

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
 Data File : BF098206.D
 Acq On : 31 Aug 2017 20:40
 Operator : SJ/JU
 Sample : I4963-18
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3837-DB

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-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	4.969	474	490	493	rBV	2980426	8110625	100.00%	23.127%
2	5.334	548	552	558	rVB	909613	769717	9.49%	2.195%
3	6.351	719	725	733	rBV2	683945	713746	8.80%	2.035%
4	6.487	744	748	751	rBV	1695016	1483412	18.29%	4.230%
5	6.716	783	787	790	rBV	1058759	844339	10.41%	2.408%
6	6.875	809	814	817	rBV	2852218	2698348	33.27%	7.694%
7	6.904	817	819	823	rVB	198039	155450	1.92%	0.443%
8	7.287	878	884	887	rBV	2031132	2378574	29.33%	6.782%
9	7.681	947	951	953	rBV	104014	98994	1.22%	0.282%
10	7.792	965	970	975	rBV	94603	101162	1.25%	0.288%
11	7.998	1001	1005	1009	rVV	1166866	1148760	14.16%	3.276%
12	8.498	1084	1090	1092	rBV	337381	345940	4.27%	0.986%
13	8.516	1092	1093	1098	rVB	145460	99635	1.23%	0.284%
14	8.992	1170	1174	1182	rVB3	66942	95437	1.18%	0.272%
