

Data Path : Z:\HPCHEM1\BNA_F\Data\BF032618\
 Data File : BF103941.D
 Acq On : 26 Mar 2018 22:33
 Operator : JU/SJ
 Sample : J2044-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEST-PIT-LOC#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_F\METHODS\8270-BF031518.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	2.322	34	40	48	rVB	108434	141864	4.07%	0.470%
2	5.222	529	533	541	rVB	121991	153383	4.40%	0.508%
3	5.604	593	598	601	rBV	2997259	2998018	85.99%	9.929%
4	6.598	762	767	778	rBV	2703677	3219697	92.35%	10.663%
5	6.745	787	792	795	rBV	3245168	3147092	90.27%	10.422%
6	6.975	827	831	834	rBV	1050681	820332	23.53%	2.717%
7	7.134	853	858	861	rBV	2752968	2496573	71.61%	8.268%
8	7.539	921	927	930	rBV	2069805	1946590	55.84%	6.447%
9	7.604	934	938	950	rVB2	29638	46465	1.33%	0.154%
10	8.257	1045	1049	1052	rBV	1322378	1072330	30.76%	3.551%
11	9.328	1227	1231	1235	rBV	3529107	3486285	100.00%	11.546%
12	9.716	1294	1297	1305	rBV	270105	254455	7.30%	0.843%
13	9.928	1329	1333	1336	rBV	95367	72045	2.07%	0.239%
14	10.016	1344	1348	1356	rBV	1371262	1203867	34.53%	3.987%
15	10.428	1416	1418	1421	rVB	140826	99901	2.87%	0.331%
16	10.645	1449	1455	1458	rBV	36624	46983	1.35%	0.156%
17	10.810	1478	1483	1486	rBV	2212253	2062746	59.17%	6.831%
18	10.904	1496	1499	1504	rBV	109877	112880	3.24%	0.374%
19	11.351	1572	1575	1578	rBV	70417	56450	1.62%	0.187%
20	11.510	1598	1602	1605	rBV	1264599	1127234	32.33%	3.733%
21	11.533	1605	1606	1609	rVB	64922	36443	1.05%	0.121%
22	12.727	1805	1809	1813	rBV	177215	162590	4.66%	0.538%
