

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010419\
 Data File : BF111855.D
 Acq On : 4 Jan 2019 20:03
 Operator : JU/SJ
 Sample : K1041-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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	2.216	18	22	28	rVB	84016	113296	2.82%	0.329%
2	5.122	510	516	523	rVB	170480	213145	5.30%	0.619%
3	5.534	581	586	589	rBV	3434194	3343972	83.22%	9.709%
4	6.540	751	757	767	rBV	3315061	3808824	94.78%	11.059%
5	6.669	774	779	782	rBV	3842603	3640092	90.59%	10.569%
6	6.893	813	817	821	rBV	1199671	949228	23.62%	2.756%
7	7.051	840	844	847	rBV	3332315	2829550	70.41%	8.216%
8	7.451	907	912	915	rBV	2360273	2322775	57.80%	6.744%
9	8.175	1031	1035	1038	rBV	1408137	1158688	28.83%	3.364%
10	9.251	1213	1218	1221	rBV	4669339	4018394	100.00%	11.667%
11	9.639	1280	1284	1288	rVB	312629	278874	6.94%	0.810%
12	9.934	1329	1334	1337	rBV	1276377	1224090	30.46%	3.554%
13	10.722	1463	1468	1471	rBV	2536527	2259979	56.24%	6.562%
14	11.416	1582	1586	1589	rBV	1190773	1020623	25.40%	2.963%
15	11.439	1589	1590	1594	rVB	185818	103907	2.59%	0.302%
16	11.939	1673	1675	1681	rVB2	64131	77671	1.93%	0.226%
17	12.028	1687	1690	1693	rBV	55490	60802	1.51%	0.177%
18	12.469	1759	1765	1768	rBV3	53493	76740	1.91%	0.223%
19	12.627	1788	1792	1796	rBV	369432	330387	8.22%	0.959%
20	12.857	1825	1831	1837	rBV	314625	339187	8.44%	0.985%
21	12.998	1851	1855	1859	rVB	3443748	3269055	81.35%	9.492%
22	13.186	1885	1887	1889	rVB2	62826	47681	1.19%	0.138%
23	13.292	1901	1905	1908	rBV2	45443	53238	1.32%	0.155%
24	13.898	2004	2008	2017	rVB2	80070	122338	3.04%	0.355%
25	14.057	2030	2035	2038	rBV	1113019	1120803	27.89%	3.254%
26	14.080	2038	2039	2041	rVB	134039	70188	1.75%	0.204%
27	14.445	2097	2101	2103	rBV2	44703	48198	1.20%	0.140%