15	9.081	1182	1189	1192	rBV	3781542	4204338	51.84%	11.989%
16	9.510	1258	1262	1268	rBV3	59327	81135	1.00%	0.231%
17	9.751	1298	1303	1311	rVB	1383682	1356456	16.72%	3.868%
18	10.539	1431	1437	1440	rBV	1506374	1402922	17.30%	4.000%
19	10.645	1452	1455	1460	rVB	95108	97024	1.20%	0.277%
20	11.233	1548	1555	1559	rBV	1673929	1505471	18.56%	4.293%
21	12.827	1818	1826	1829	rBV	3773730	4574626	56.40%	13.044%
22	13.868	1997	2003	2006	rBV	1393898	1410579	17.39%	4.022%
23	15.280	2238	2243	2246	rBV	679782	814194	10.04%	2.322%
24	15.310	2246	2248	2252	rVB	97513	106168	1.31%	0.303%
25	15.715	2312	2317	2323	rVB	98066	138863	1.71%	0.396%
26	16.186	2392	2397	2404	rVB2	86078	143663	1.77%	0.410%
27	16.733	2485	2490	2496	rVB2	51706	98935	1.22%	0.282%
28	17.380	2594	2600	2608	rVB2	40122	91181	1.12%	0.260%

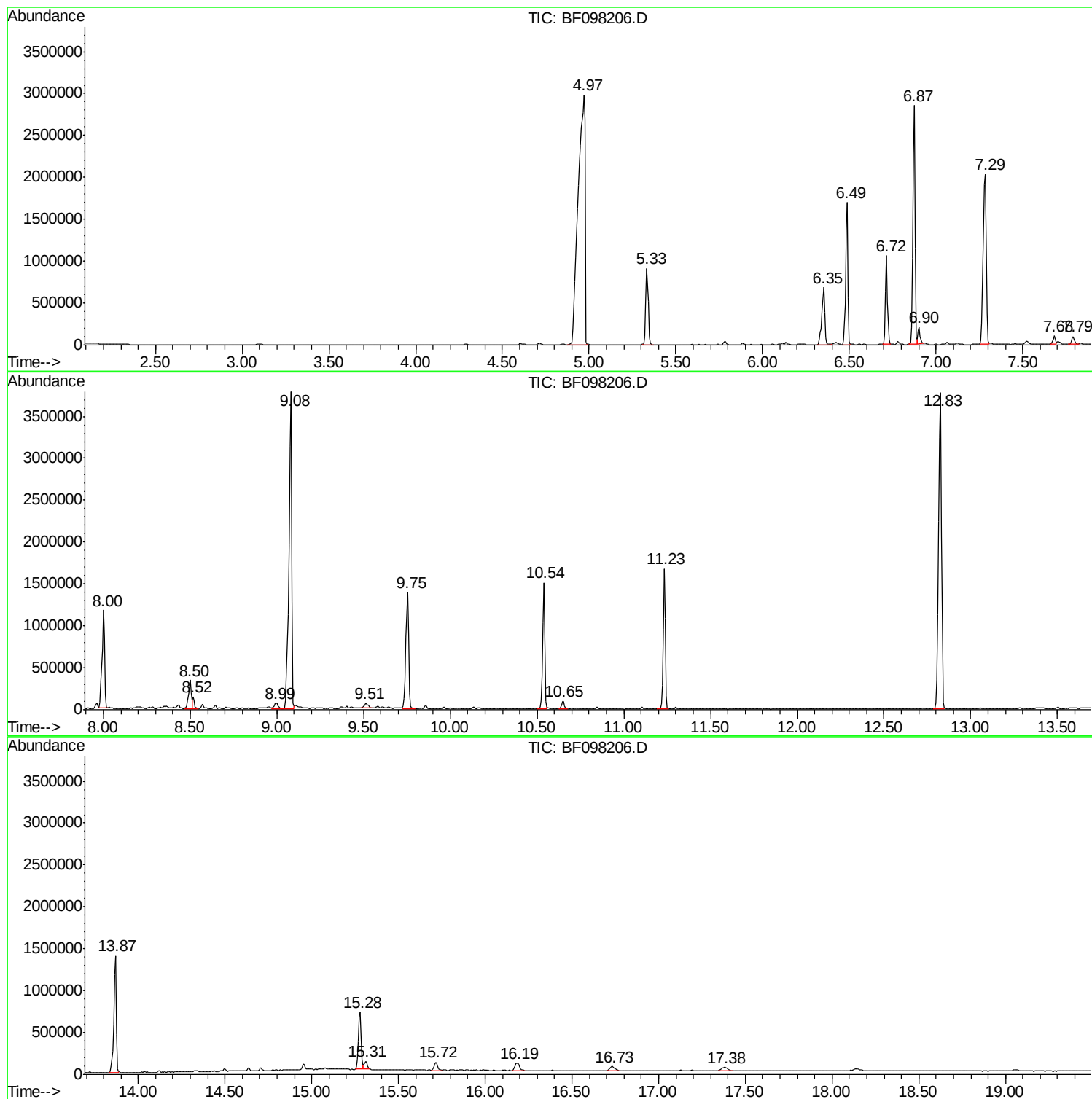
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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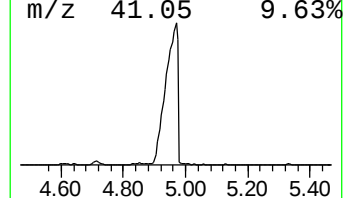
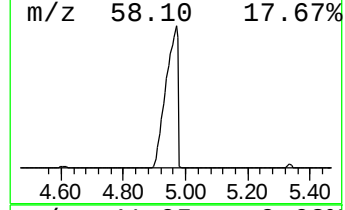
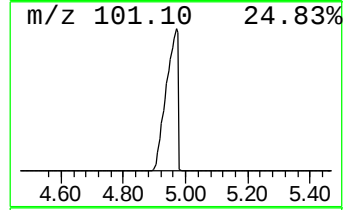
