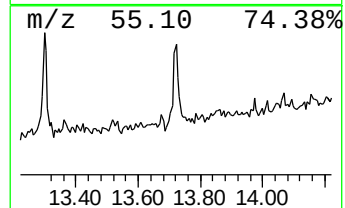
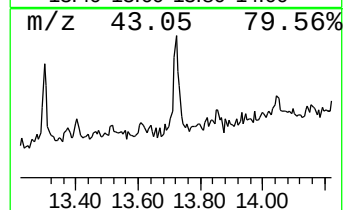
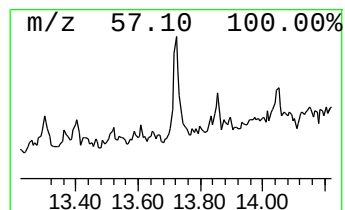
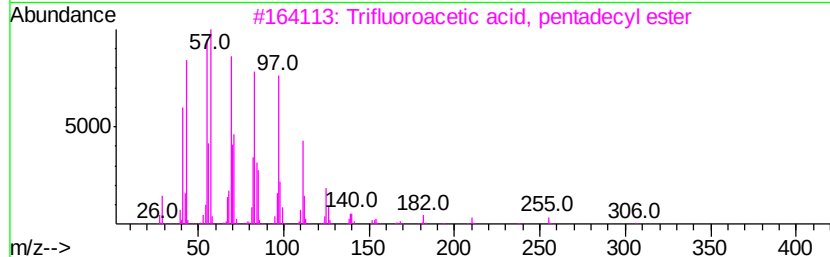
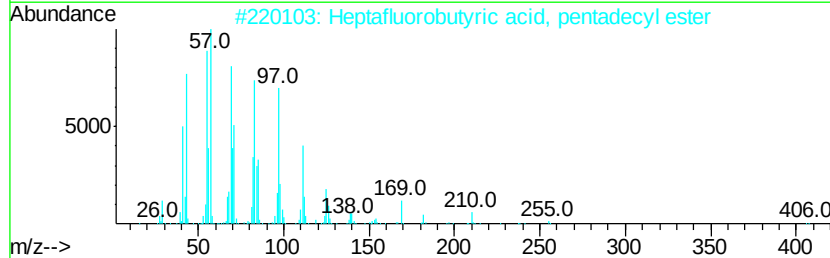
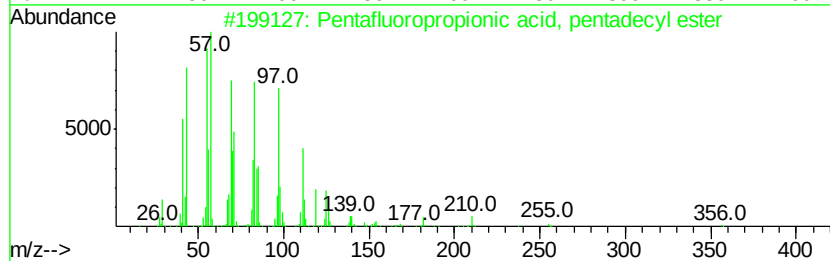
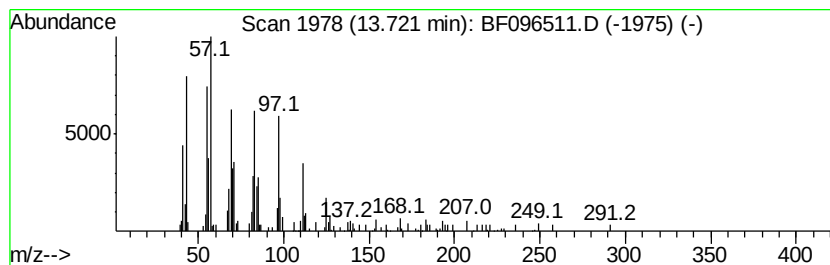
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.33 ng	84820	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87



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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...	4.89	8.4	ng	296109	1	6.72	704168	20.0
unknown6.48	6.48	57.6	ng	2029130	1	6.72	704168	20.0
Hexadecane	10.67	2.5	ng	81436	4	11.23	646965	20.0
Hexadecanamide	13.30	4.3	ng	154832	5	13.86	728303	20.0
Pentafluoropropio...	13.72	2.3	ng	84820	5	13.86	728303	20.0