

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
 Data File : BF109707.D
 Acq On : 9 Oct 2018 20:55
 Operator : JU/SJ
 Sample : J5329-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 POND-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-BF100818.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	4.898	475	478	488	rBV	43104	61638	3.25%	0.387%
2	5.316	546	549	576	rBV	1236377	1591673	84.03%	10.000%
3	6.345	720	724	741	rBV	1301398	1731505	91.42%	10.878%
4	6.469	741	745	768	rVB	1702349	1873711	98.92%	11.772%
5	6.698	780	784	794	rBV	335249	434885	22.96%	2.732%
6	6.851	806	810	836	rVB	1456685	1406536	74.26%	8.837%
7	7.257	876	879	914	rBV	749830	1159090	61.20%	7.282%
8	7.975	998	1001	1025	rBV	449741	566605	29.91%	3.560%
9	9.051	1180	1184	1209	rBV	1835140	1894091	100.00%	11.900%
10	9.445	1248	1251	1261	rBV	132220	128401	6.78%	0.807%
11	9.722	1294	1298	1319	rBV	546041	547747	28.92%	3.441%
12	10.510	1428	1432	1451	rBV	761928	925585	48.87%	5.815%
13	11.204	1546	1550	1568	rBV	355189	482242	25.46%	3.030%
14	11.739	1638	1641	1648	rBV2	16417	23618	1.25%	0.148%
15	12.780	1814	1818	1834	rBV	1501666	1457016	76.92%	9.154%
16	13.698	1969	1974	1985	rBV4	29220	81491	4.30%	0.512%
17	13.827	1992	1996	2009	rBV	516977	555596	29.33%	3.491%
18	13.998	2022	2025	2029	rVB	19403	19055	1.01%	0.120%
19	14.304	2073	2077	2081	rVB	35857	34903	1.84%	0.219%
20	14.598	2123	2127	2130	rBV	62506	65418	3.45%	0.411%
21	14.662	2135	2138	2141	rVB	26393	23817	1.26%	0.150%
22	14.904	2175	2179	2184	rBV	89056	100188	5.29%	0.629%
23	15.227	2229	2234	2237	rBV	317140	444780	23.48%	2.794%
24	15.651	2301	2306	2311	rBV	95428	139603	7.37%	0.877%
25	16.103	2378	2383	2392	rVB	60471	106070	5.60%	0.666%
26	16.633	2467	2473	2479	rBV2	27909	61941	3.27%	0.389%

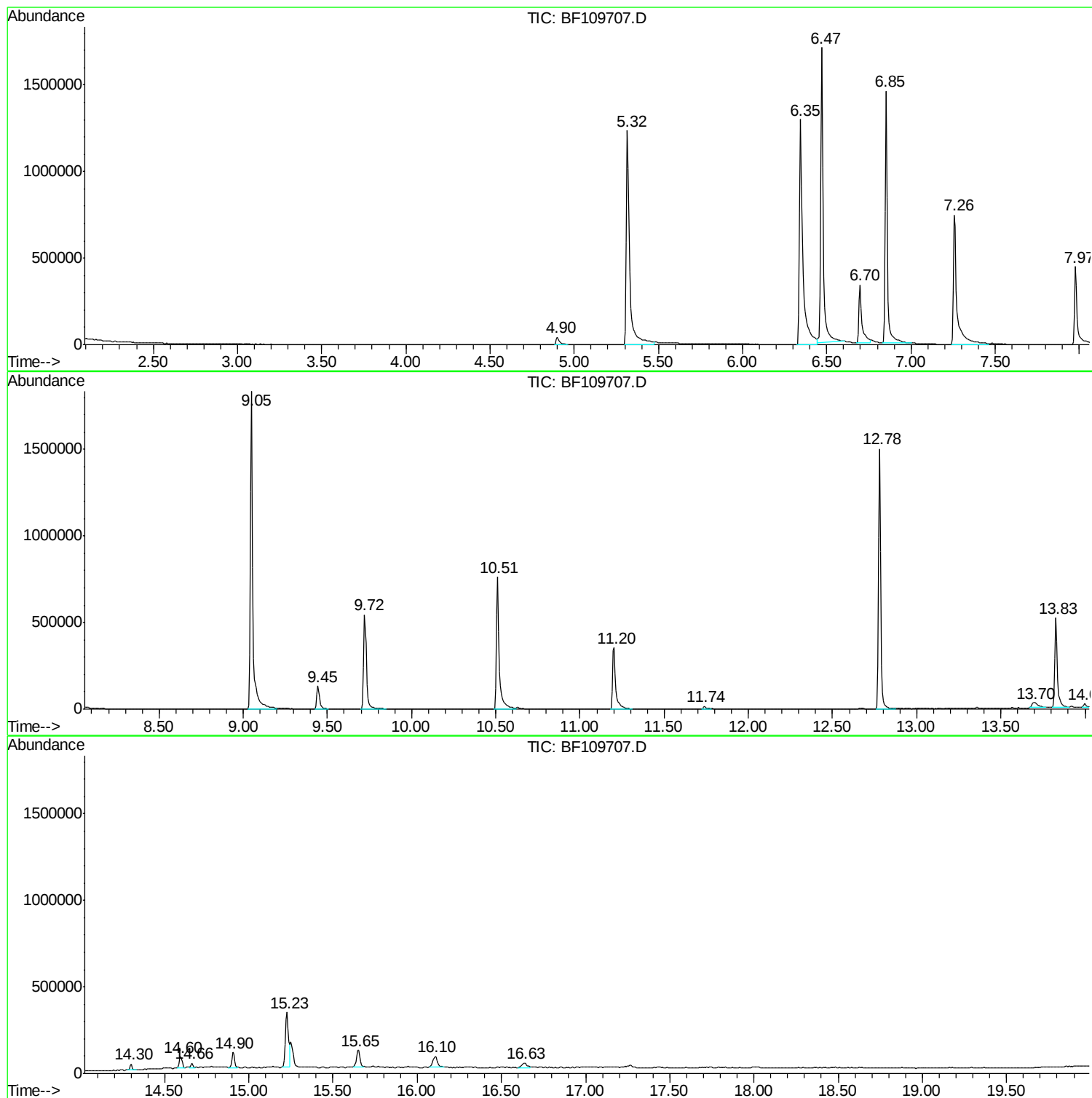