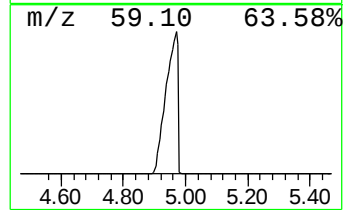
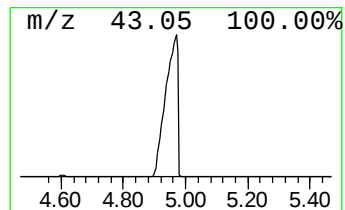
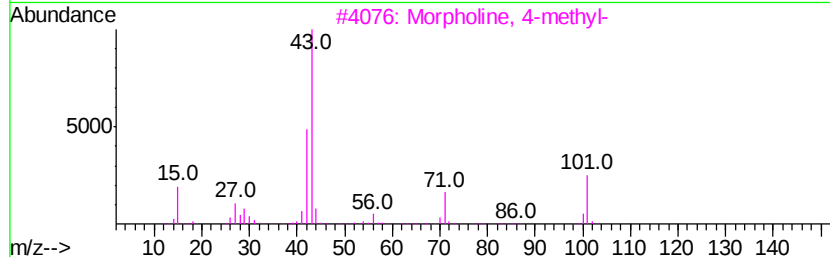
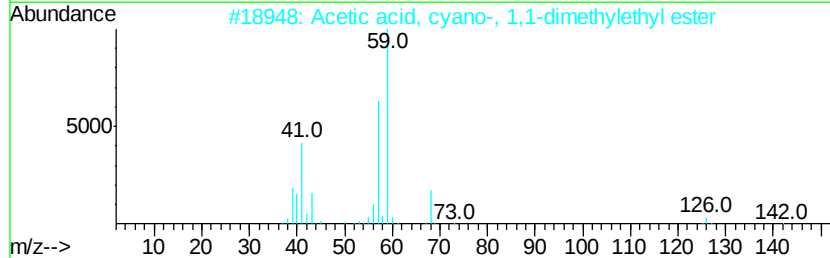
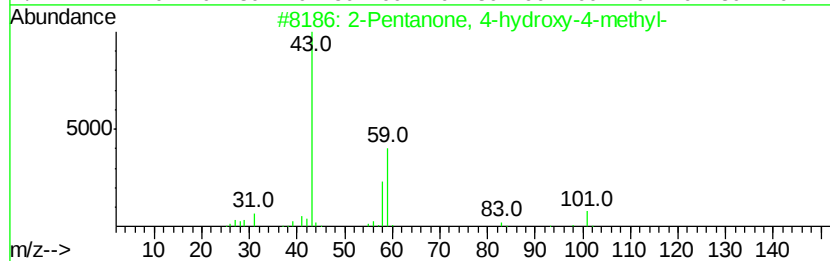
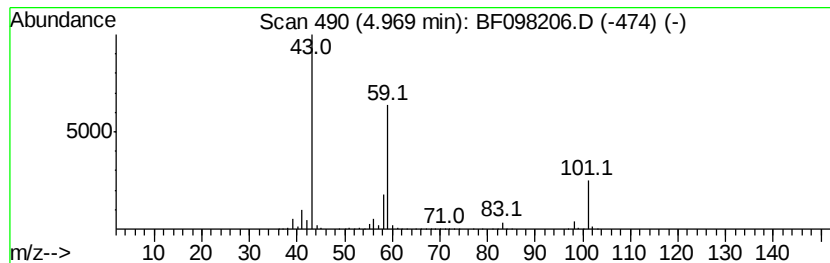
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	192.12 ng	8110630	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	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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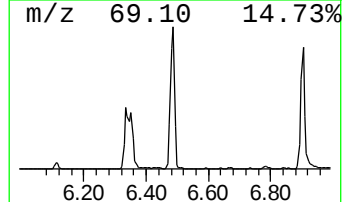
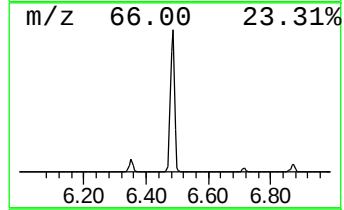
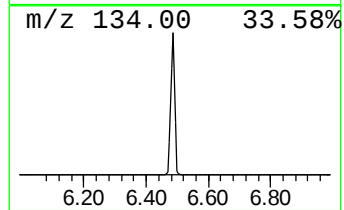
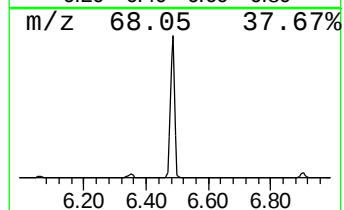
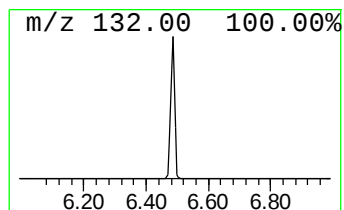
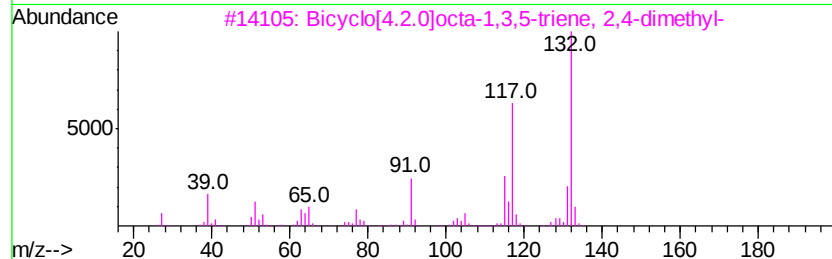
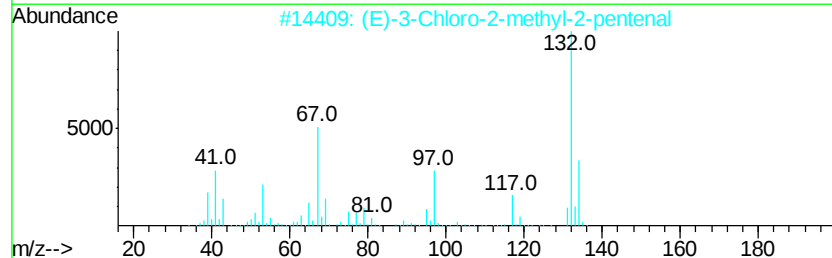
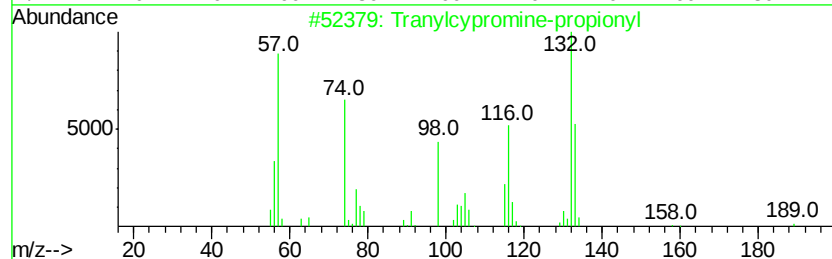
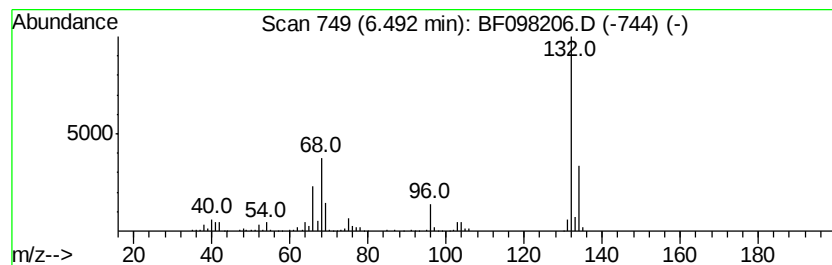
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	35.14 ng	1483410	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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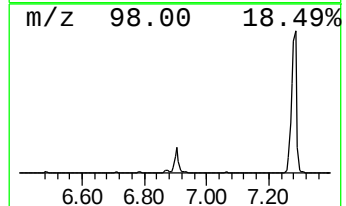
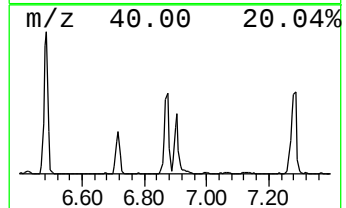
