

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
 Data File : BF109987.D
 Acq On : 19 Oct 2018 4:12
 Operator : JU/SJ
 Sample : J5579-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 7-1-ROLLOFFS

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-BF101518.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	16	rVB	320589	470624	12.89%	1.424%
2	2.328	35	41	47	rVB	525339	694738	19.03%	2.103%
3	3.610	257	259	267	rBV2	18278	41167	1.13%	0.125%
4	5.216	529	532	540	rVB	117170	140531	3.85%	0.425%
5	5.598	592	597	601	rBV	3312032	3363347	92.14%	10.180%
6	6.598	761	767	776	rBV2	3424159	3650228	100.00%	11.048%
7	6.745	787	792	795	rBV	3772944	3383136	92.68%	10.240%
8	6.975	828	831	835	rBV	1291364	1088015	29.81%	3.293%
9	7.134	854	858	861	rBV	3029566	2445739	67.00%	7.402%
10	7.540	922	927	930	rBV	2264272	1980749	54.26%	5.995%
11	8.263	1046	1050	1053	rBV	1362449	1268318	34.75%	3.839%
12	9.334	1227	1232	1235	rBV	3539271	2901527	79.49%	8.782%
13	9.675	1286	1290	1292	rBV	46793	46870	1.28%	0.142%
14	9.722	1295	1298	1306	rVB	439491	384193	10.53%	1.163%
15	9.881	1322	1325	1328	rVB2	64807	55314	1.52%	0.167%
16	10.022	1345	1349	1352	rBV	1292326	1178534	32.29%	3.567%
17	10.051	1352	1354	1357	rVB	85619	63892	1.75%	0.193%
18	10.428	1413	1418	1423	rBV6	34734	59416	1.63%	0.180%
19	10.569	1439	1442	1448	rVB3	33035	42301	1.16%	0.128%
20	10.810	1479	1483	1486	rBV	1894501	1638469	44.89%	4.959%
21	10.916	1497	1501	1506	rBV2	149929	173193	4.74%	0.524%
22	11.363	1574	1577	1579	rBV2	45344	52585	1.44%	0.159%
23	11.386	1579	1581	1584	rVB	53443	47224	1.29%	0.143%
24	11.510	1598	1602	1605	rBV	1311985	1147278	31.43%	3.472%
25	11.533	1605	1606	1611	rVB	215689	139175	3.81%	0.421%
26	11.586	1612	1615	1617	rVB	48139	41918	1.15%	0.127%
27	12.016	1685	1688	1690	rBV2	121735	107144	2.94%	0.324%
28	12.039	1690	1692	1698	rVB2	59088	50302	1.38%	0.152%
29	12.127	1704	1707	1709	rBV2	66506	70570	1.93%	0.214%
30	12.727	1806	1809	1812	rBV	278020	244154	6.69%	0.739%
31	12.763	1812	1815	1818	rVB	168746	142878	3.91%	0.432%
32	12.822	1823	1825	1828	rVV2	42544	44991	1.23%	0.136%
33	12.957	1845	1848	1854	rVB	287271	258797	7.09%	0.783%
34	13.069	1865	1867	1868	rBV	56495	44054	1.21%	0.133%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.098	1868	1872	1875	rVB	2540573	2297017	62.93%	6.952%
36	13.974	2019	2021	2026	rVB2	256947	247270	6.77%	0.748%
37	14.121	2043	2046	2048	rBV	163070	157598	4.32%	0.477%
38	14.157	2048	2052	2055	rBV	1137475	1071213	29.35%	3.242%
39	14.927	2181	2183	2187	rVB	162000	140571	3.85%	0.425%
40	15.286	2241	2244	2248	rVB	245604	268937	7.37%	0.814%
41	15.686	2308	2312	2322	rVB	790191	1083724	29.69%	3.280%
42	16.157	2389	2392	2397	rVB	235497	311806	8.54%	0.944%