23	12.898	1828	1838	1841	rBV7	18160	45609	1.31%	0.151%
24	12.957	1845	1848	1853	rVB	167629	159581	4.58%	0.528%
25	13.098	1867	1872	1875	rBV	2958206	2841936	81.52%	9.412%
26	13.286	1896	1904	1906	rBV3	39867	75194	2.16%	0.249%
27	13.974	2017	2021	2025	rBV2	212077	236775	6.79%	0.784%
28	14.163	2048	2053	2056	rBV	909597	923587	26.49%	3.059%
29	14.186	2056	2057	2062	rVB	100129	64814	1.86%	0.215%
30	15.245	2234	2237	2248	rVB	92994	212128	6.08%	0.703%
31	15.639	2301	2304	2308	rVB	72738	86754	2.49%	0.287%
32	15.704	2310	2315	2324	rBV	532712	784615	22.51%	2.598%

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

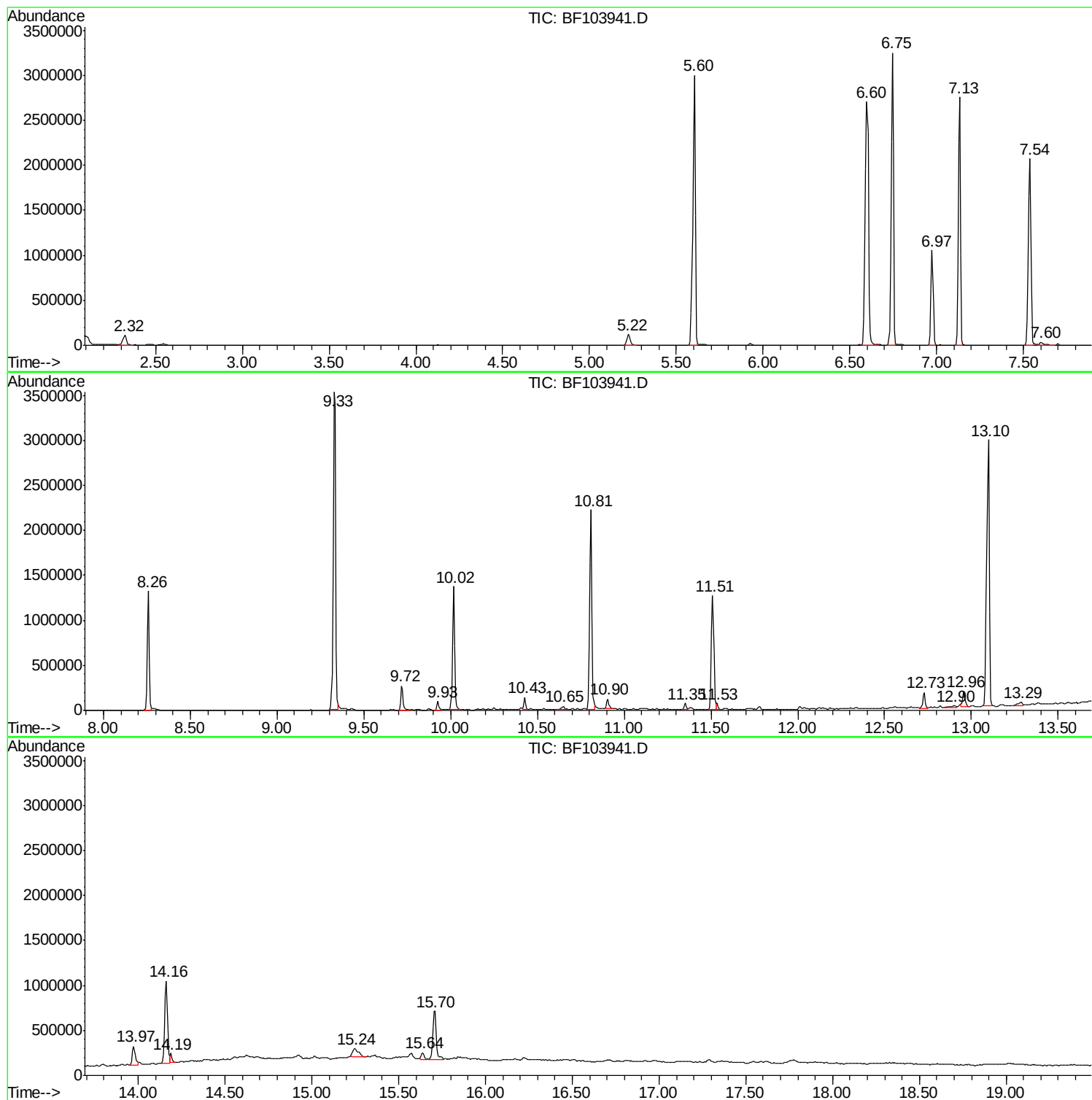
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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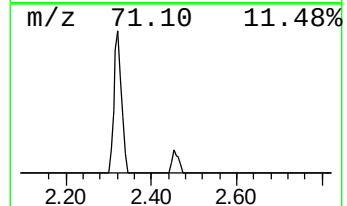