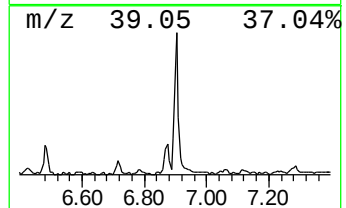
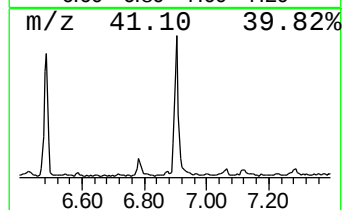
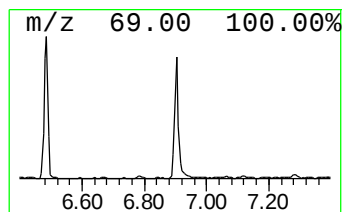
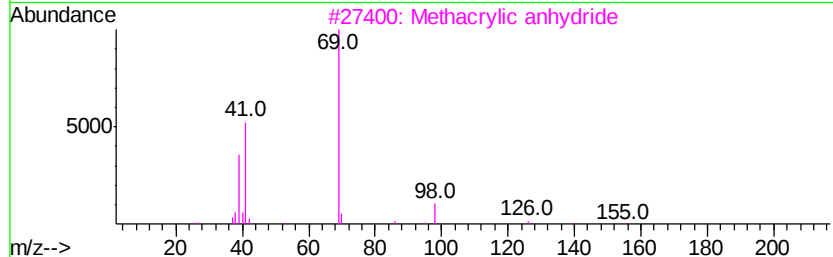
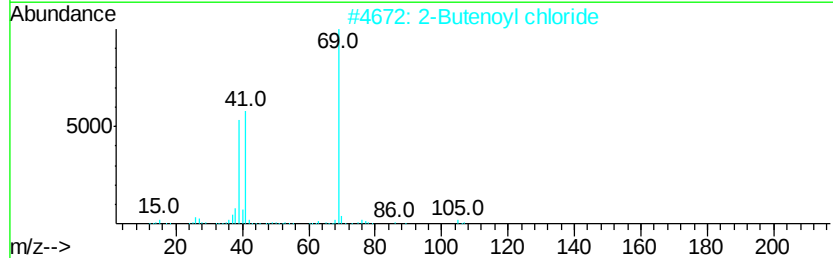
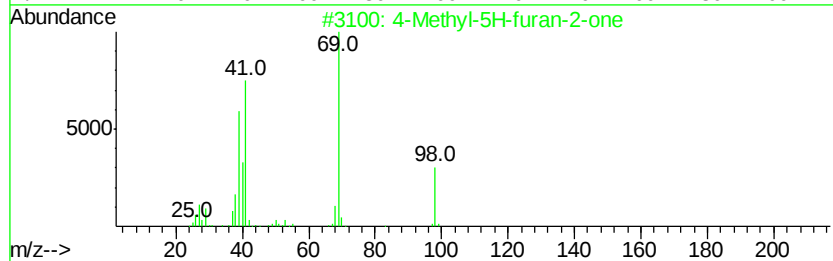
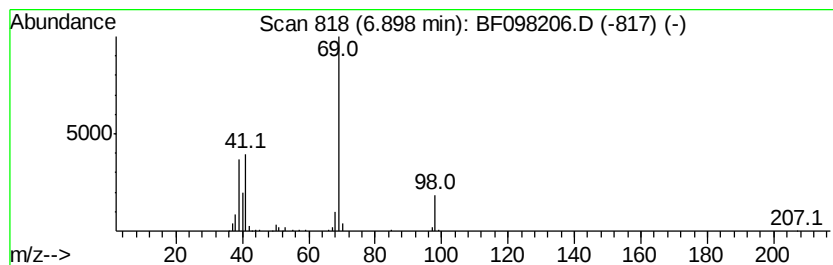
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Peak Number 4 4-Methyl-5H-furan-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	3.68 ng	155450	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-5H-furan-2-one	98	C5H6O2	006124-79-4	91
2		2-Butenoyl chloride	104	C4H5ClO	010487-71-5	59
3		Methacrylic anhydride	154	C8H10O3	000760-93-0	56
4		Isoxazole	69	C3H3NO	000288-14-2	53
5		2-Butenoic acid, ethyl ester, (Z)-	114	C6H10O2	006776-19-8	39



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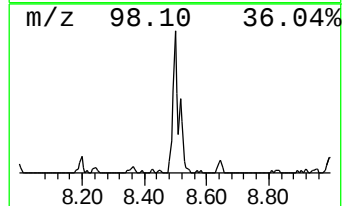
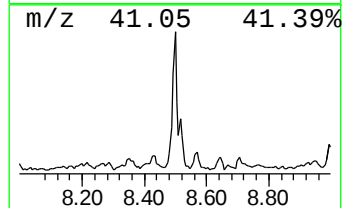
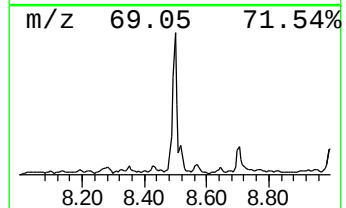
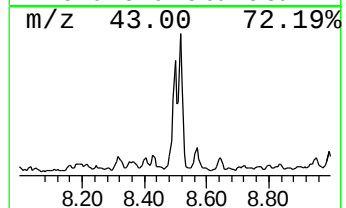
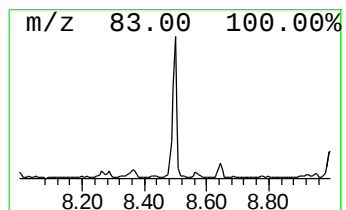
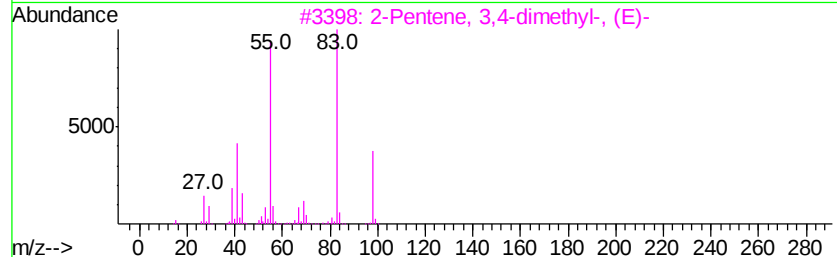