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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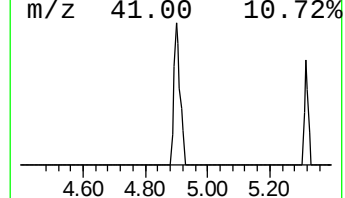
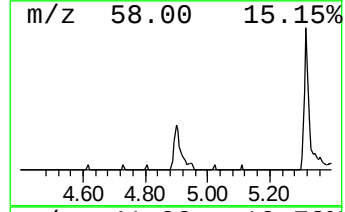
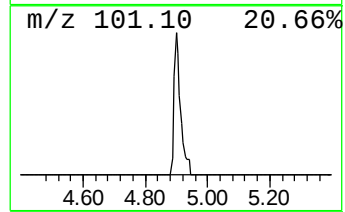
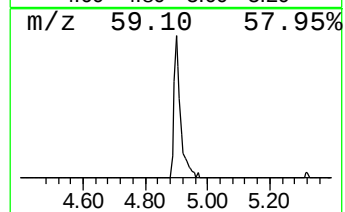
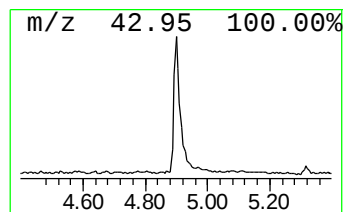
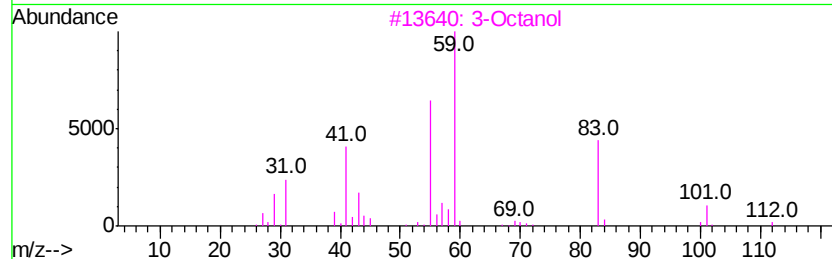
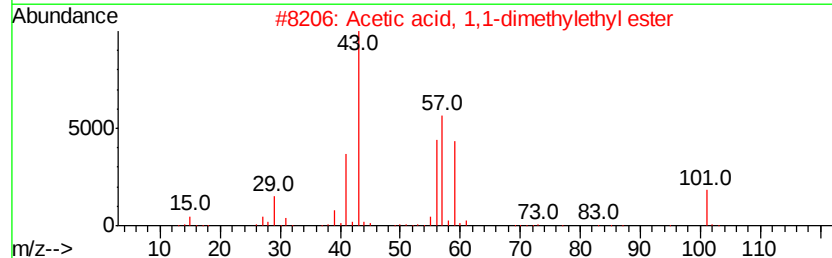
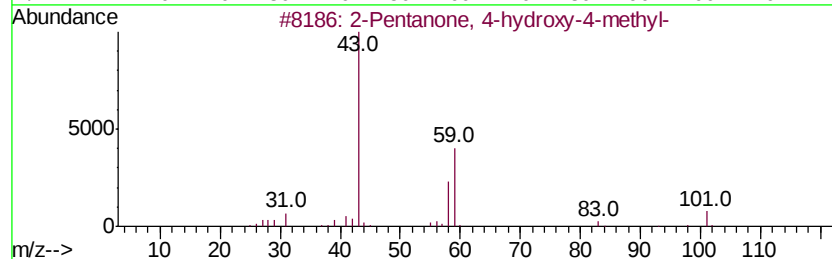
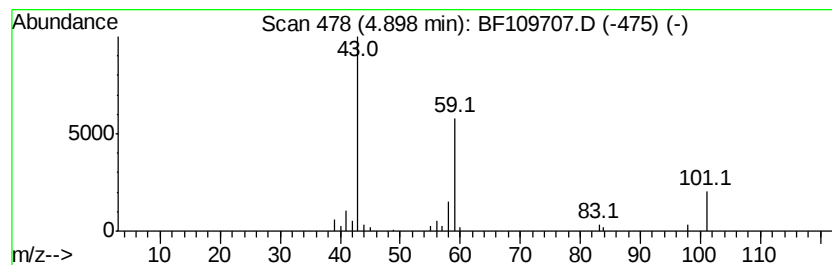
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.83 ng	61638	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	39
3			3-Octanol	130	C8H18O	000589-98-0	28
4			3-Pentanol	88	C5H12O	000584-02-1	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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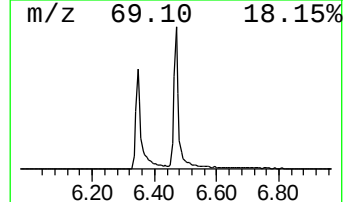
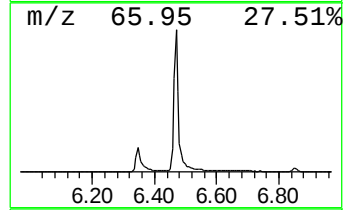
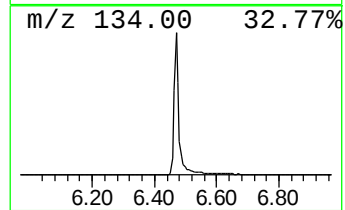
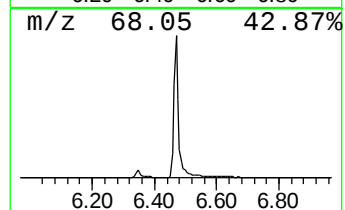
