

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
 Data File : BF097877.D
 Acq On : 19 Aug 2017 14:30
 Operator : SJ/JU
 Sample : I4846-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PI-2(3)

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-BF081517.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	2.116	3	5	18	rVB2	78973	134744	3.67%	0.457%
2	3.534	240	246	256	rBV	69484	111652	3.04%	0.379%
3	4.951	483	487	495	rVB	311562	381924	10.41%	1.295%
4	5.369	553	558	561	rBV	2301614	2155329	58.75%	7.308%
5	6.392	726	732	735	rBV	2385057	2276014	62.04%	7.717%
6	6.528	750	755	758	rBV	2511799	2268497	61.84%	7.691%
7	6.763	791	795	798	rBV	1015892	930710	25.37%	3.156%
8	6.916	817	821	824	rBV	2057977	1763471	48.07%	5.979%
9	7.322	882	890	893	rBV	1616581	1475134	40.21%	5.001%
10	8.045	1008	1013	1016	rBV	1312654	1288782	35.13%	4.370%
11	9.122	1190	1196	1199	rBV	2799963	2613315	71.24%	8.860%
12	9.510	1259	1262	1267	rBV	293920	230889	6.29%	0.783%
13	9.792	1304	1310	1314	rBV	1483877	1387301	37.82%	4.704%
14	10.580	1439	1444	1447	rBV	2157563	2086504	56.88%	7.074%
15	10.704	1462	1465	1471	rBV	62260	79307	2.16%	0.269%
16	11.275	1558	1562	1564	rBV	1479849	1251681	34.12%	4.244%
17	11.298	1564	1566	1569	rVV	289727	221085	6.03%	0.750%
18	11.345	1572	1574	1577	rVB	58185	51129	1.39%	0.173%
19	11.804	1649	1652	1657	rBV3	89030	86146	2.35%	0.292%
20	11.886	1662	1666	1668	rBV3	65403	74604	2.03%	0.253%
21	12.322	1738	1740	1744	rBV2	53791	54546	1.49%	0.185%
22	12.404	1752	1754	1759	rVB4	37140	42596	1.16%	0.144%
23	12.480	1764	1767	1771	rVB	376426	323989	8.83%	1.098%
24	12.710	1799	1806	1809	rBV	343536	359090	9.79%	1.217%
25	12.869	1828	1833	1836	rVB	3366687	3668562	100.00%	12.438%