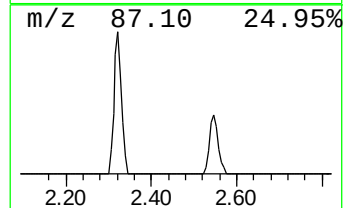
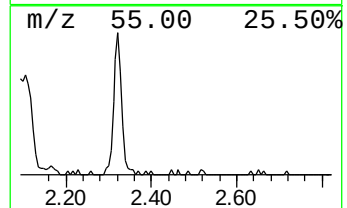
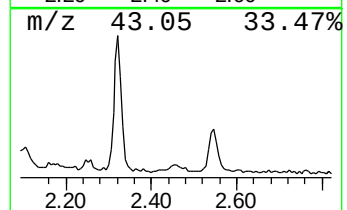
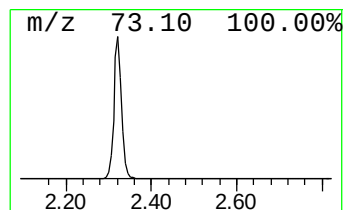
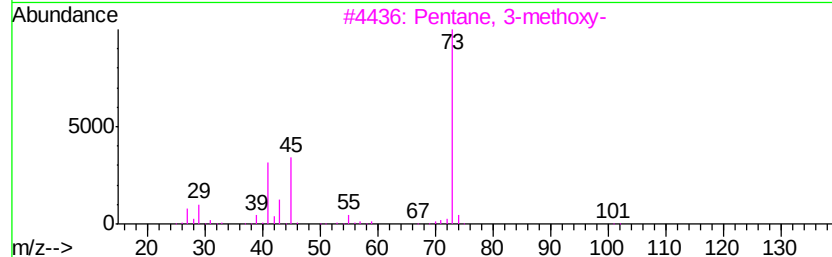
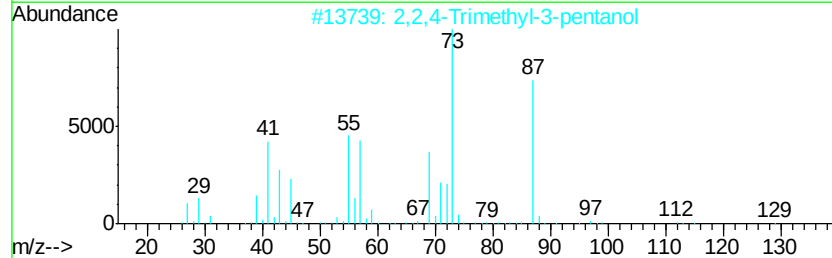
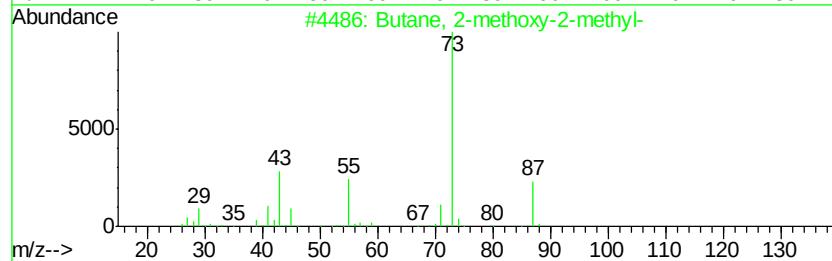
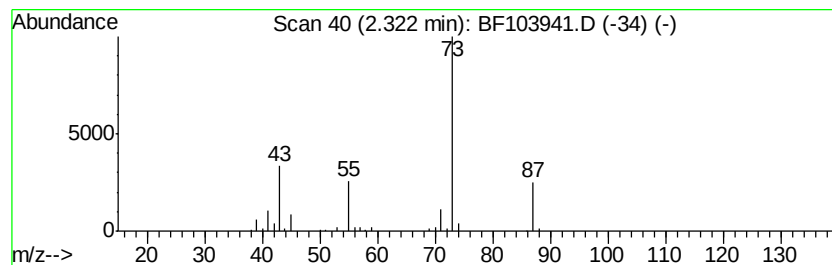
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	3.46 ng	141864	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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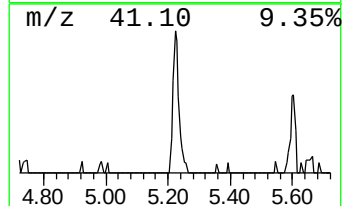
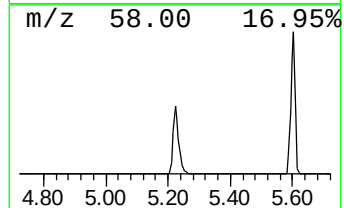
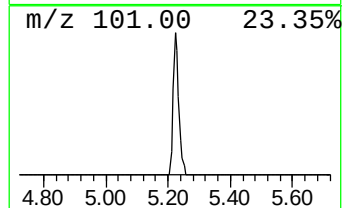
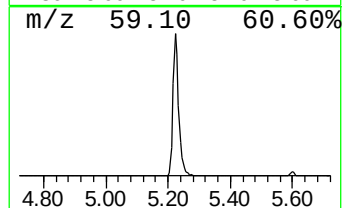
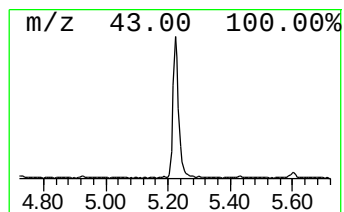
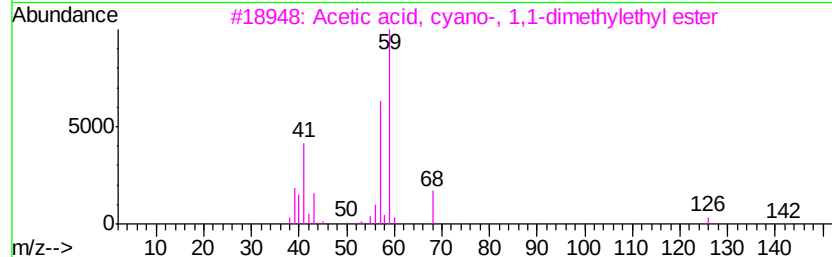