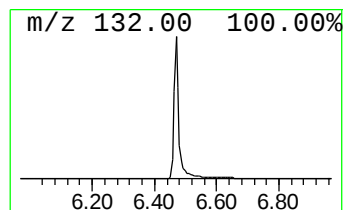
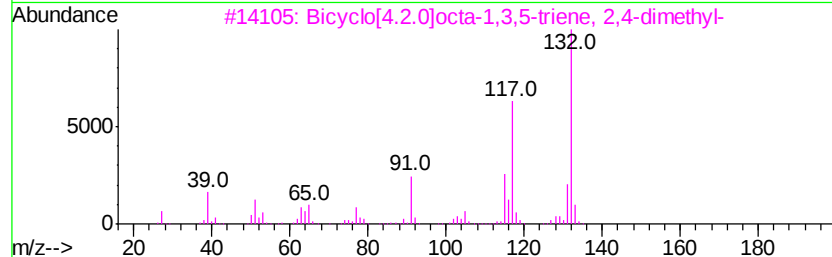
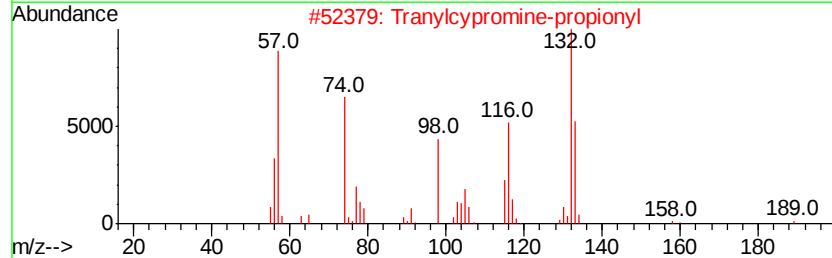
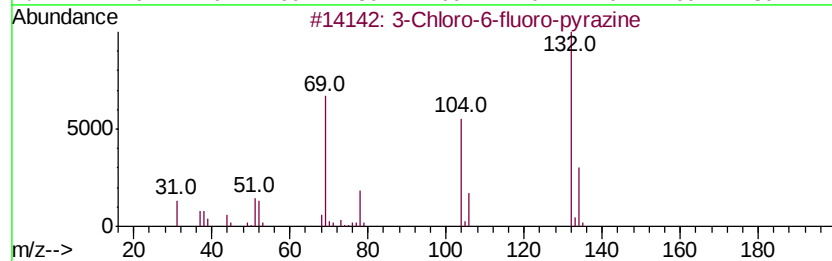
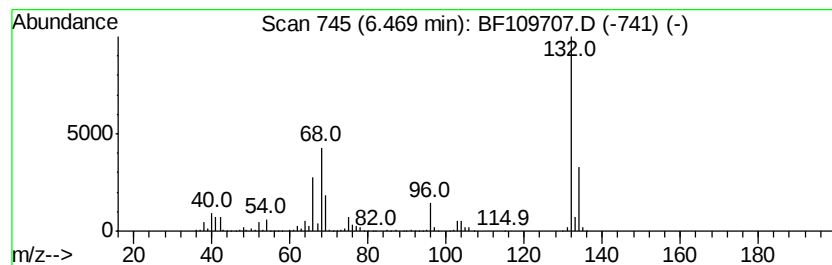
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	86.17 ng	1873710	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-			132	C10H12	005379-20-4	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...			132	C3H4N2S2	029490-19-5	9



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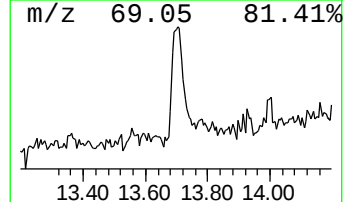
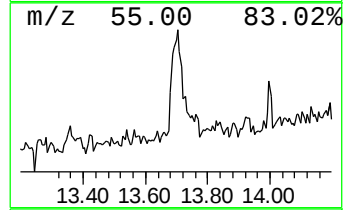
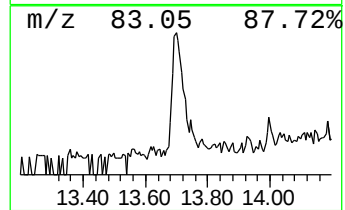
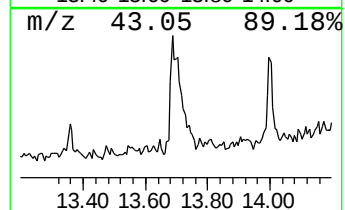
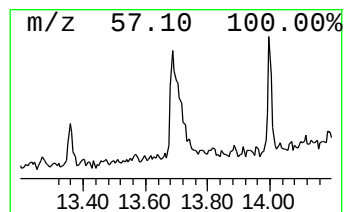
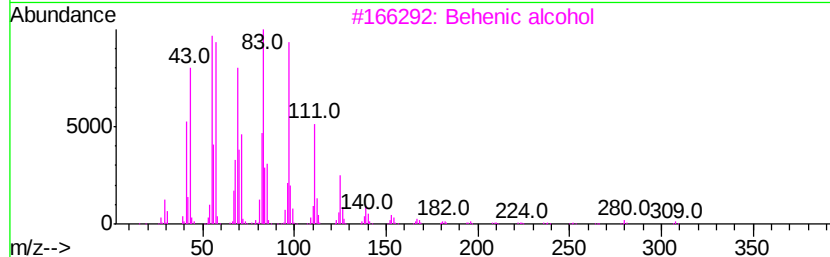
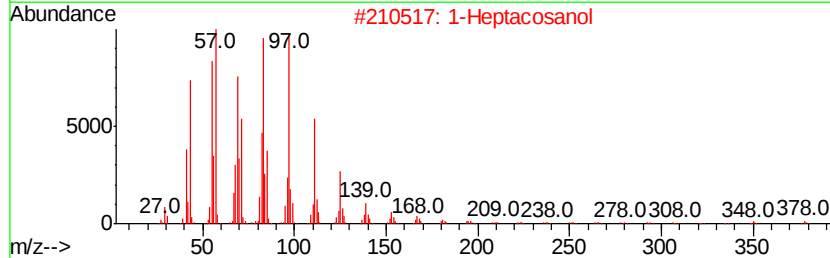
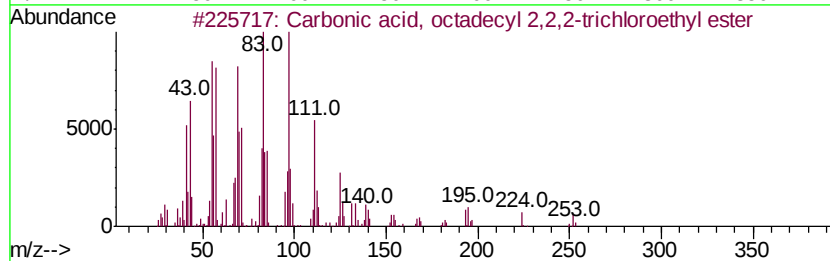
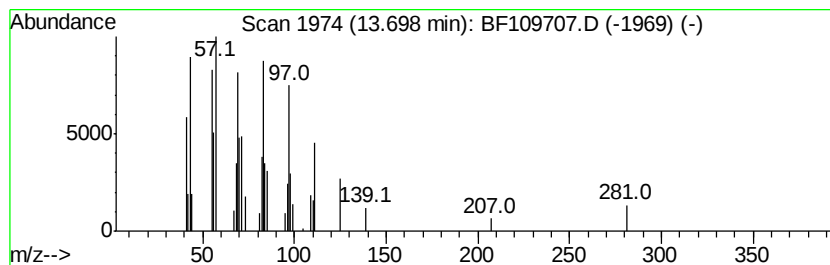