26	13.039	1860	1862	1865	rVB	54476	42627	1.16%	0.145%
27	13.104	1870	1873	1876	rVV2	49678	46629	1.27%	0.158%
28	13.139	1877	1879	1882	rVB	43527	39475	1.08%	0.134%
29	13.545	1945	1948	1952	rVB4	35729	51052	1.39%	0.173%
30	13.757	1980	1984	1991	rVB2	286257	327536	8.93%	1.111%
31	13.904	2004	2009	2012	rBV2	944593	996731	27.17%	3.379%
32	13.927	2012	2013	2016	rVB	137896	86131	2.35%	0.292%
33	14.392	2089	2092	2099	rVB2	132616	150044	4.09%	0.509%
34	14.757	2151	2154	2159	rVB3	52981	72139	1.97%	0.245%

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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

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35	14.827	2163	2166	2170	rVB2	52994	55475	1.51%	0.188%
36	14.921	2177	2182	2185	rBV	130608	214102	5.84%	0.726%
37	15.015	2194	2198	2199	rBV2	121073	142248	3.88%	0.482%
38	15.204	2227	2230	2236	rVB	88233	108610	2.96%	0.368%
39	15.262	2236	2240	2246	rVB	109800	131815	3.59%	0.447%
40	15.327	2246	2251	2255	rBV	611328	739193	20.15%	2.506%
41	15.562	2288	2291	2298	rVB4	42852	60885	1.66%	0.206%
42	15.792	2326	2330	2334	rBV2	97026	139520	3.80%	0.473%
43	15.839	2334	2338	2346	rVB2	119241	202788	5.53%	0.688%
44	16.545	2454	2458	2466	rVB9	45811	82581	2.25%	0.280%
45	16.704	2481	2485	2492	rVB2	42708	73956	2.02%	0.251%
46	16.839	2503	2508	2512	rBV2	48086	88006	2.40%	0.298%
47	17.115	2552	2555	2566	rVB2	39501	89662	2.44%	0.304%
48	17.280	2576	2583	2589	rBV6	73637	169993	4.63%	0.576%
49	18.245	2742	2747	2755	rBV10	26137	65907	1.80%	0.223%

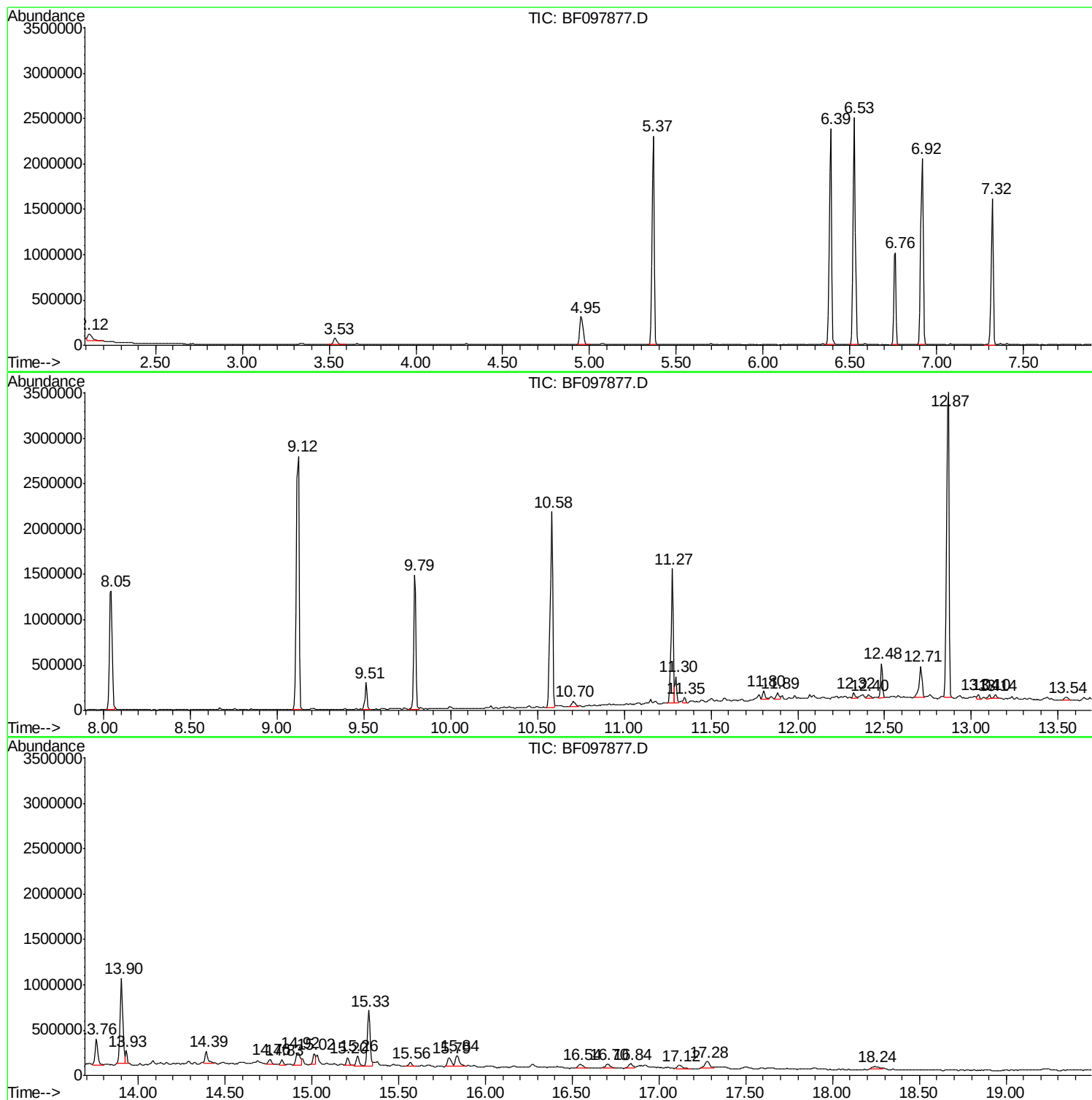
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ClientSampled :
PI-2(3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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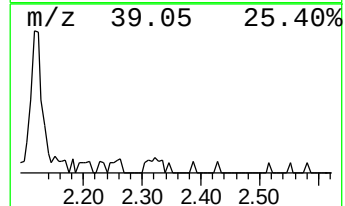