28	14.521	2111	2114	2119	rBV4	54670	82770	2.06%	0.240%
29	14.833	2164	2167	2169	rBV	63738	58890	1.47%	0.171%
30	15.104	2209	2213	2216	rBV	106483	165365	4.12%	0.480%
31	15.174	2222	2225	2229	rBV2	49108	63667	1.58%	0.185%
32	15.210	2229	2231	2237	rVV5	37997	65321	1.63%	0.190%
33	15.410	2263	2265	2272	rVB	85843	115306	2.87%	0.335%
34	15.474	2272	2276	2281	rVB	81479	96295	2.40%	0.280%

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Misc :
ALS Vial : 15 Sample Multiplier: 1

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

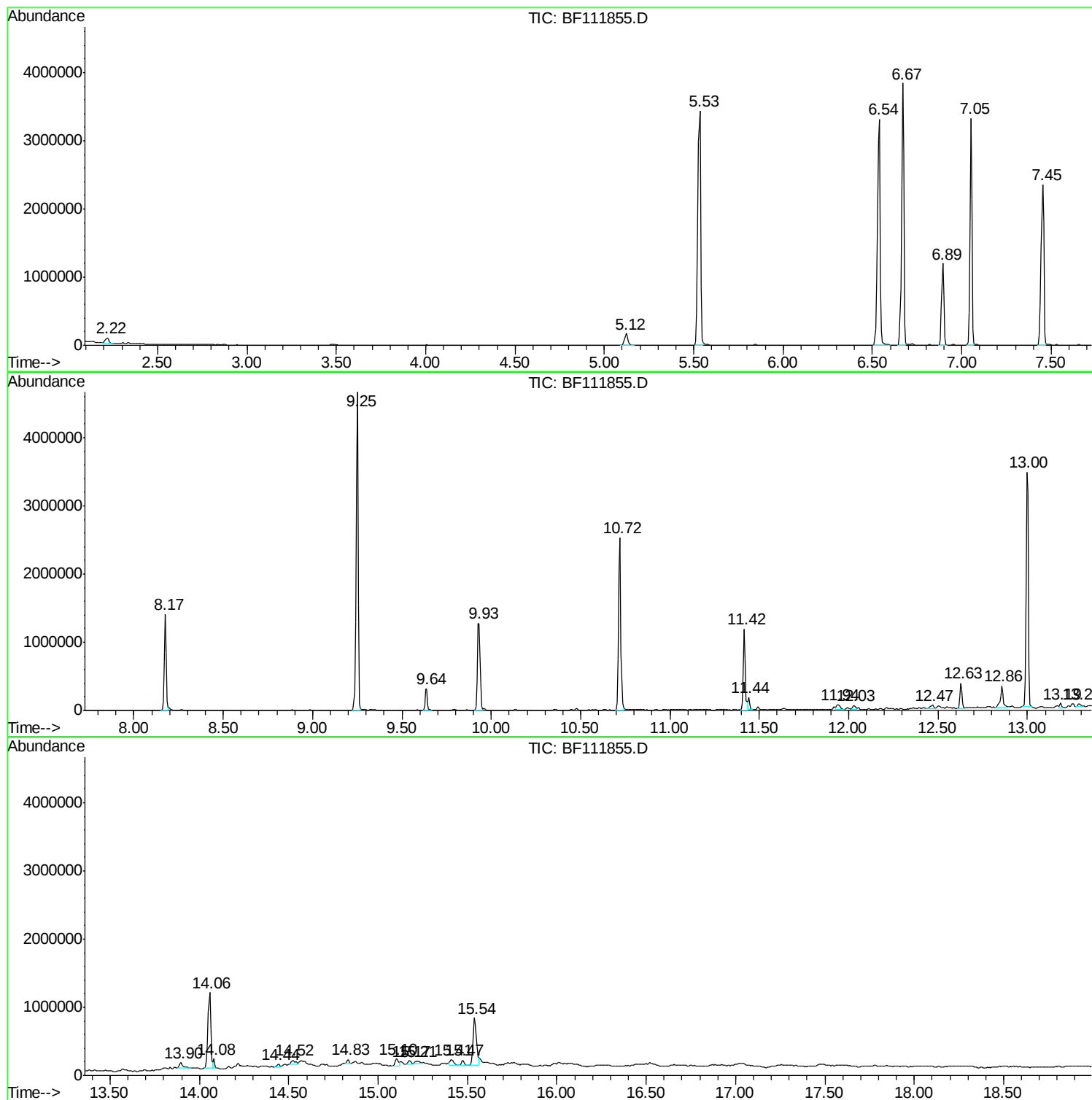
35	15.539	2282	2287	2291	rbV	696254	891694	22.19%	2.589%
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Sum of corrected areas: 34441033

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.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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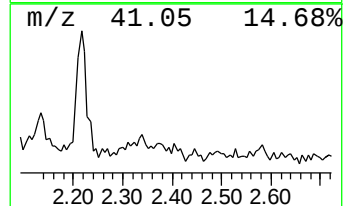