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Peak Number 4 Carbonic acid, octadecyl 2,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.93 ng	81491	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91



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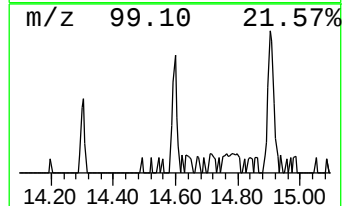
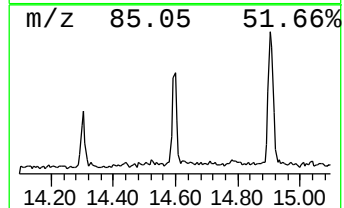
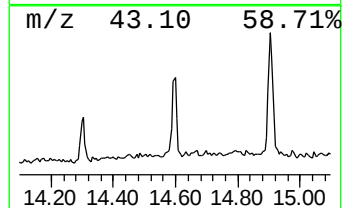
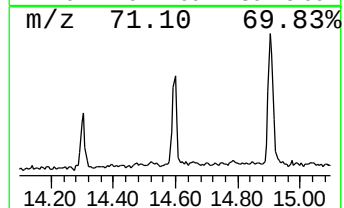
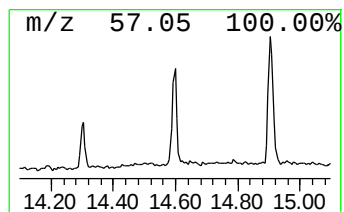
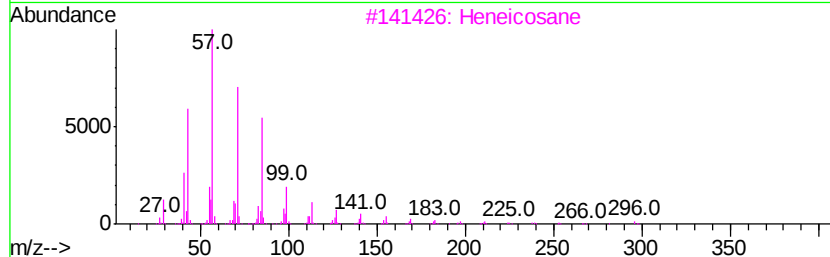
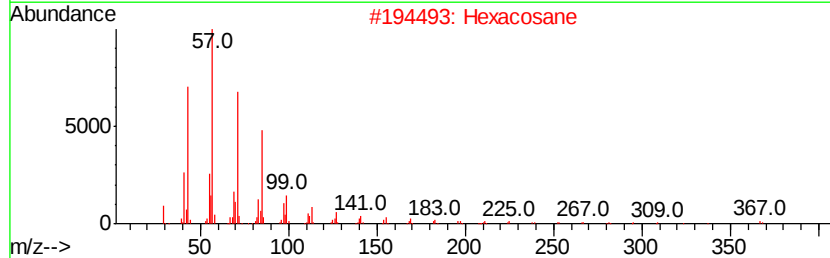
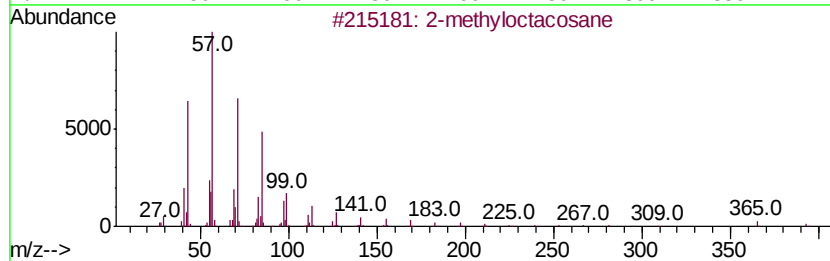
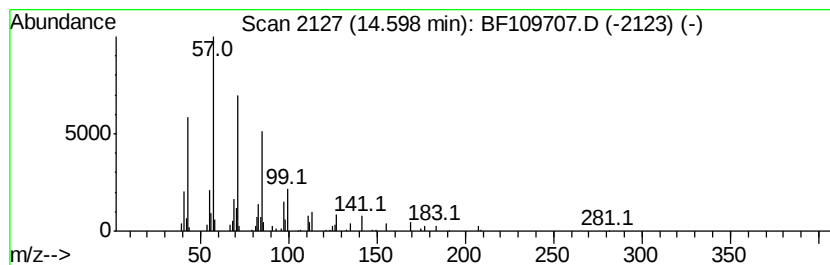
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Peak Number 5 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.60	2.94 ng	65418	Perylene-d12		15.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane			408	C29H60	1000376-72-8	91
2	Hexacosane			366	C26H54	000630-01-3	87
3	Heneicosane			296	C21H44	000629-94-7	87