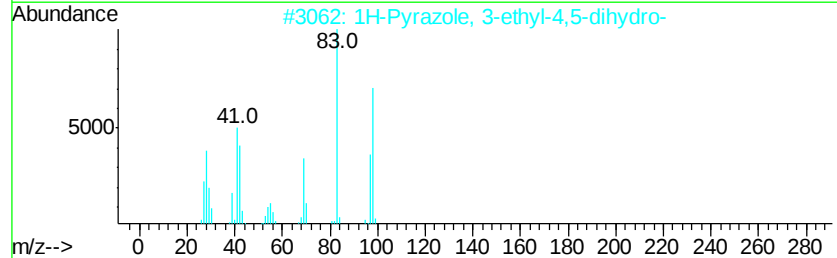
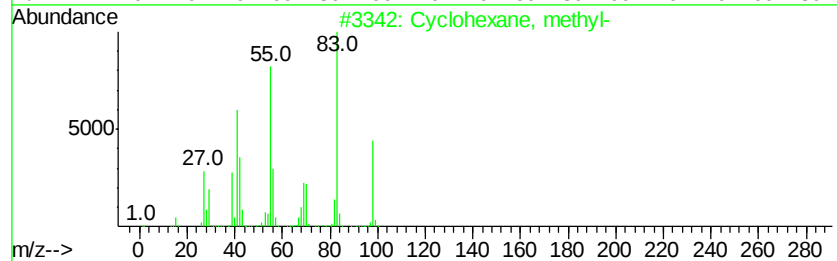
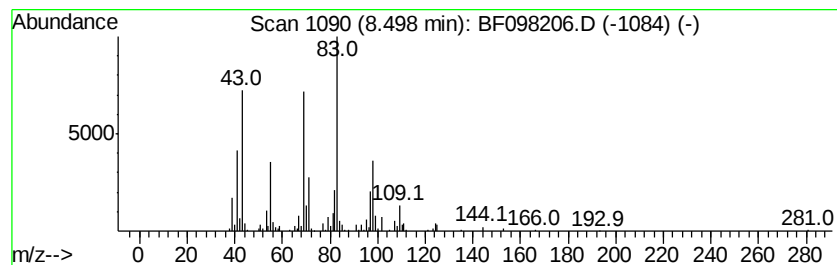
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Peak Number 5 unknown8.50 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.50	6.02 ng	345940	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, methyl-	98	C7H14	000108-87-2	47
2		1H-Pyrazole, 3-ethyl-4,5-dihydro-	98	C5H10N2	005920-29-6	47
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	43
4		3-Hexen-2-one	98	C6H10O	000763-93-9	43
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	38



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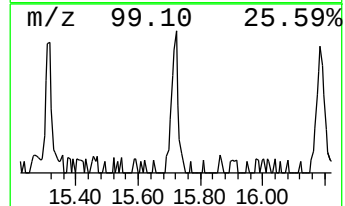
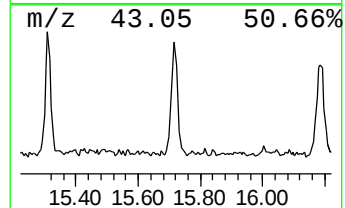
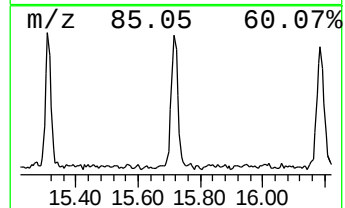
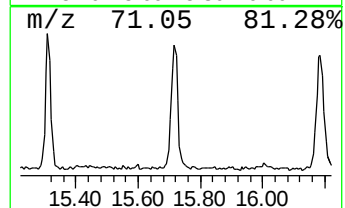
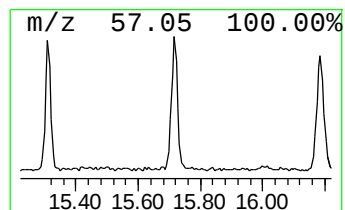
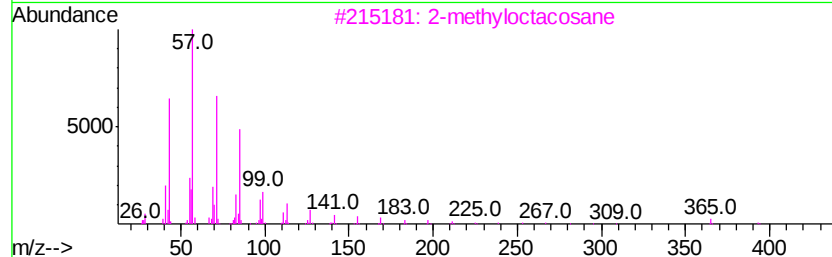
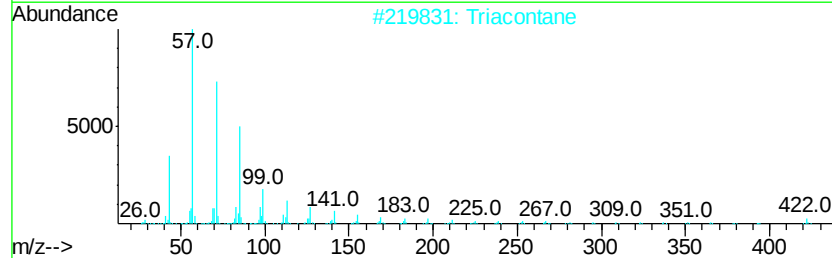
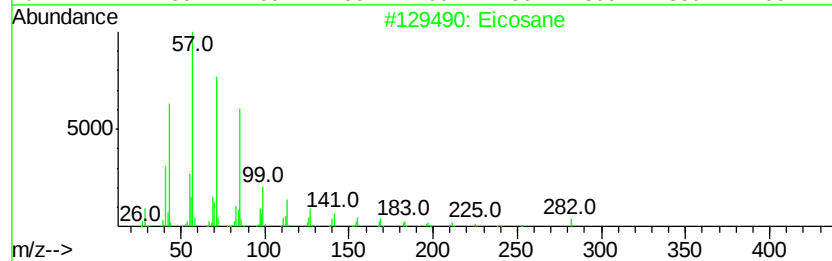
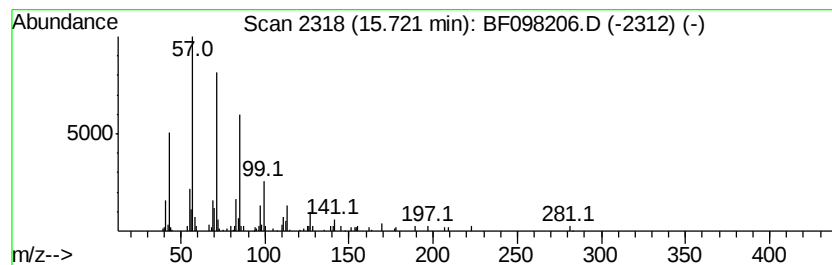