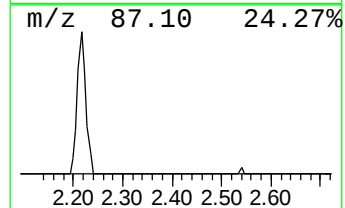
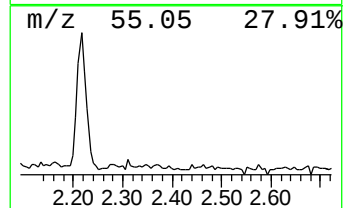
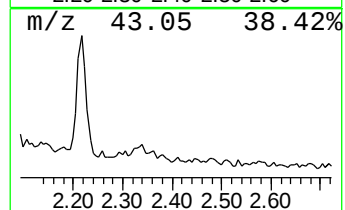
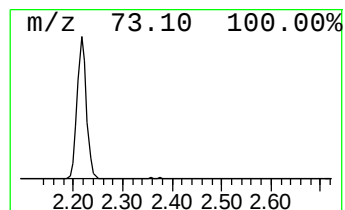
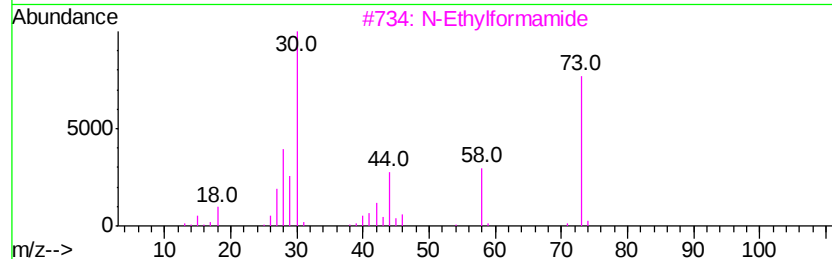
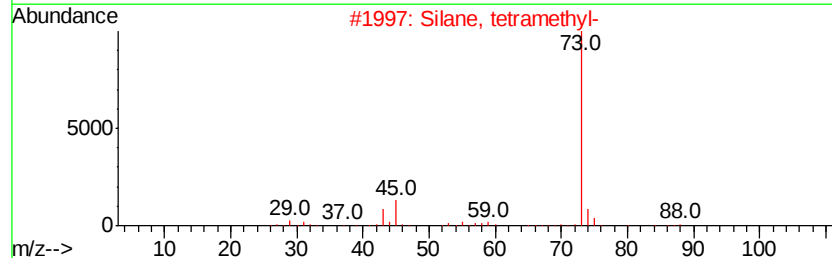
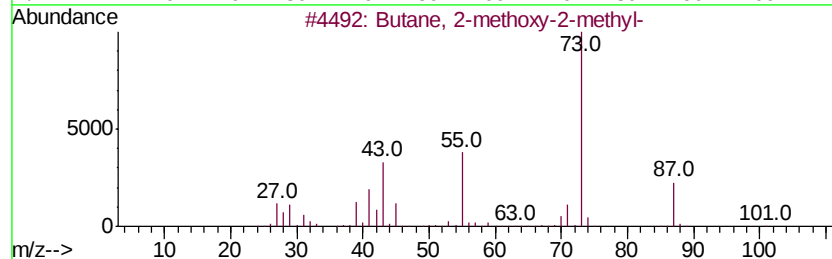
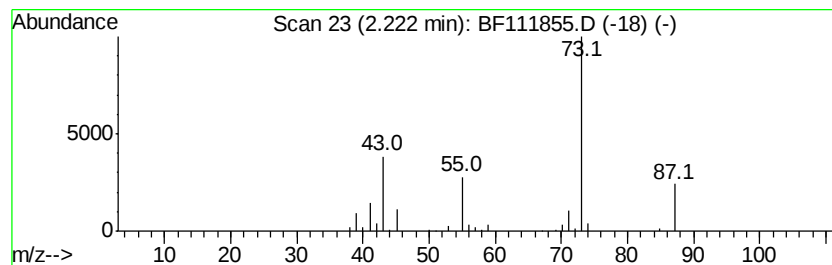
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.22	2.39 ng	113296	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	9



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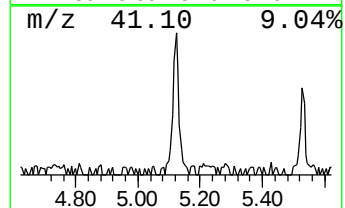
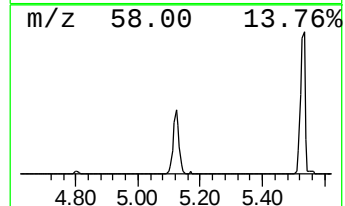
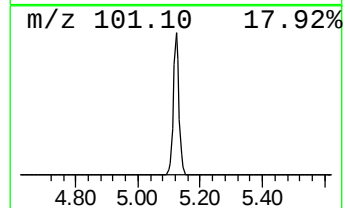
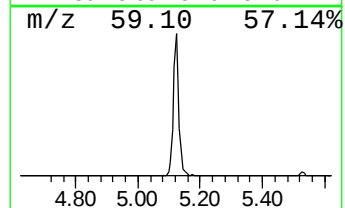
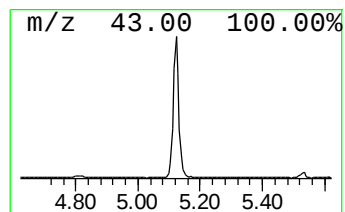
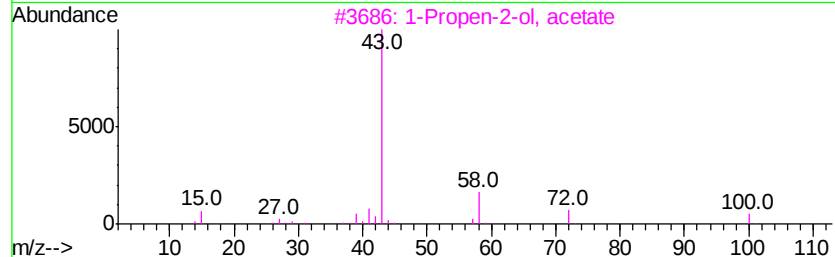
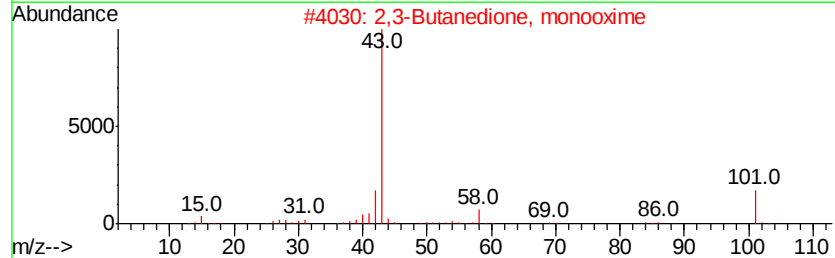
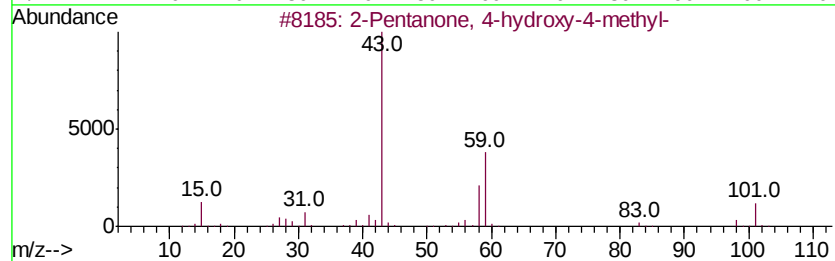
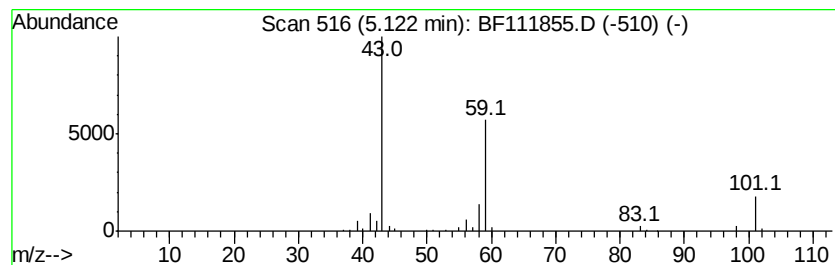