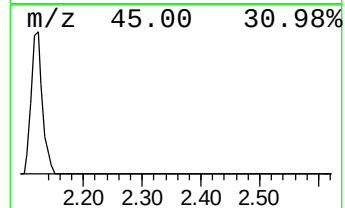
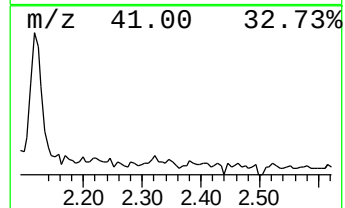
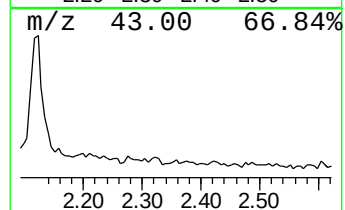
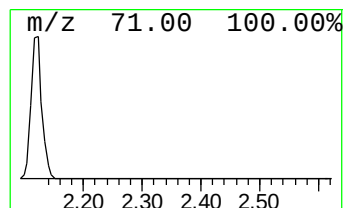
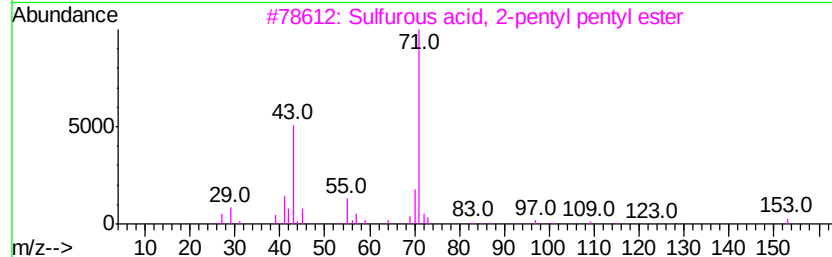
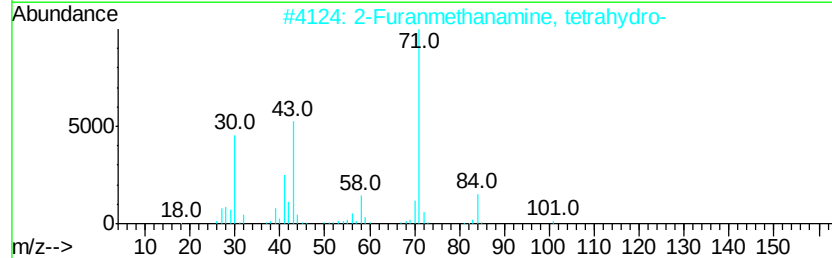
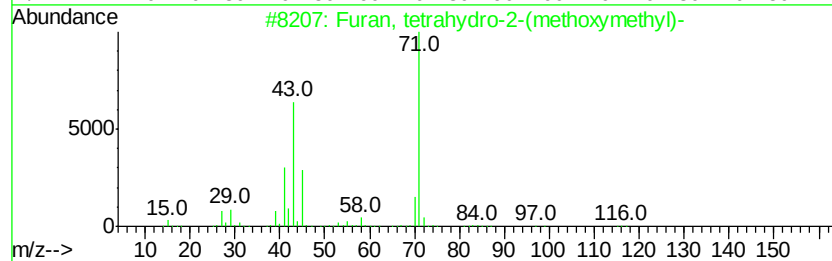
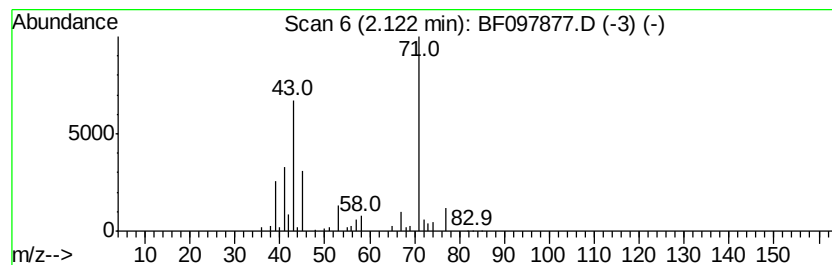
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	2.90 ng	134744	1,4-Dichlorobenzene-d4	6.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	59
2		2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	50
3		Sulfurous acid, 2-pentyl pentyl ...	222	C10H22O3S	1000309-15-4	50
4		2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	47
5		Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	47



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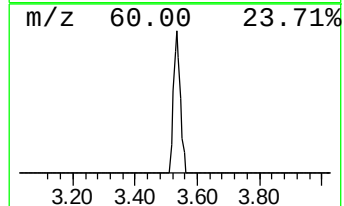
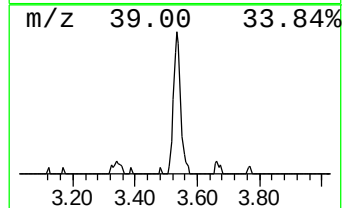
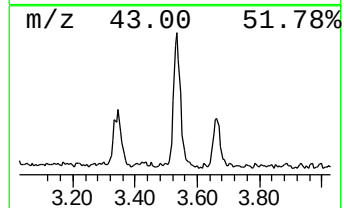
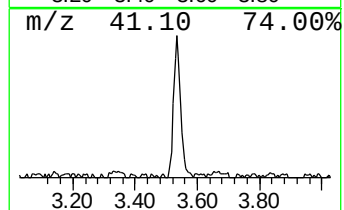
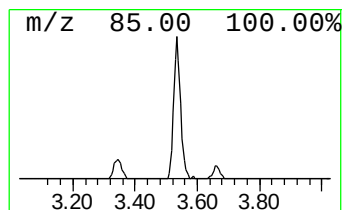
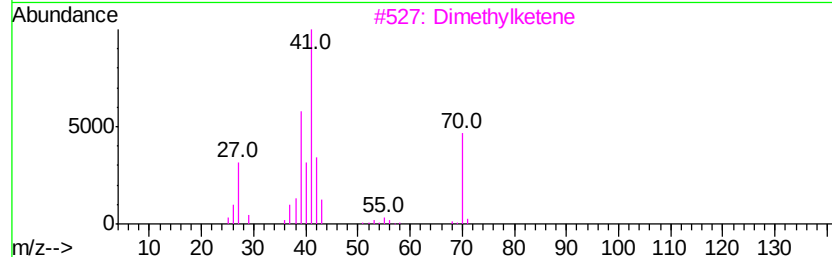
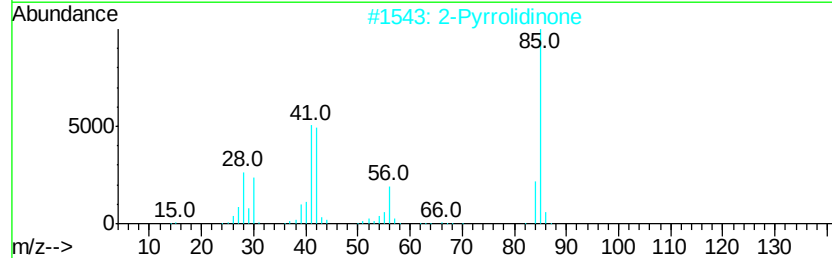
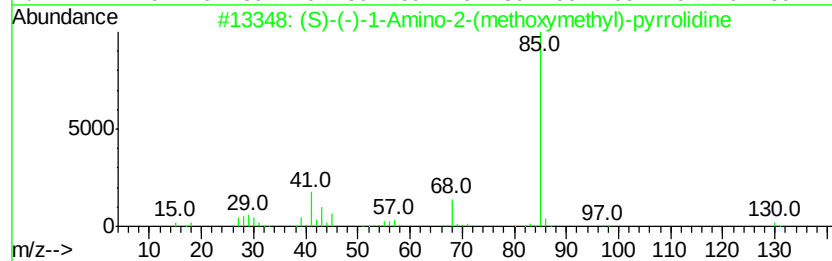
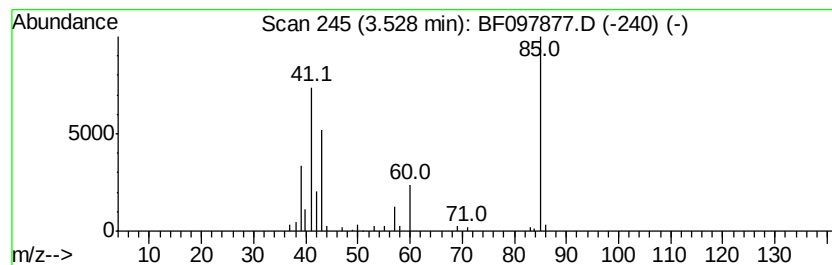
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.53 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	2.40 ng	111652	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(-)-1-Amino-2-(methoxymethyl)pyrrolidine	130	C6H14N2O	059983-39-0	23
2		2-Pyrrolidinone	85	C4H7NO	000616-45-5	9
3		Dimethylketene	70	C4H6O	000598-26-5	9
4		2-Furanmethanol, tetrahydro-5-methoxy-	116	C6H12O2	054774-28-6	9
5		Ethyl 2,4-dioxovalerate	158	C7H10O4	000615-79-2	9



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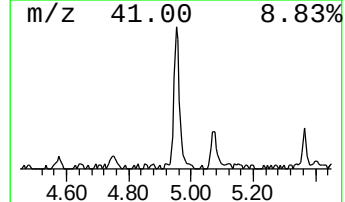