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Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.41 ng	138863	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Triacontane	422	C30H62	000638-68-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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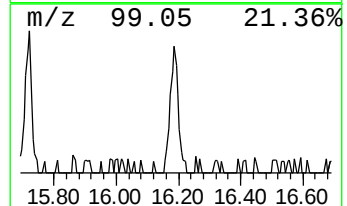
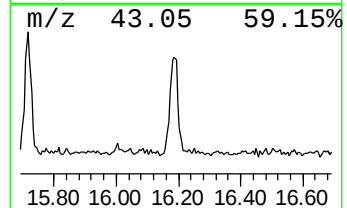
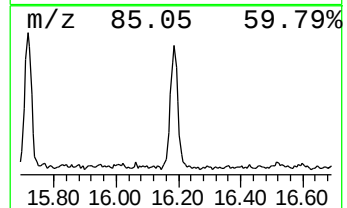
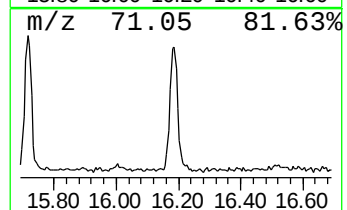
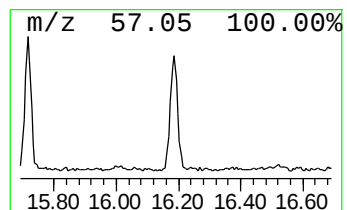
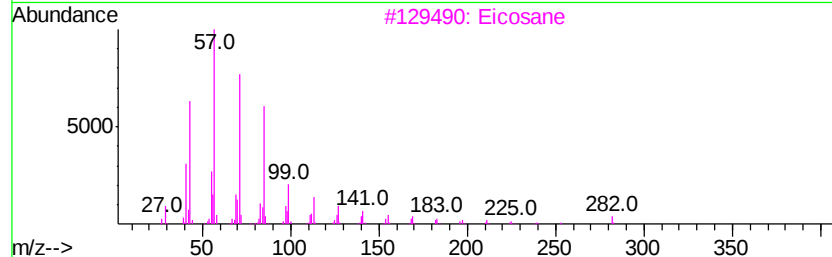
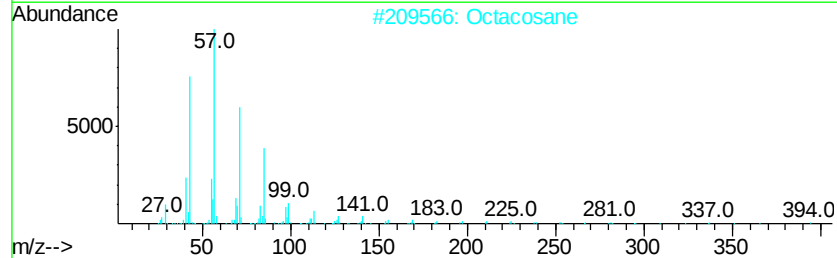
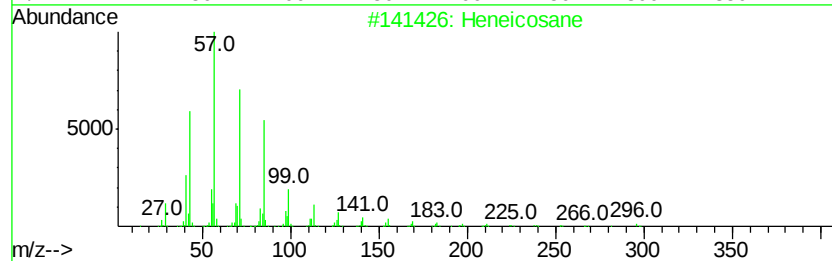
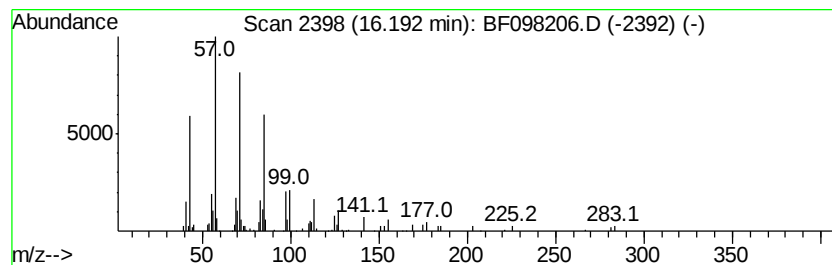
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	3.53 ng	143663	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Eicosane		282	C20H42	000112-95-8	91
4	triacontane		422	C30H62	000638-68-6	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083117\
 Data File : BF098206.D
 Acq On : 31 Aug 2017 20:40
 Operator : SJ/JU
 Sample : I4963-18
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

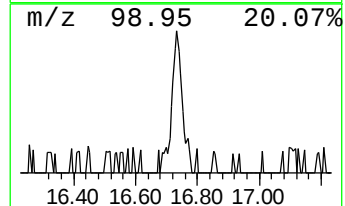
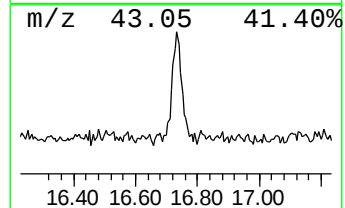