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.49 ng	213145	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane	58	C4H10	000106-97-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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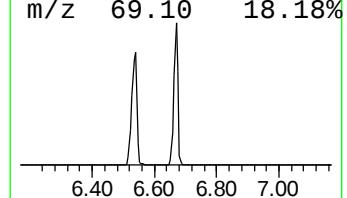
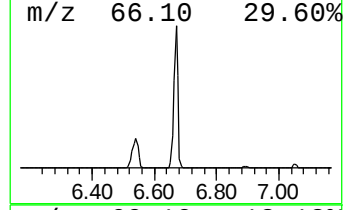
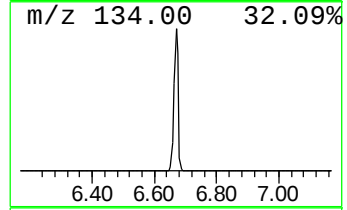
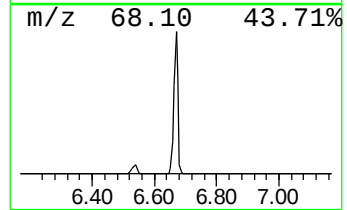
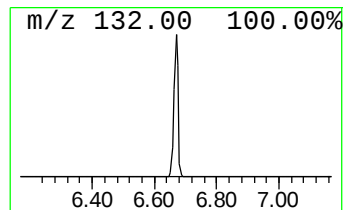
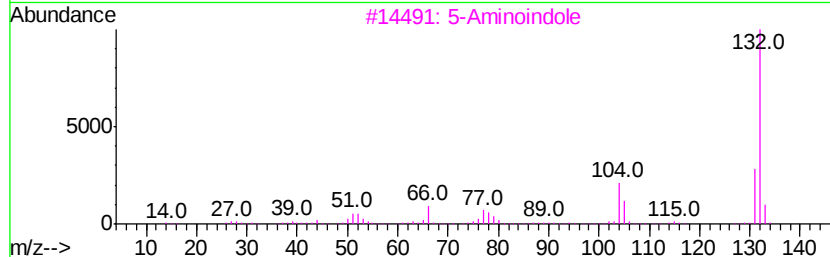
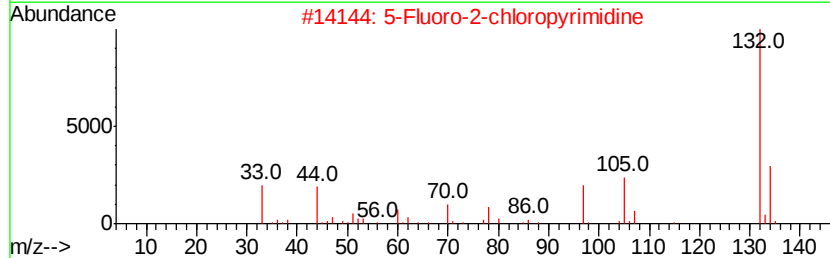
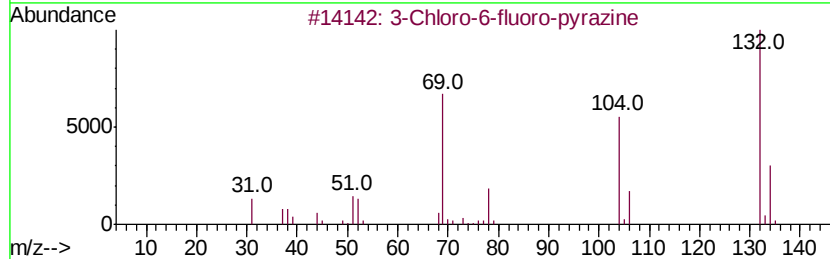
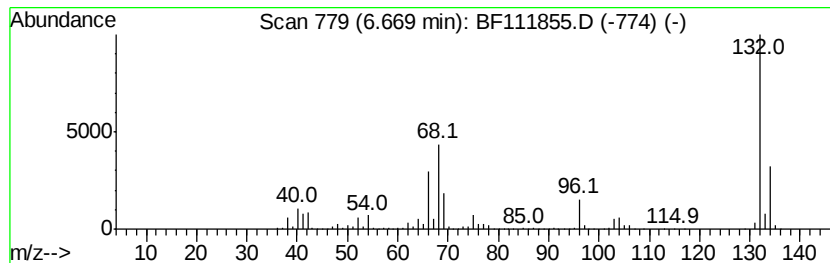
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	76.70 ng	3640090	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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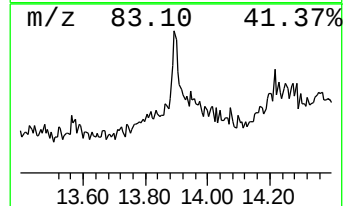
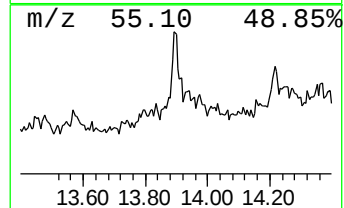