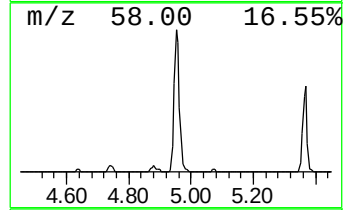
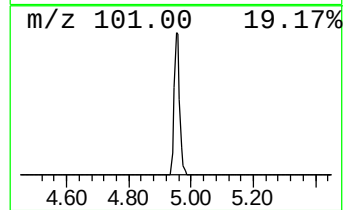
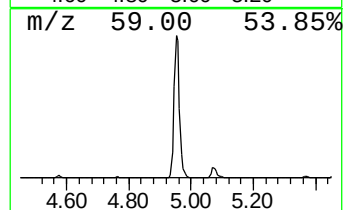
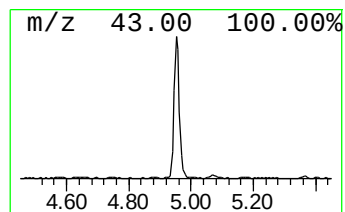
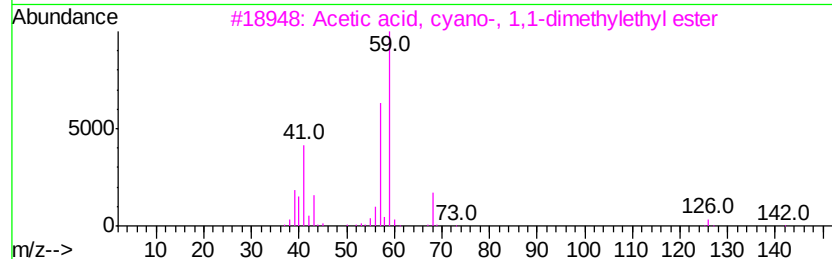
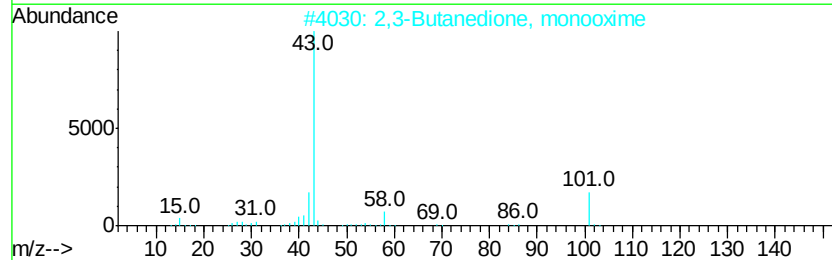
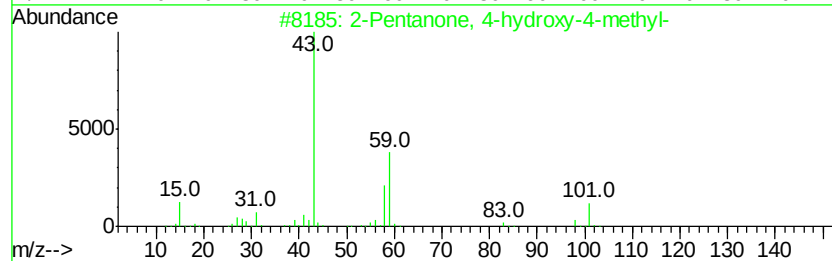
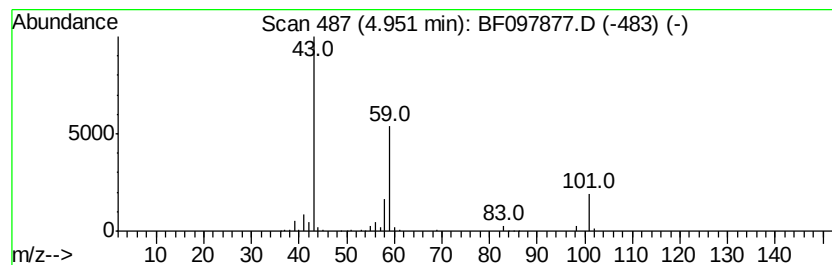
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	8.21 ng	381924	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	53
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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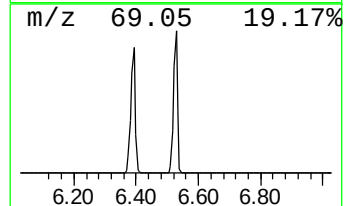
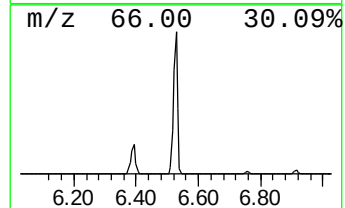
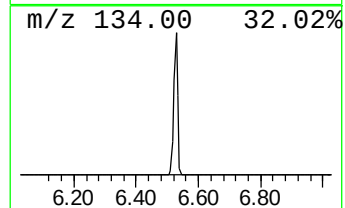
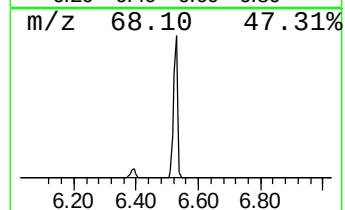
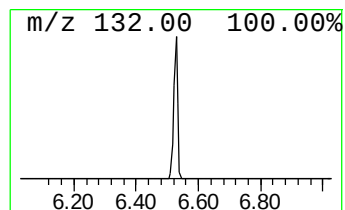
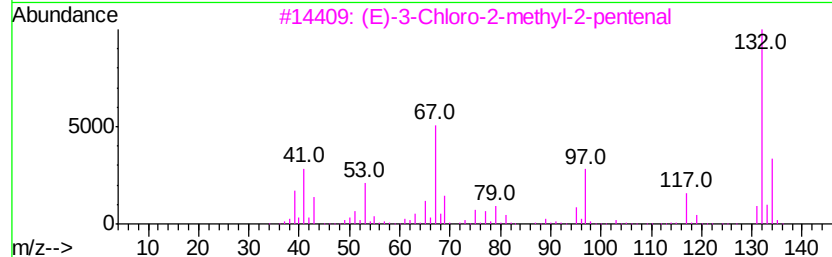
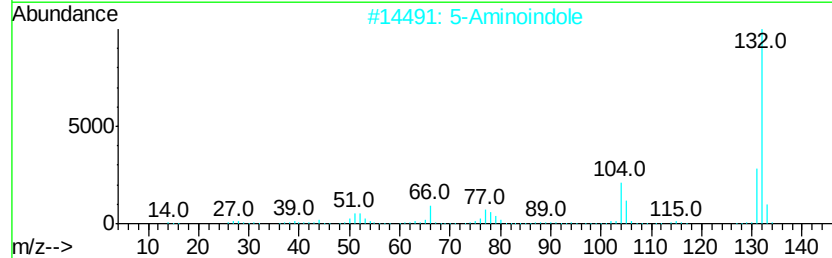
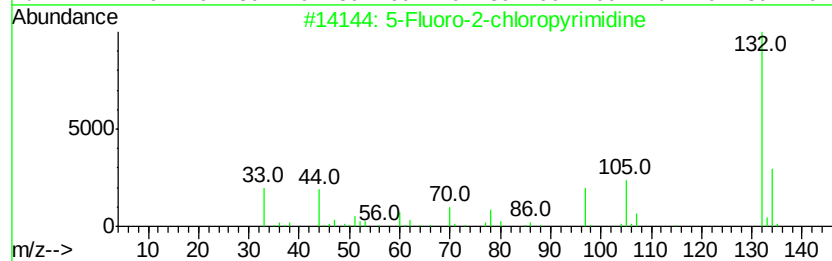
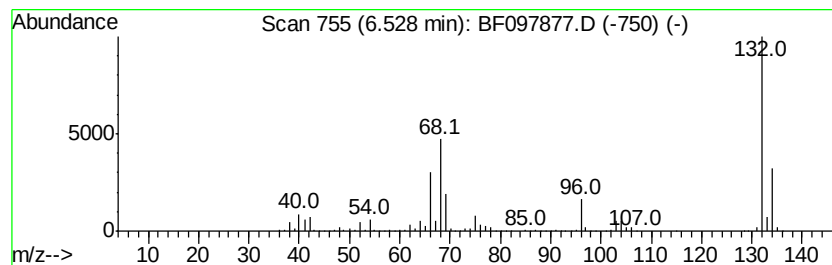
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	48.75 ng	2268500	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	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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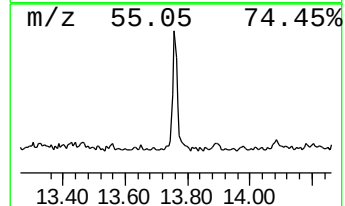
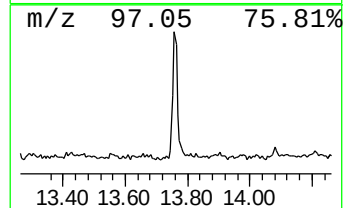
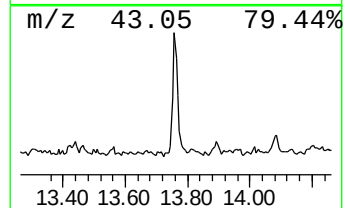
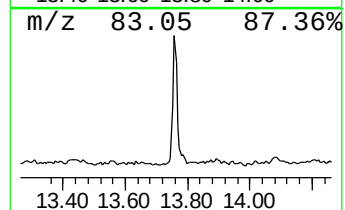
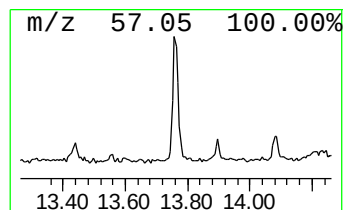
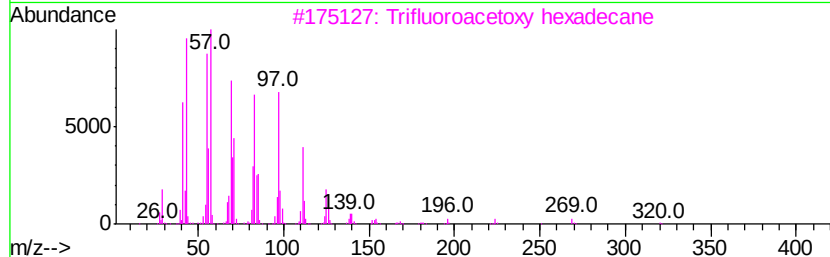
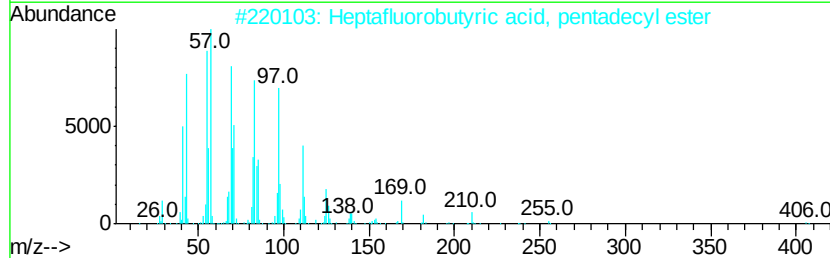
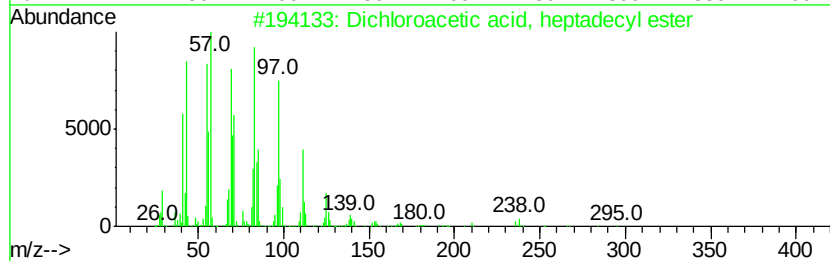
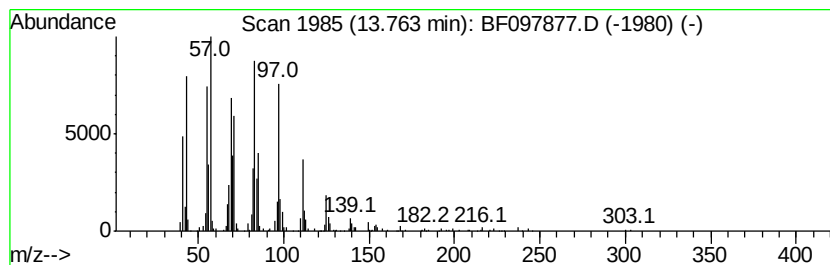
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.57 ng	327536	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