4	Tetratetracontane			619	C44H90	007098-22-8	87
5	Hentriacontane			437	C31H64	000630-04-6	86



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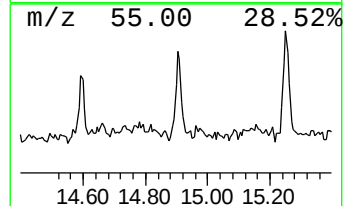
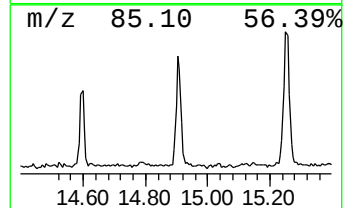
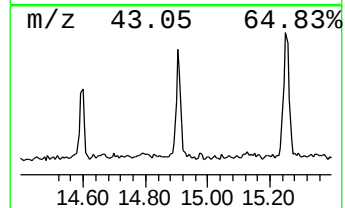
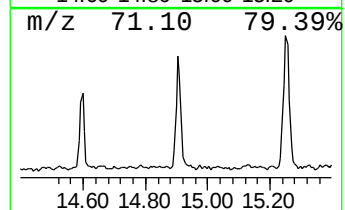
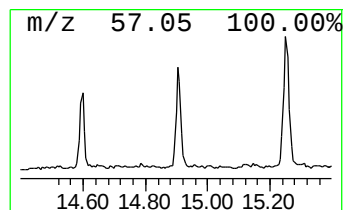
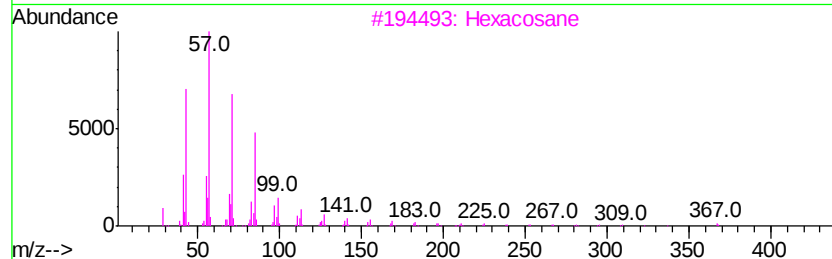
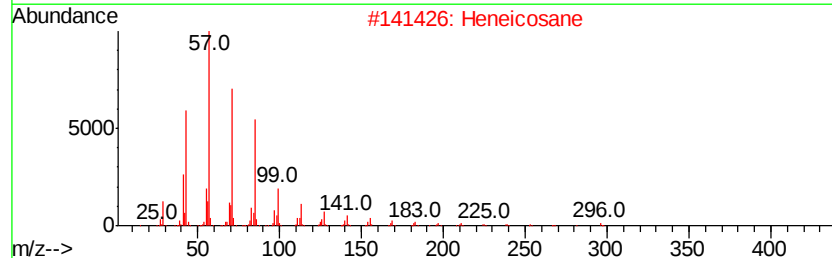
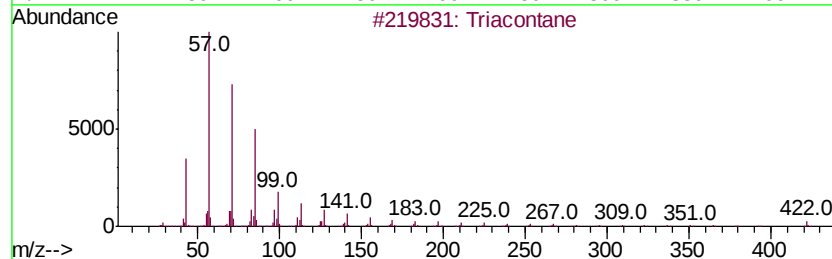
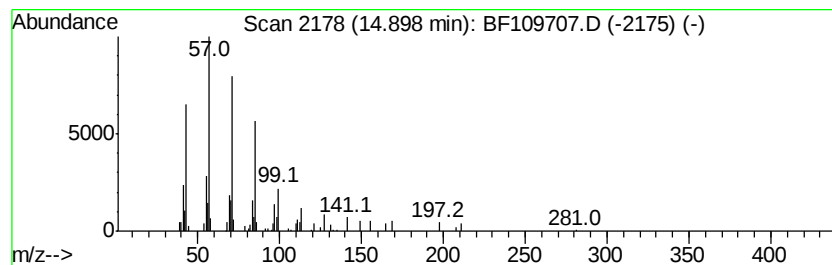
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	4.51 ng	100188	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90



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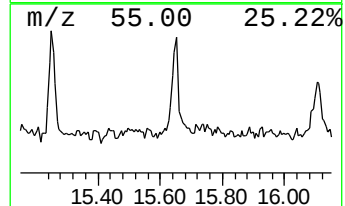
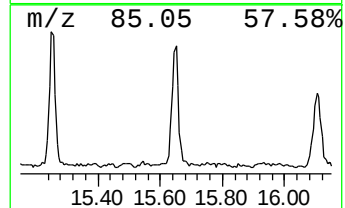
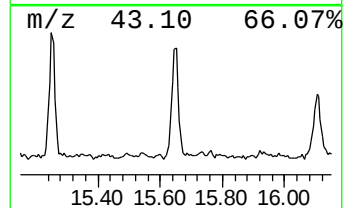
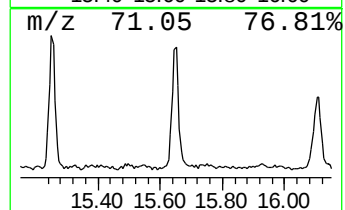
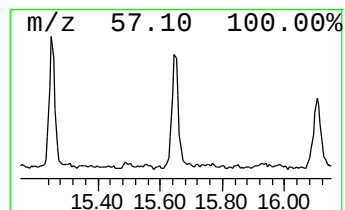