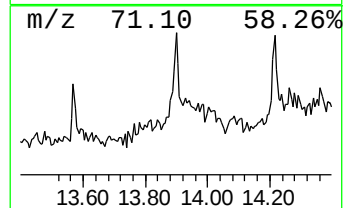
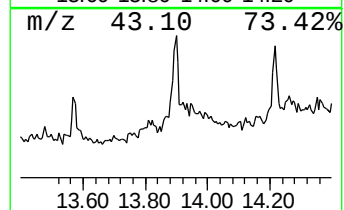
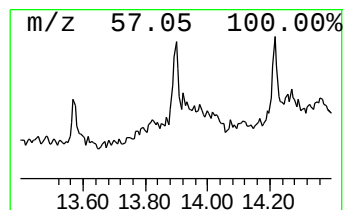
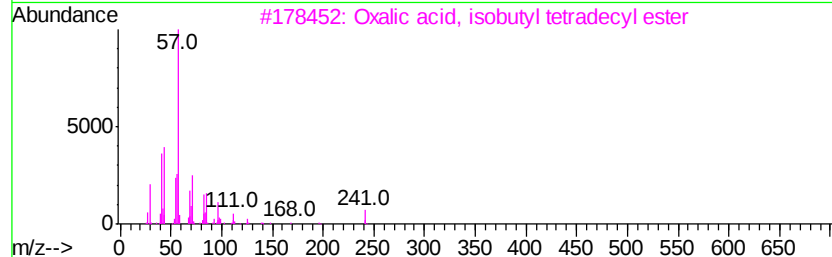
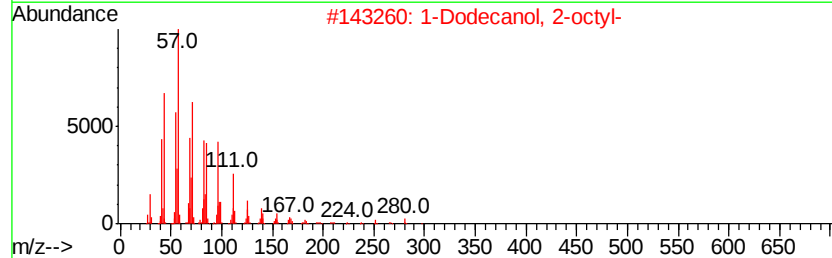
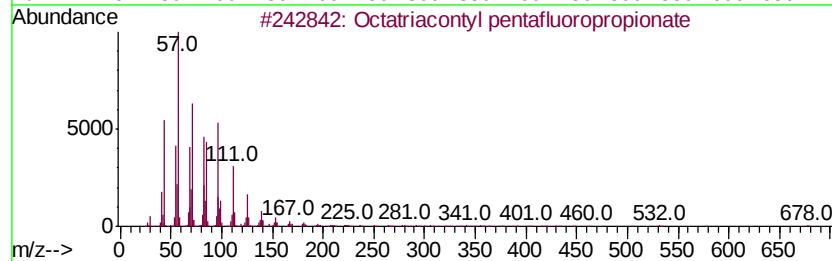
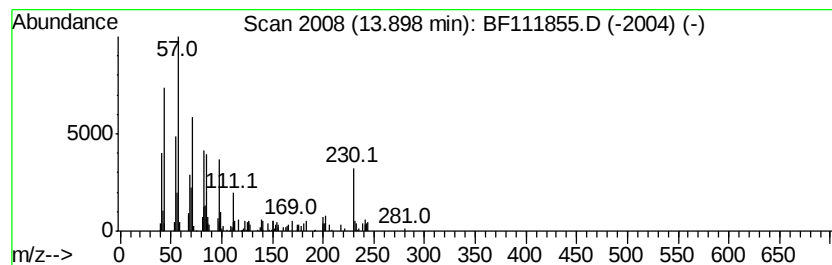
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octatriacontyl pentafluorop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.18 ng	122338	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	80
2		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	80
3		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	80
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	72
5		Undecane	156	C11H24	001120-21-4	46



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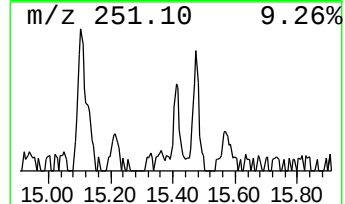
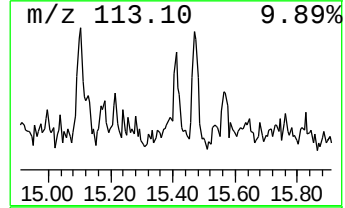
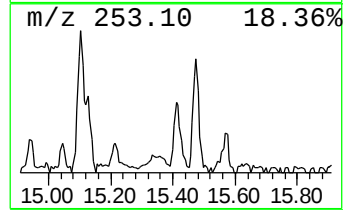