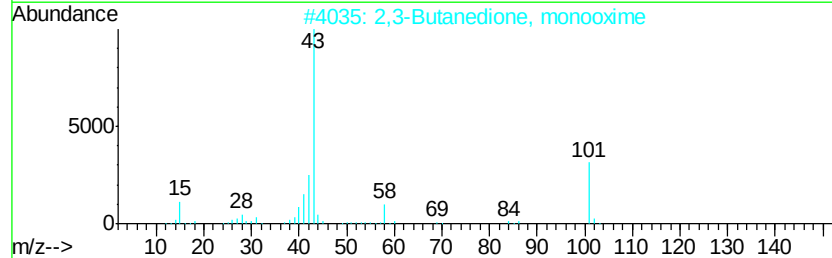
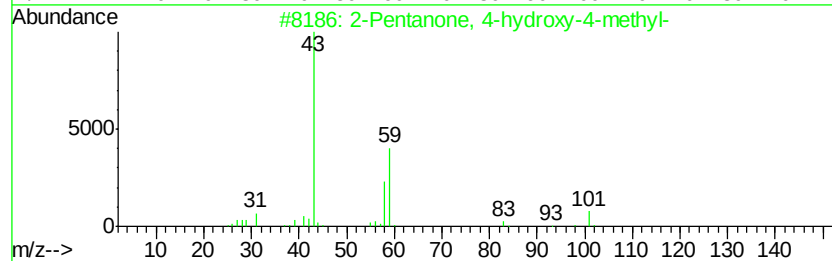
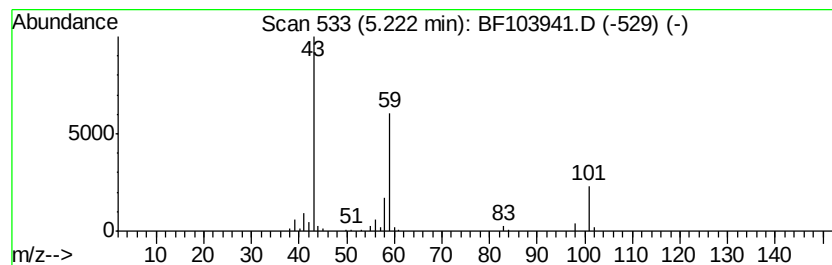
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.74 ng	153383	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
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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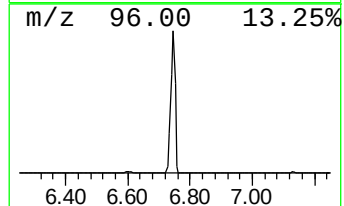
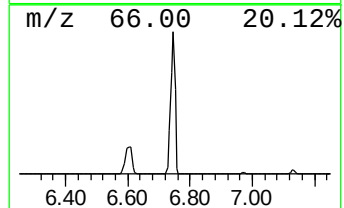
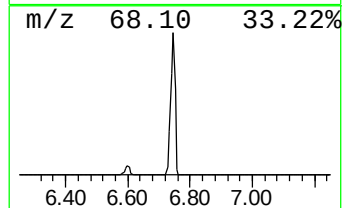
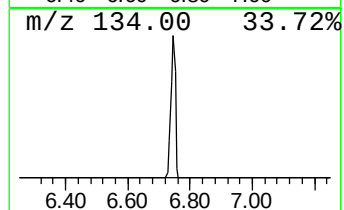
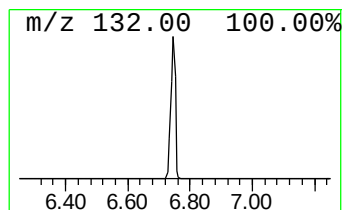
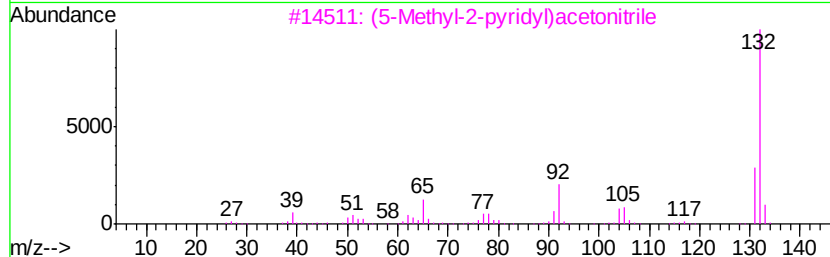
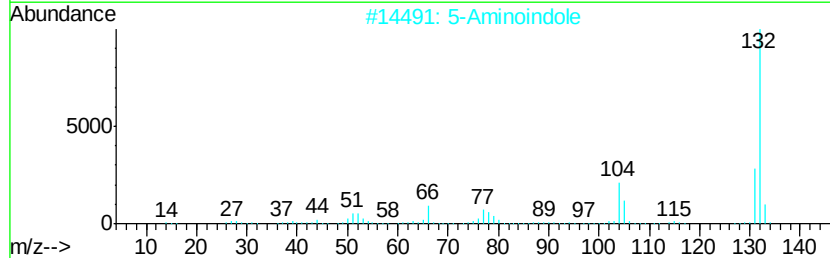
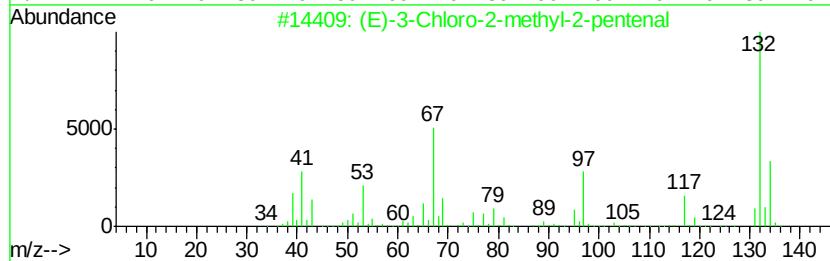
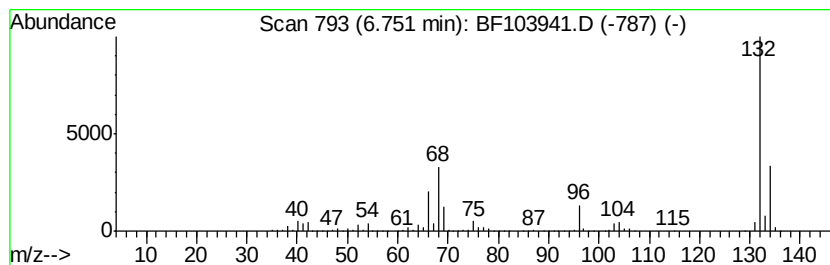