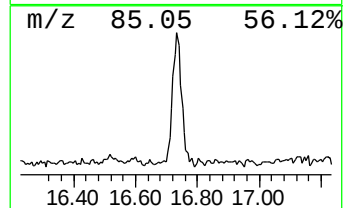
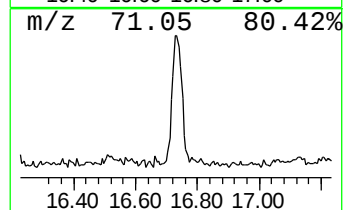
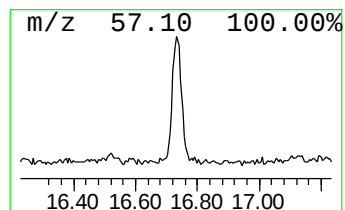
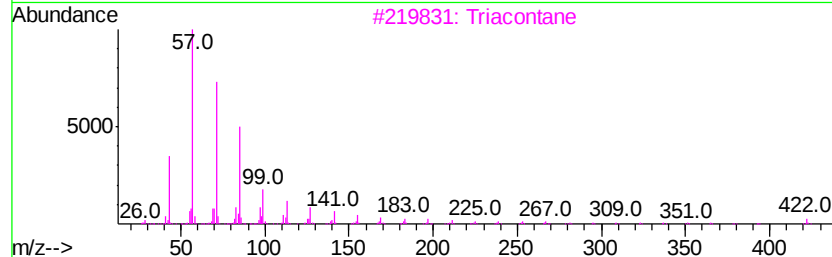
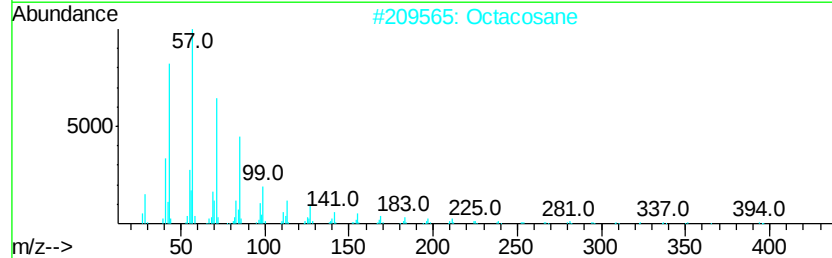
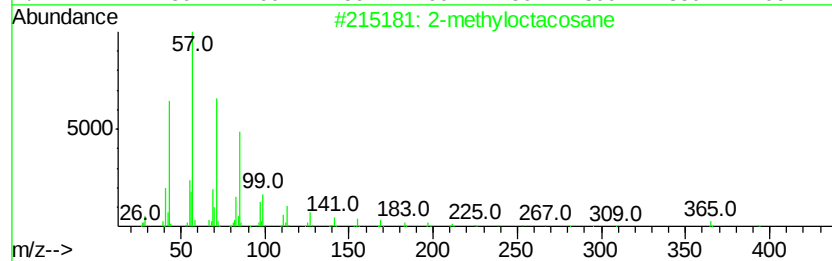
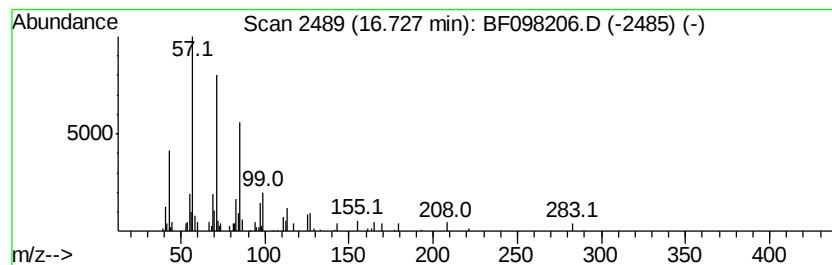
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.73	2.43 ng	98935	Perylene-d12		15.28	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	86
2	Octacosane		394	C28H58	000630-02-4	86
3	Triacontane		422	C30H62	000638-68-6	86
4	Hexatriacontane		507	C36H74	000630-06-8	83
5	Hentriacontane		437	C31H64	000630-04-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098206.D
Acq On : 31 Aug 2017 20:40
Operator : SJ/JU
Sample : I4963-18
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3837-DB

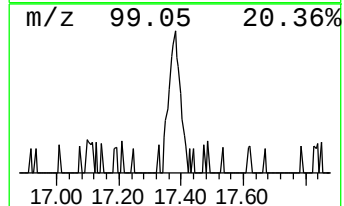
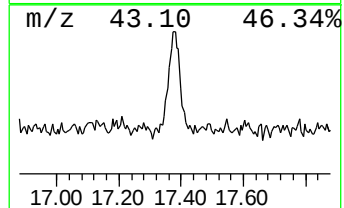
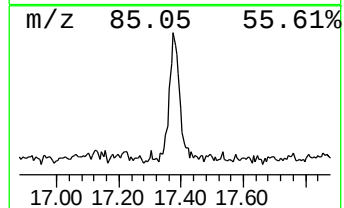
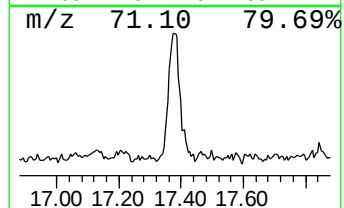
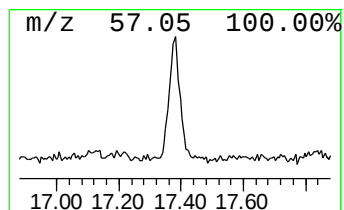
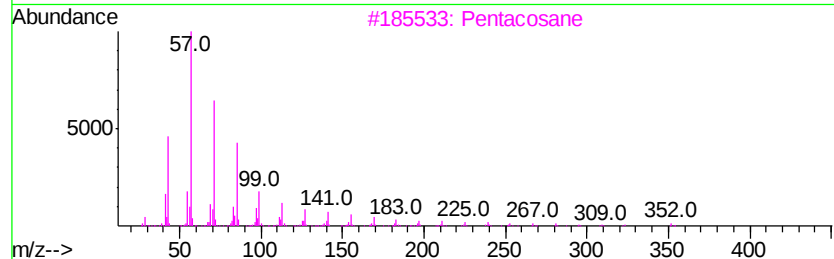
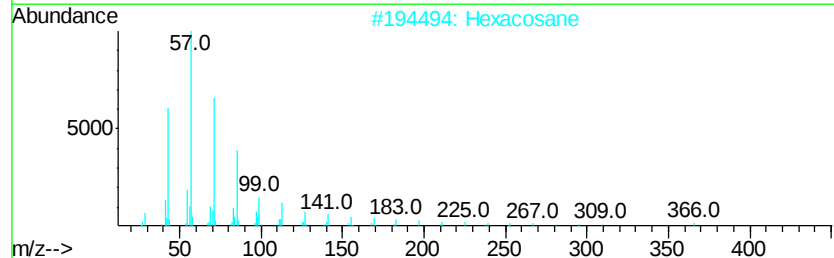