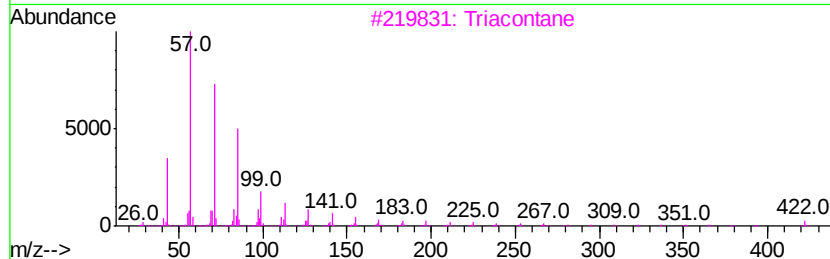
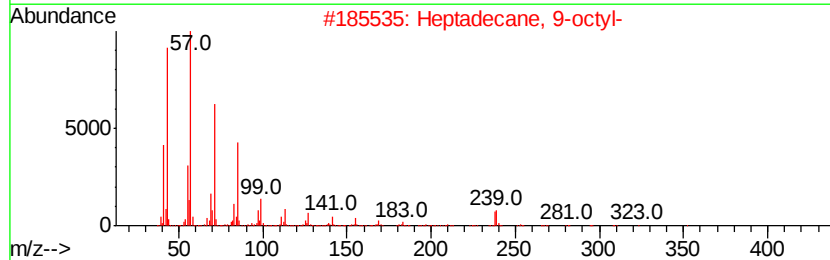
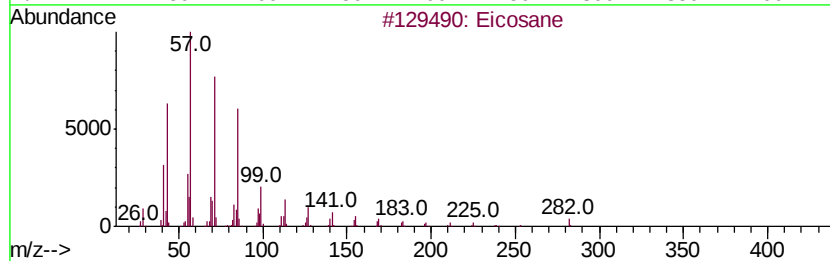
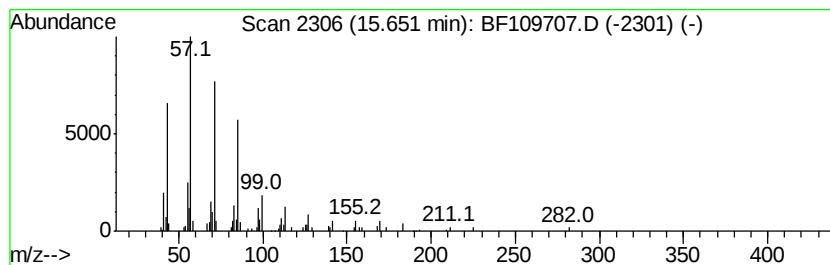
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	6.28 ng	139603	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Triacontane		422	C30H62	000638-68-6	91
4	Docosane		310	C22H46	000629-97-0	91
5	Octacosane		394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109707.D
Acq On : 9 Oct 2018 20:55
Operator : JU/SJ
Sample : J5329-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POND-1

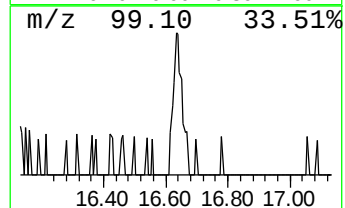
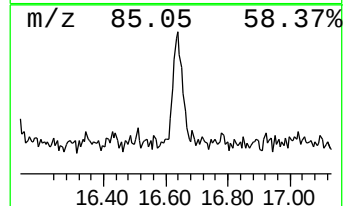
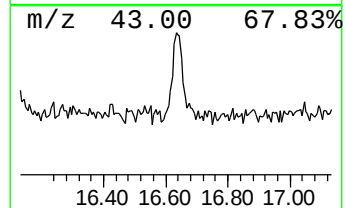
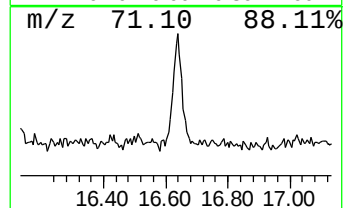
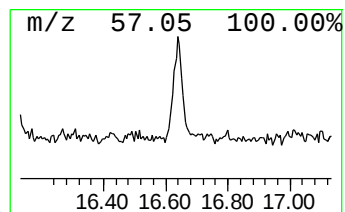
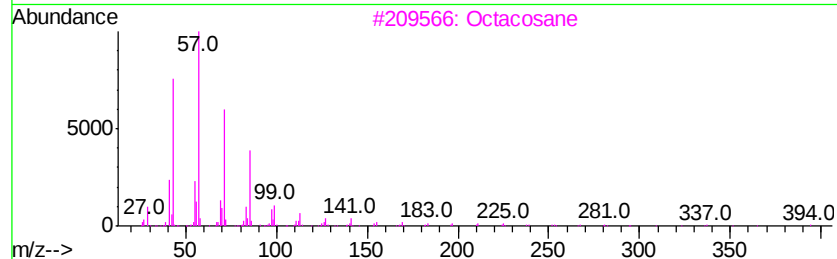
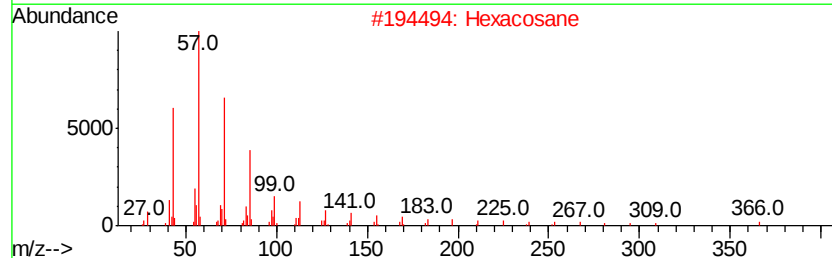
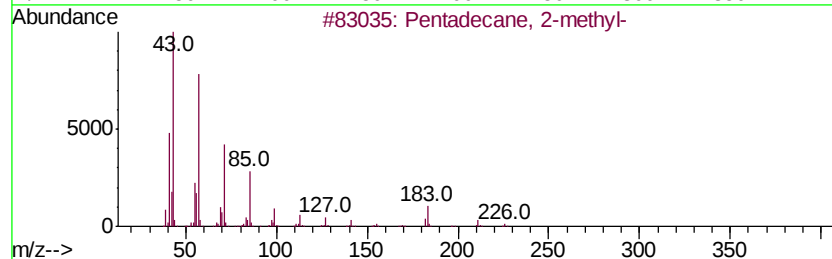
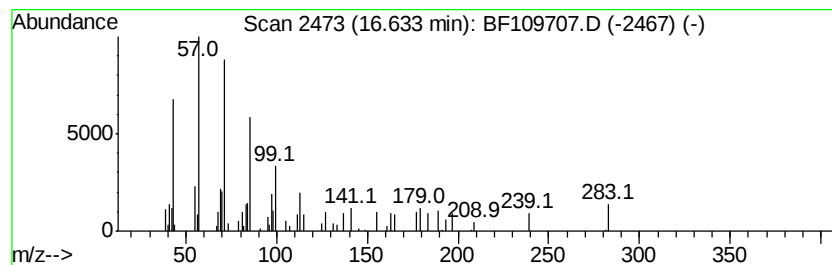
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.79 ng	61941	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	59
2		Hexacosane	366	C26H54	000630-01-3	59
3		Octacosane	394	C28H58	000630-02-4	59
4		Eicosane	282	C20H42	000112-95-8	58
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100918\
Data File : BF109707.D
Acq On : 9 Oct 2018 20:55
Operator : JU/SJ
Sample : J5329-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POND-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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...	4.90	2.8	ng	61638	1	6.70	434885	20.0
unknown6.47	6.47	86.2	ng	1873710	1	6.70	434885	20.0
Carbonic acid, oc...	13.70	2.9	ng	81491	5	13.83	555596	20.0
2-methyloctacosane	14.60	2.9	ng	65418	6	15.23	444780	20.0
Triacontane	14.90	4.5	ng	100188	6	15.23	444780	20.0
Eicosane	15.65	6.3	ng	139603	6	15.23	444780	20.0
Pentadecane, 2-me...	16.63	2.8	ng	61941	6	15.23	444780	20.0