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Acq On : 19 Aug 2017 14:30
Operator : SJ/JU
Sample : I4846-01
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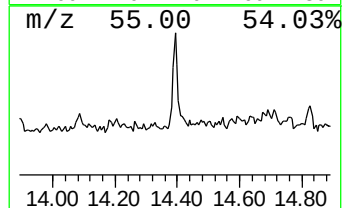
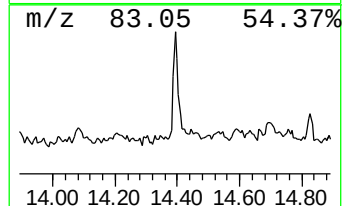
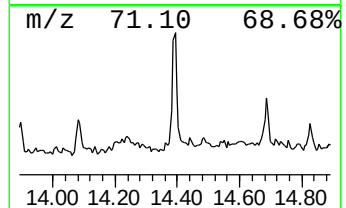
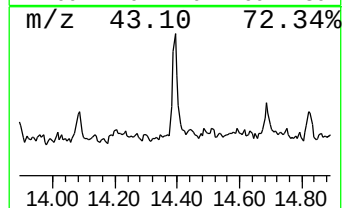
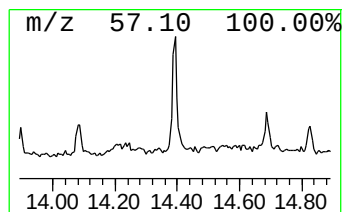
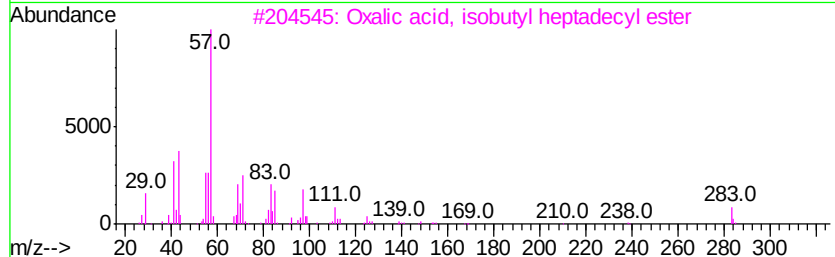
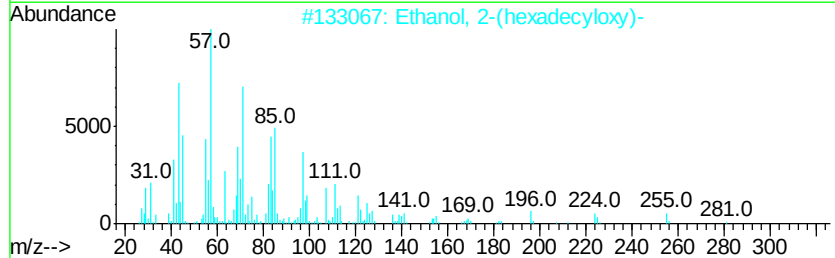
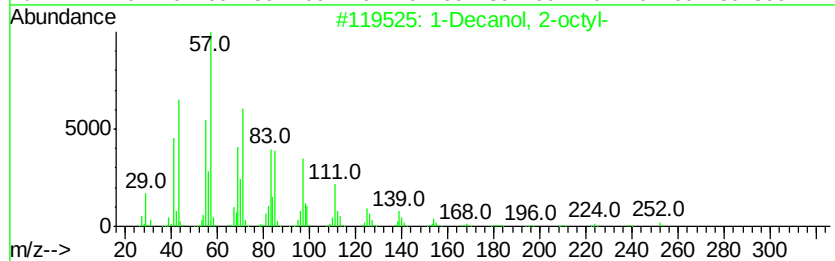
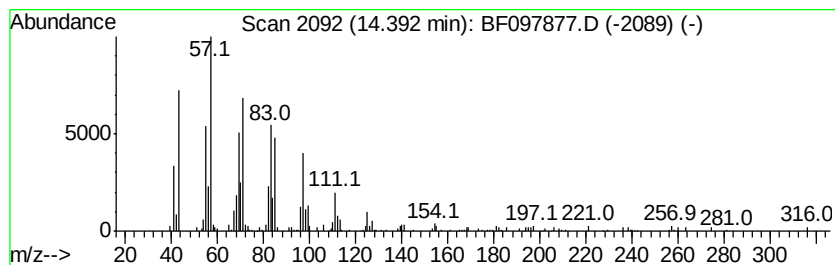
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Decanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.39	3.01 ng	150044	Chrysene-d12	13.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	91
2	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
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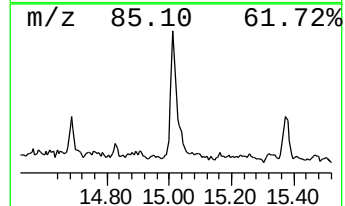
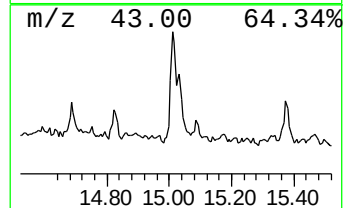
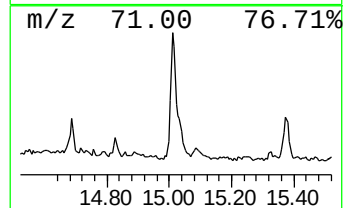
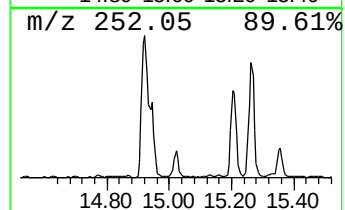
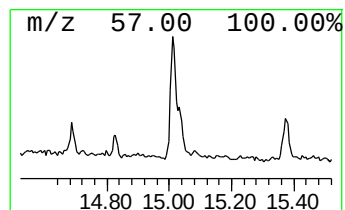
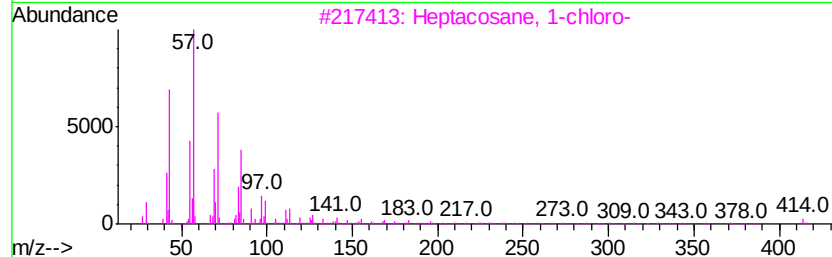
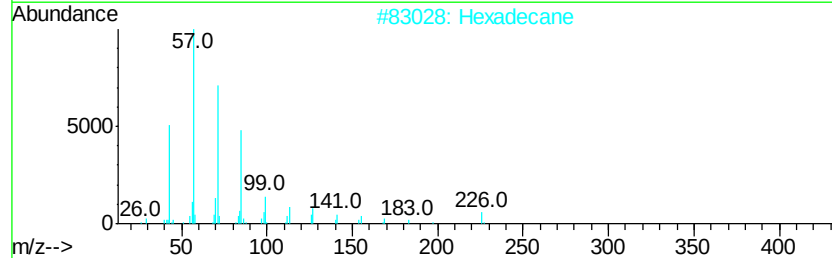
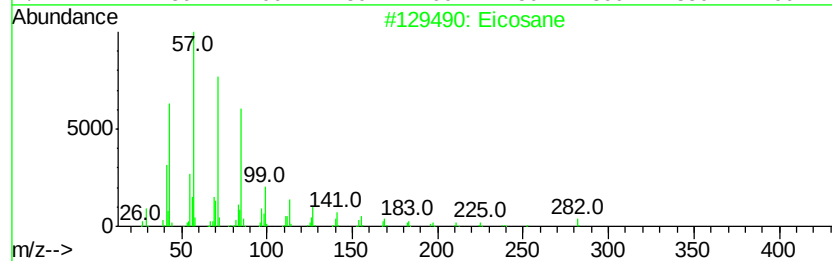
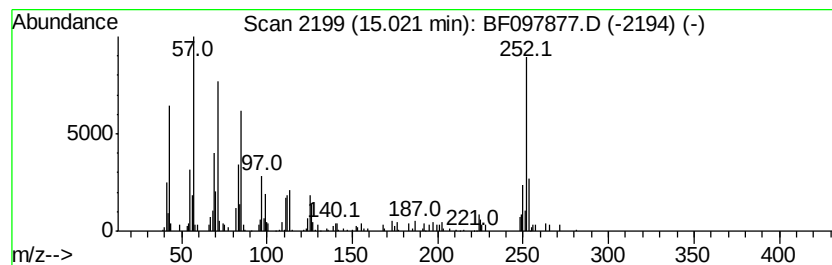
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.85 ng	142248	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	89
2	Hexadecane		226	C16H34	000544-76-3	86
3	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	68
4	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	68
5	Hexacosane		366	C26H54	000630-01-3	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
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Acq On : 19 Aug 2017 14:30