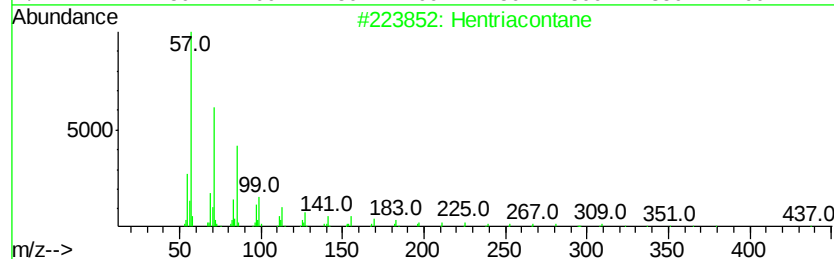
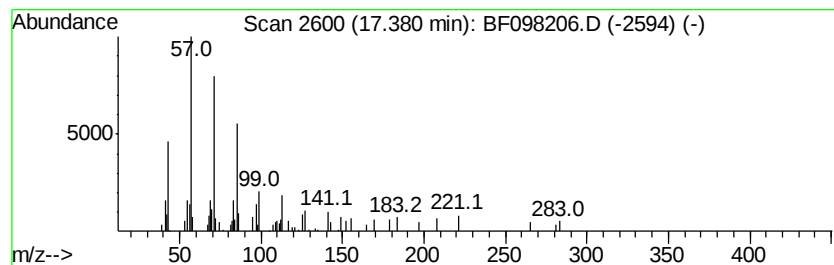
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	2.24 ng	91181	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	Hexacosane		366	C26H54	000630-01-3	87
3	Pentacosane		352	C25H52	000629-99-2	87
4	Octacosane		394	C28H58	000630-02-4	87
5	Tetratriacontane		479	C34H70	014167-59-0	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083117\
Data File : BF098206.D
Acq On : 31 Aug 2017 20:40
Operator : SJ/JU
Sample : I4963-18
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3837-DB

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
2-Pentanone, 4-hy...	4.97	192.1	ng	8110630	1	6.72	844339	20.0
unknown6.49	6.49	35.1	ng	1483410	1	6.72	844339	20.0
4-Methyl-5H-furan...	6.90	3.7	ng	155450	1	6.72	844339	20.0
unknown8.50	8.50	6.0	ng	345940	2	8.00	1148760	20.0
Eicosane	15.72	3.4	ng	138863	6	15.28	814194	20.0
Heneicosane	16.19	3.5	ng	143663	6	15.28	814194	20.0
2-methyloctacosane	16.73	2.4	ng	98935	6	15.28	814194	20.0
Hentriacontane	17.38	2.2	ng	91181	6	15.28	814194	20.0