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	76.73 ng	3147090	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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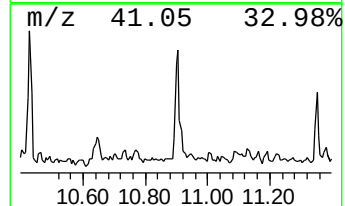
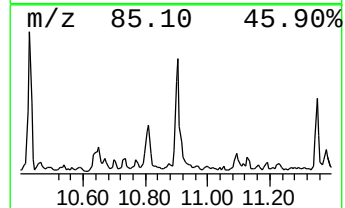
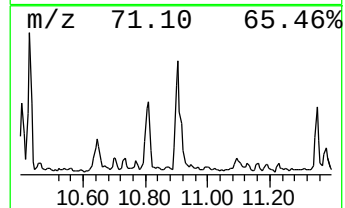
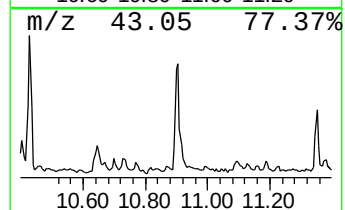
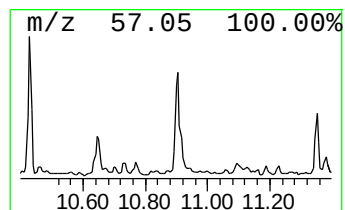
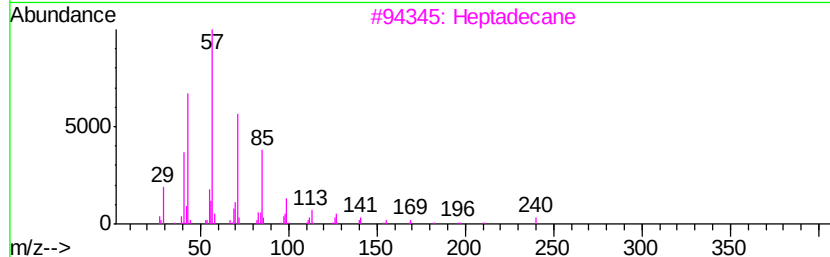
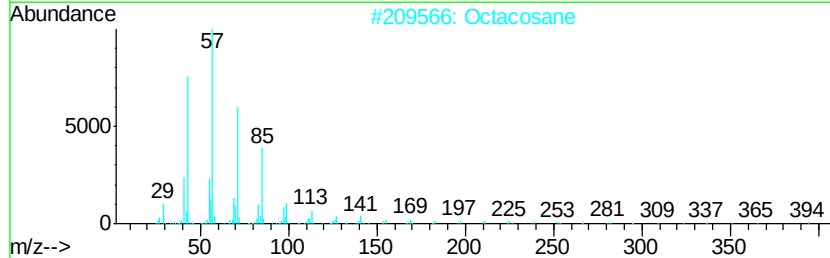
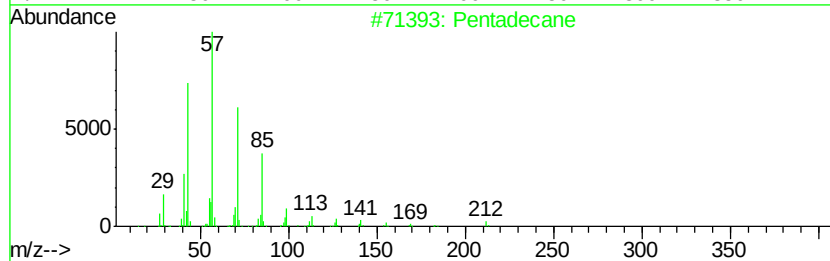
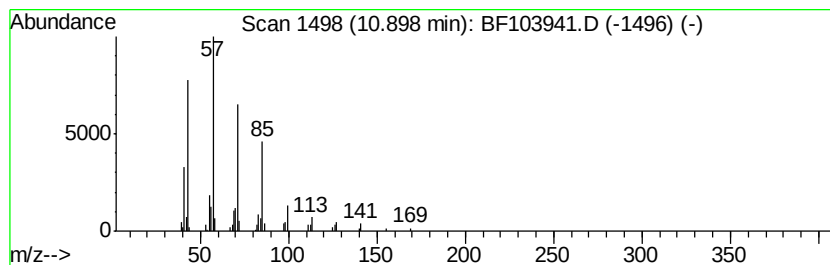
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.00 ng	112880	Phenanthrene-d10	11.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Heptadecane	240 C17H36	000629-78-7	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Tetracosane	338 C24H50	000646-31-1	91