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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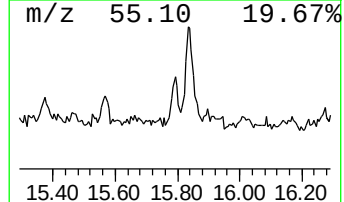
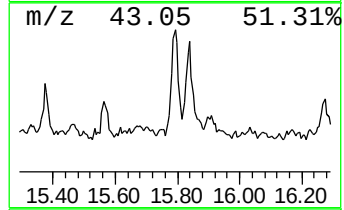
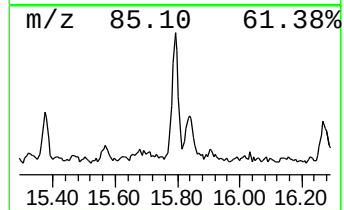
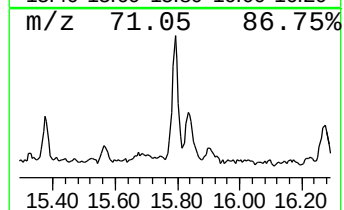
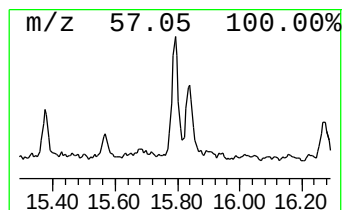
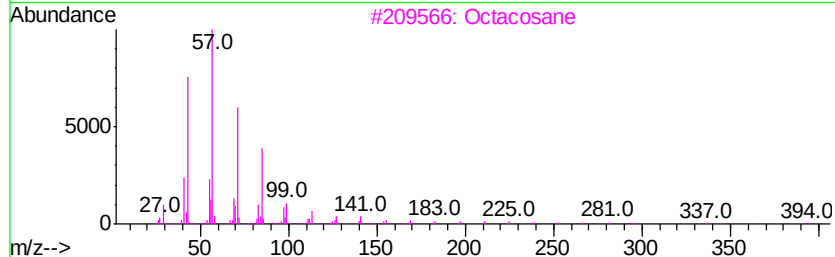
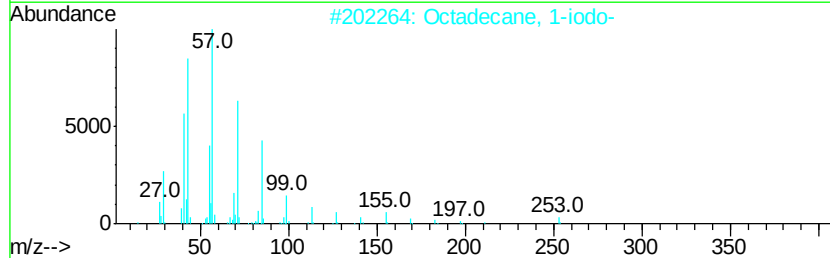
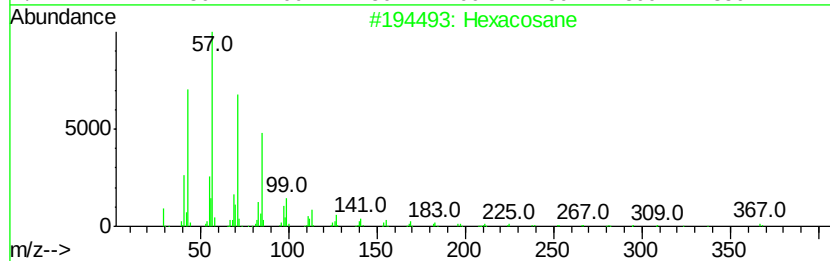
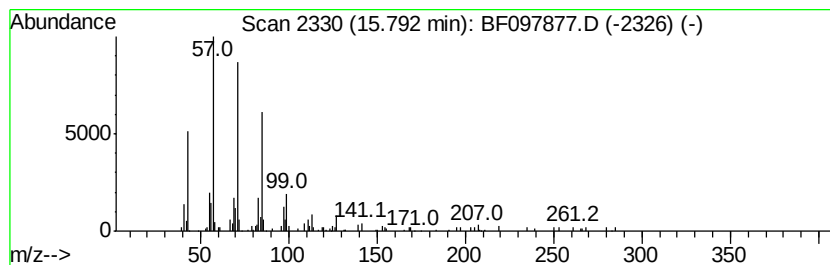
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.77 ng	139520	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3		Octacosane	394	C28H58	000630-02-4	80
4		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	80
5		Tetracosane	338	C24H50	000646-31-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
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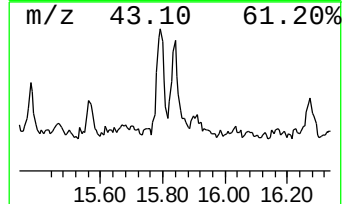
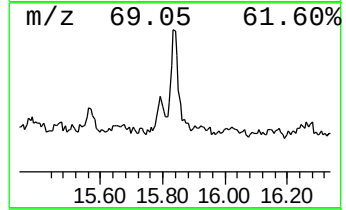
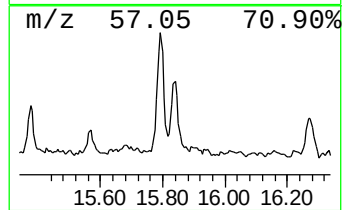
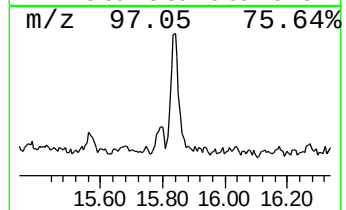
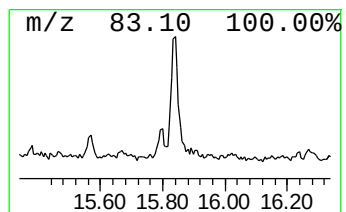
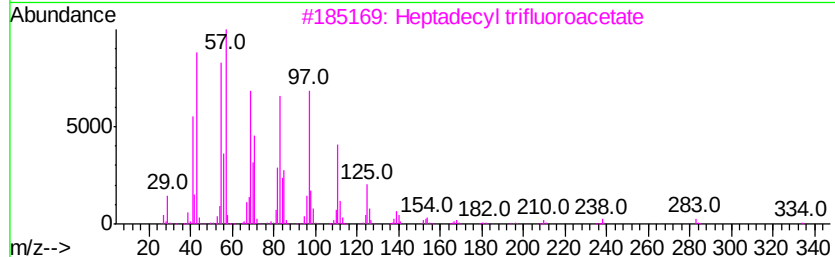
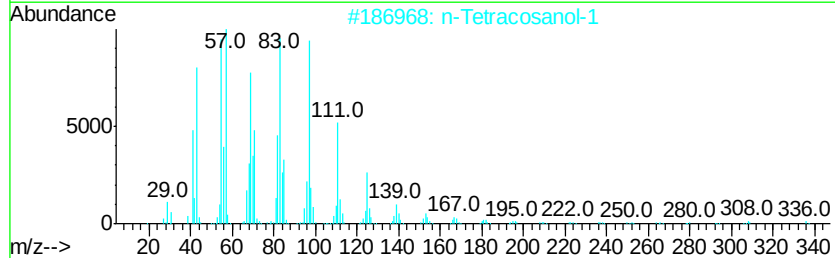
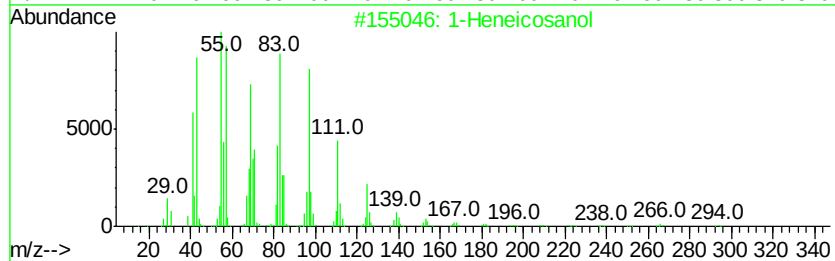
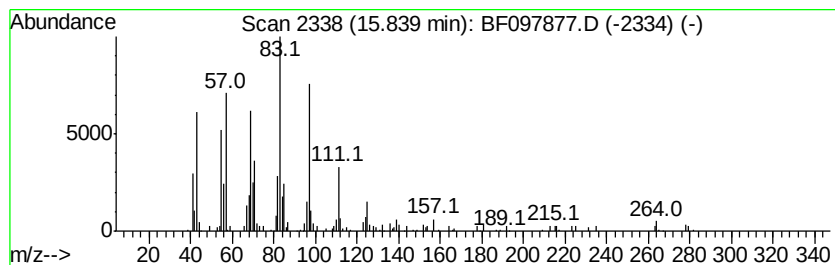
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.84	5.49 ng	202788	Perylene-d12	15.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	64
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	64
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	58
4	Behenic alcohol	326	C22H46O	000661-19-8	58
5	Cyclohexanone, 3-ethyl-	126	C8H14O	022461-89-8	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
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Misc :
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ClientSampleId :