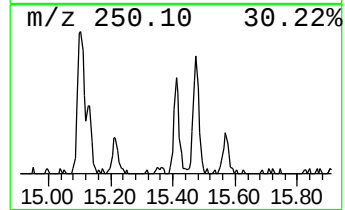
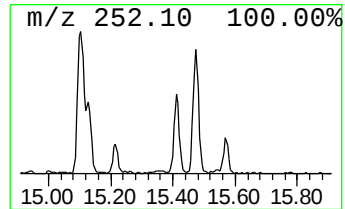
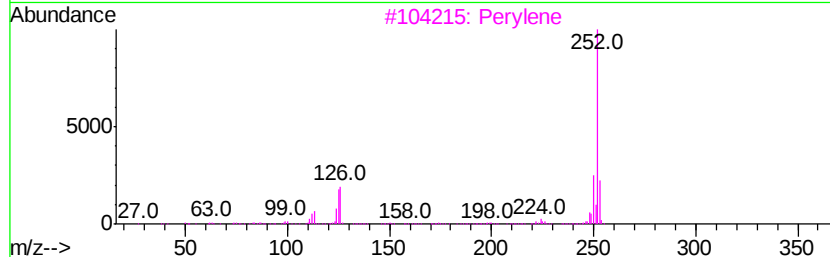
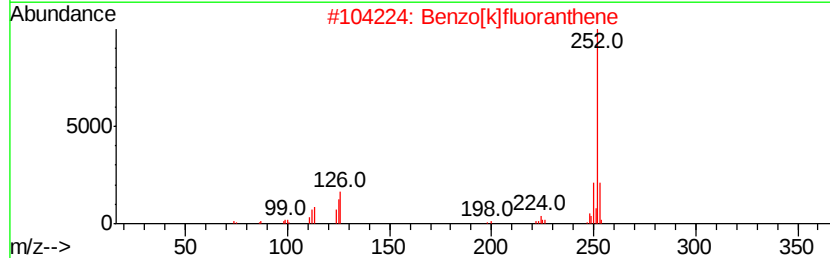
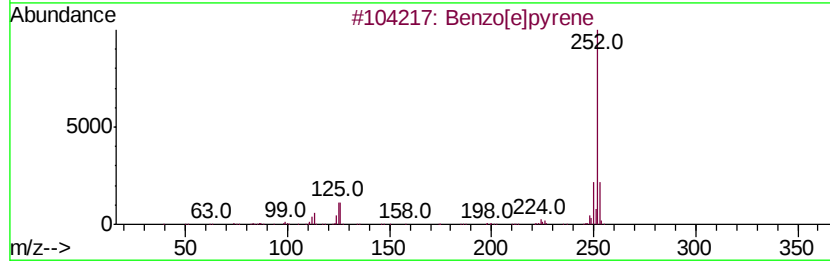
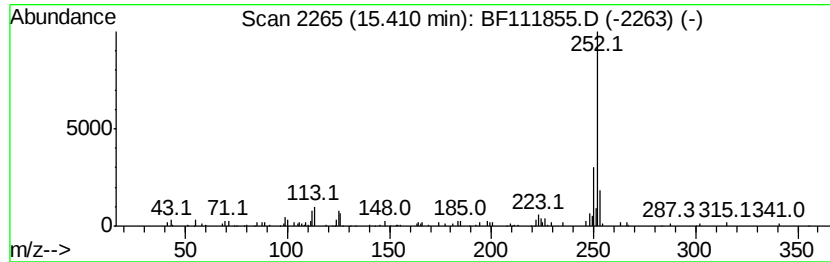
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	2.59 ng	115306	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	81
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3		Perylene	252	C20H12	000198-55-0	76
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	76
5		Benzo[a]pyrene	252	C20H12	000050-32-8	74



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	2.22	2.4	ng	113296	1	6.89	949228	20.0
2-Pentanone, 4-hy...	5.12	4.5	ng	213145	1	6.89	949228	20.0
unknown6.67	6.67	76.7	ng	3640090	1	6.89	949228	20.0
Octatriacontyl pe...	13.90	2.2	ng	122338	5	14.06	1120800	20.0
Benzo[e]pyrene	15.41	2.6	ng	115306	6	15.54	891694	20.0