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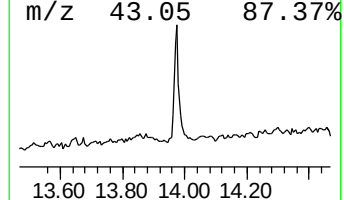
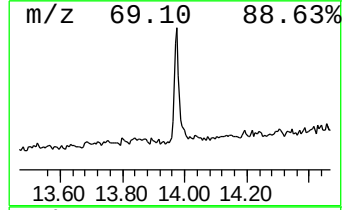
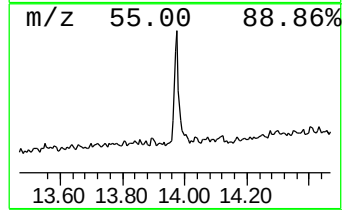
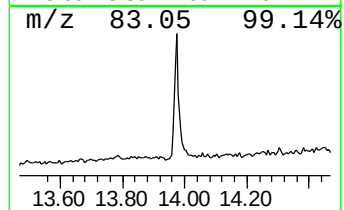
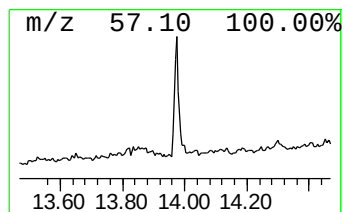
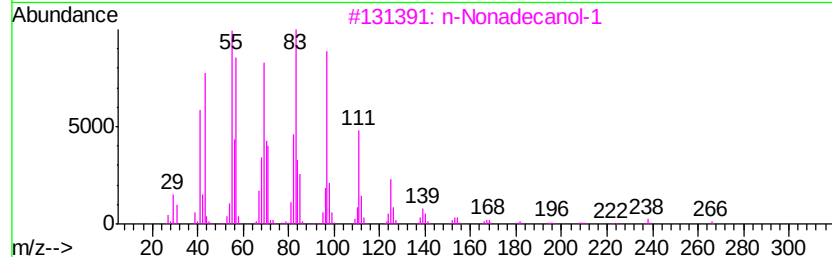
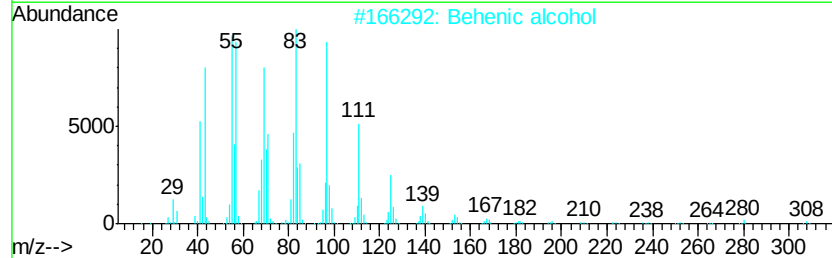
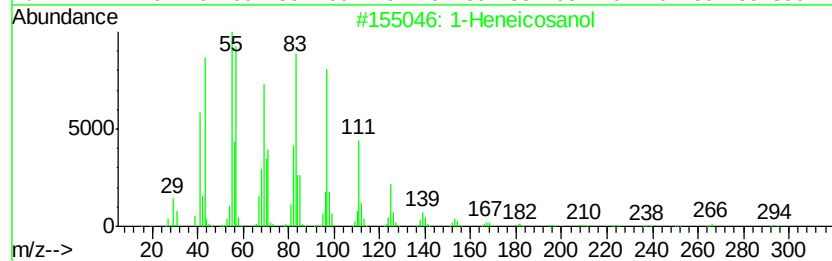
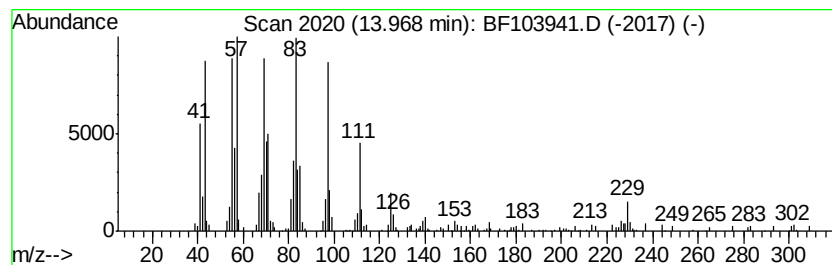
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.13 ng	236775	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.32	3.5	ng	141864	1	6.97	820332	20.0
2-Pentanone, 4-hy...	5.22	3.7	ng	153383	1	6.97	820332	20.0
unknown6.75	6.75	76.7	ng	3147090	1	6.97	820332	20.0
Pentadecane	10.90	2.0	ng	112880	4	11.51	1127230	20.0
1-Heneicosanol	13.97	5.1	ng	236775	5	14.16	923587	20.0