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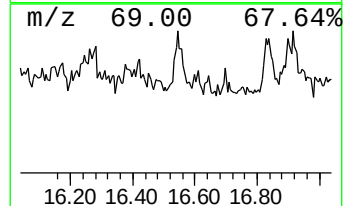
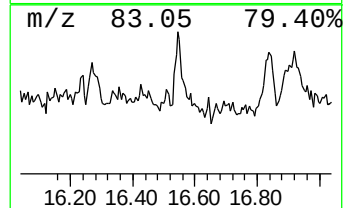
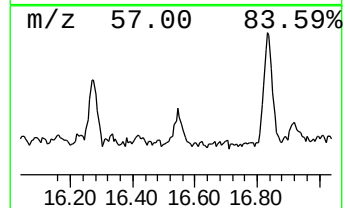
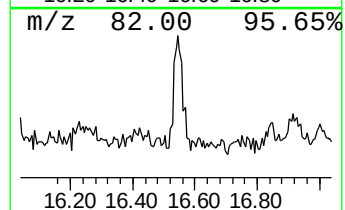
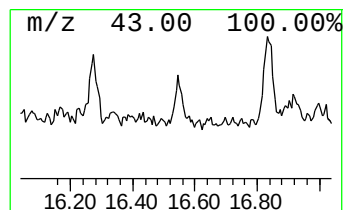
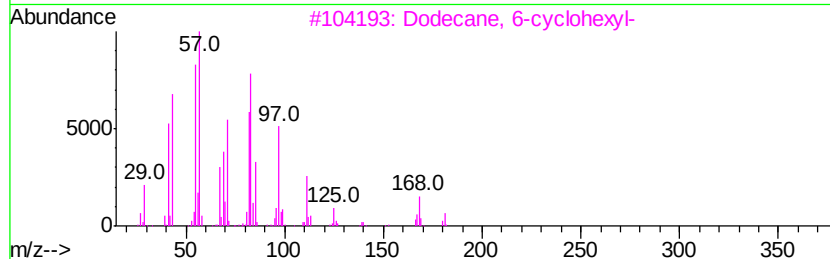
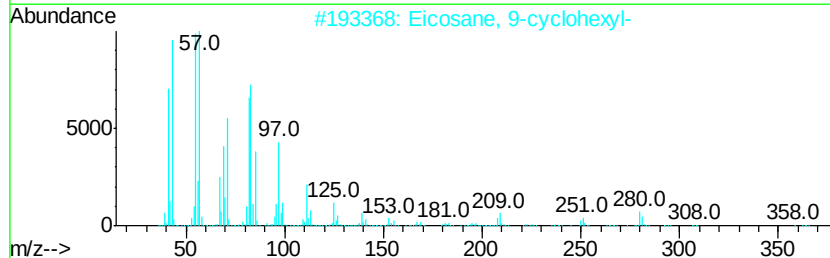
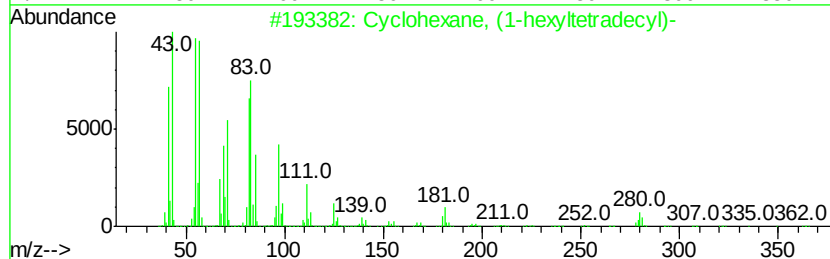
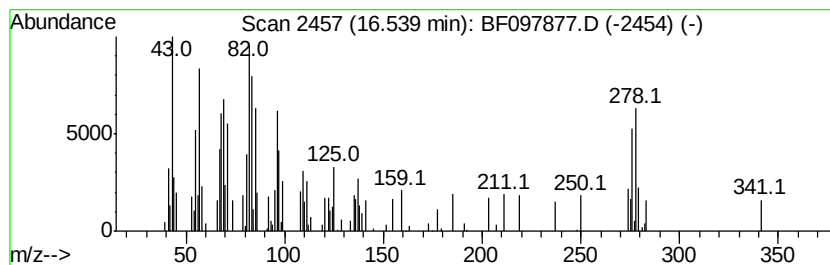
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclohexane, (1-hexyltetradecyl)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	2.23 ng	82581	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	53
2		Eicosane, 9-cyclohexyl-	364	C26H52	004443-61-2	49
3		Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	49
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	46
5		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	30



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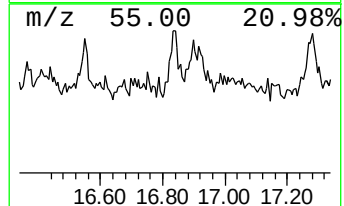
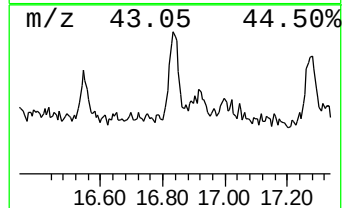
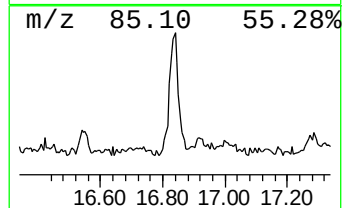
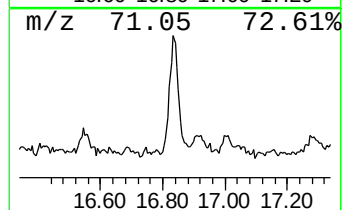
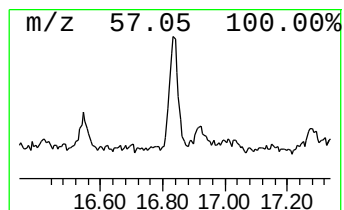
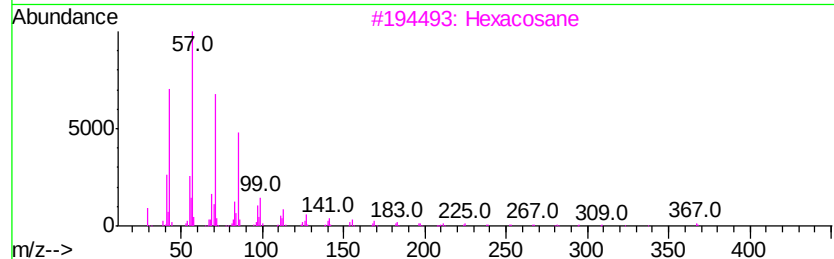
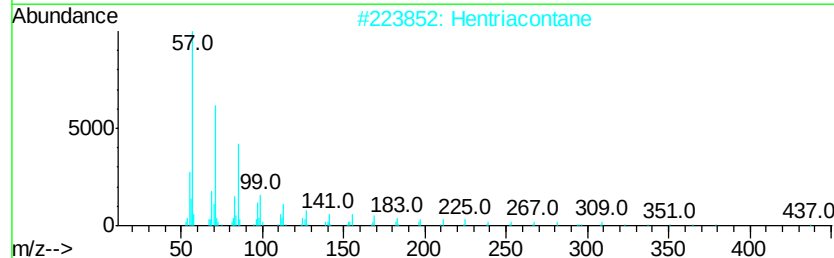
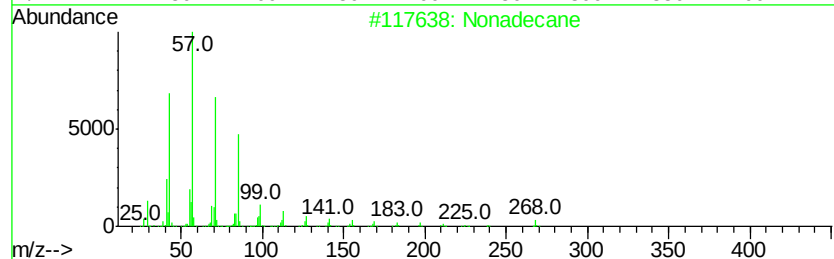
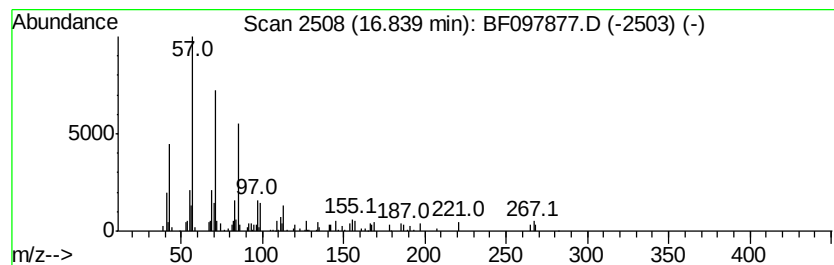
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Nonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	2.38 ng	88006	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	91
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Hexacosane	366	C26H54	000630-01-3	83
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



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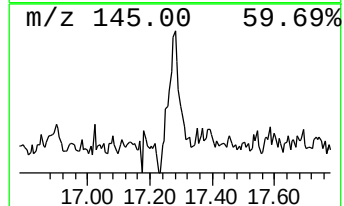
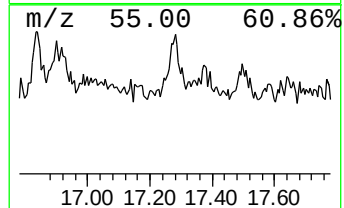
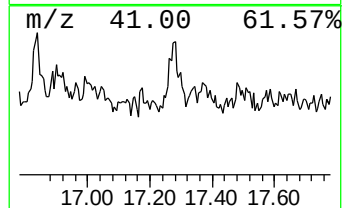
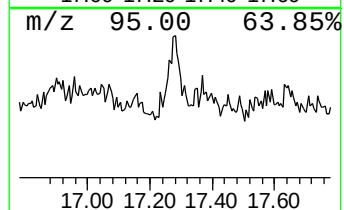
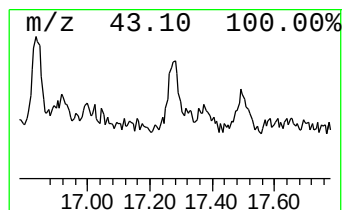
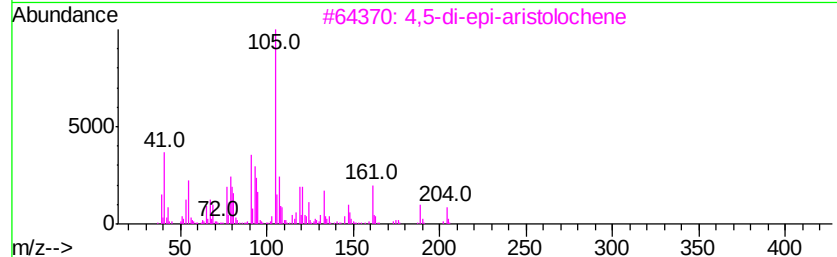
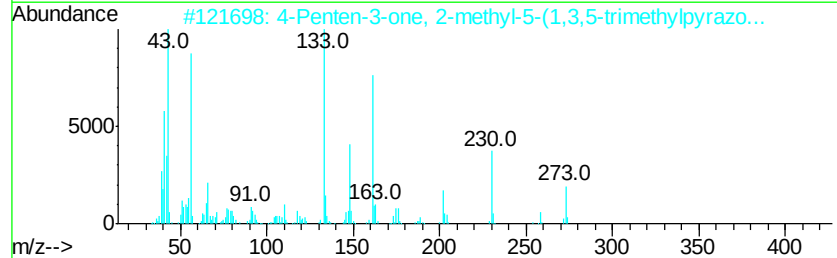
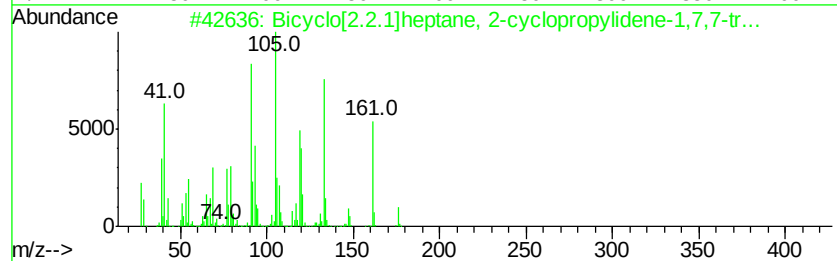
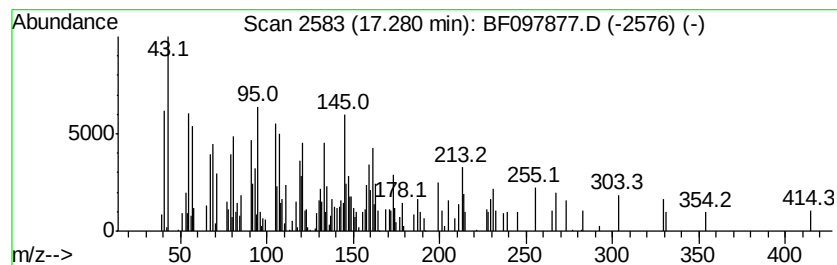
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	4.60 ng	169993	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptane, 2-cyclopr...	176	C13H20	1000159-45-7	22
2		4-Penten-3-one, 2-methyl-5-(1,3,...	273	C14H19N5O	312311-98-1	18
3		4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	16
4		1,10,25,26-Tetraaza-4,7-dioxatet...	354	C20H26N4O2	286013-88-5	14
5		Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	1000151-74-7	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
 Data File : BF097877.D
 Acq On : 19 Aug 2017 14:30
 Operator : SJ/JU
 Sample : I4846-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PI-2(3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
 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
Furan, tetrahydro...	2.12	2.9	ng	134744	1	6.76	930710	20.0
unknown3.53	3.53	2.4	ng	111652	1	6.76	930710	20.0
2-Pentanone, 4-hy...	4.95	8.2	ng	381924	1	6.76	930710	20.0
unknown6.53	6.53	48.8	ng	2268500	1	6.76	930710	20.0
Dichloroacetic ac...	13.76	6.6	ng	327536	5	13.90	996731	20.0
1-Decanol, 2-octyl-	14.39	3.0	ng	150044	5	13.90	996731	20.0
Eicosane	15.02	3.9	ng	142248	6	15.33	739193	20.0
Hexacosane	15.79	3.8	ng	139520	6	15.33	739193	20.0
1-Heneicosanol	15.84	5.5	ng	202788	6	15.33	739193	20.0
Cyclohexane, (1-h...	16.54	2.2	ng	82581	6	15.33	739193	20.0
Nonadecane	16.84	2.4	ng	88006	6	15.33	739193	20.0
unknown17.28	17.28	4.6	ng	169993	6	15.33	739193	20.0