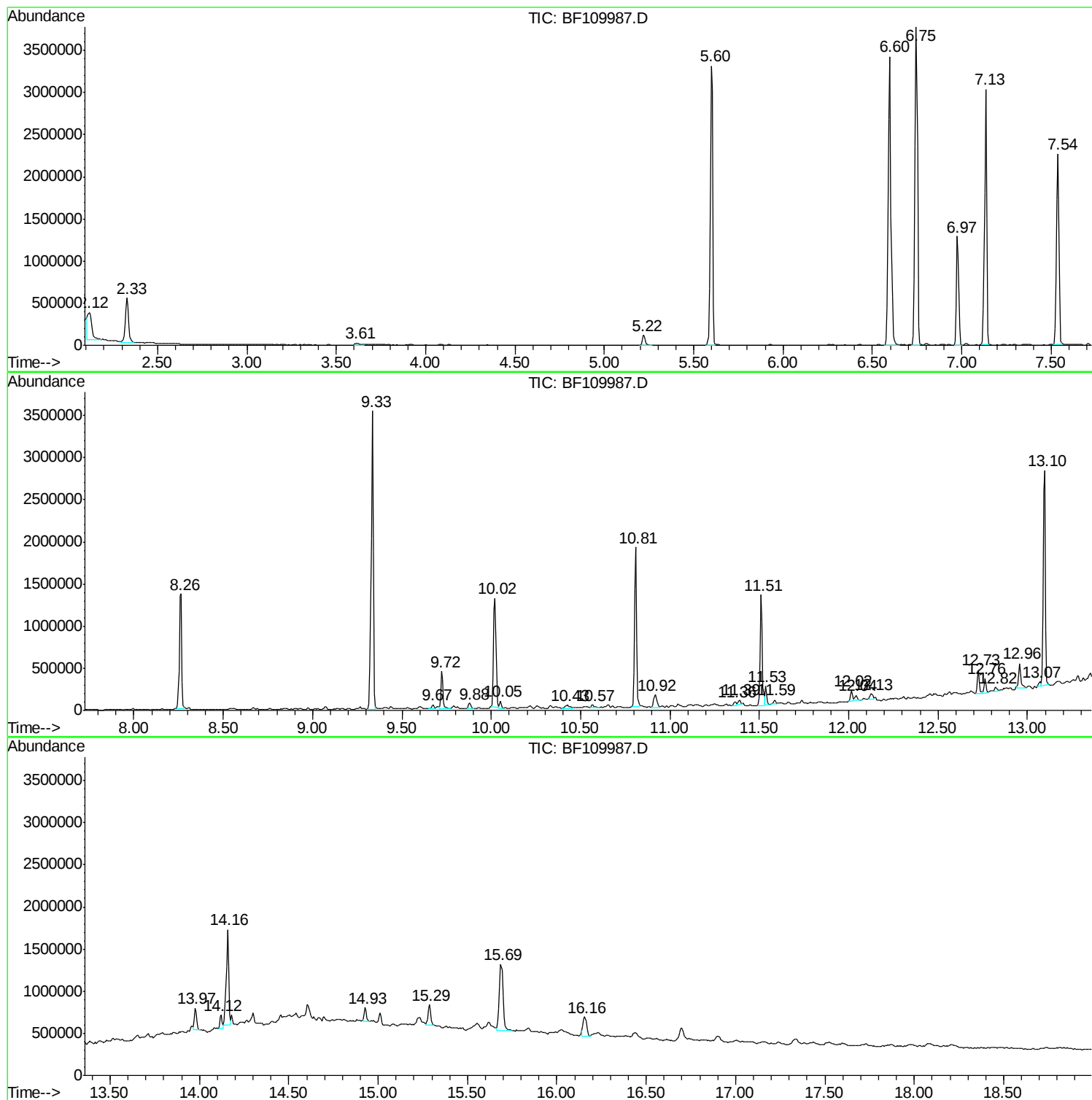
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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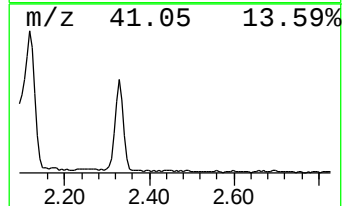
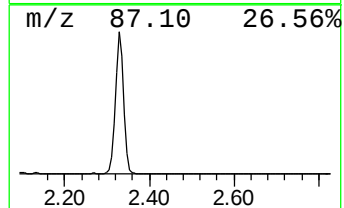
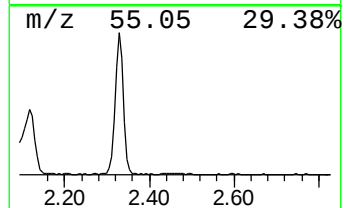
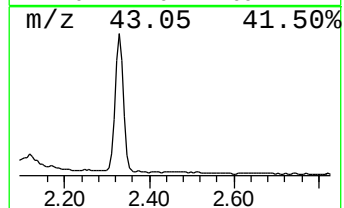
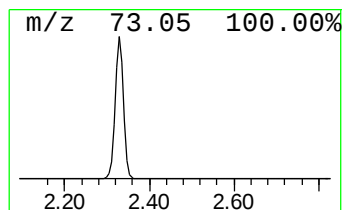
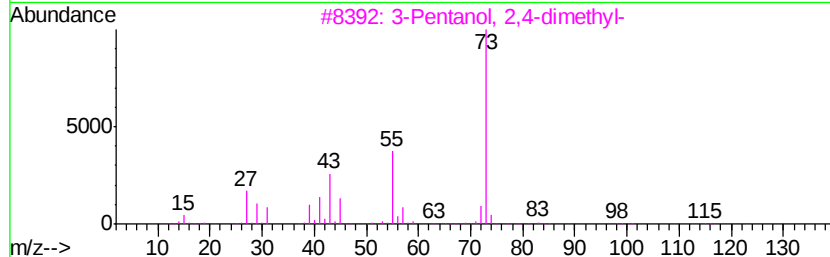
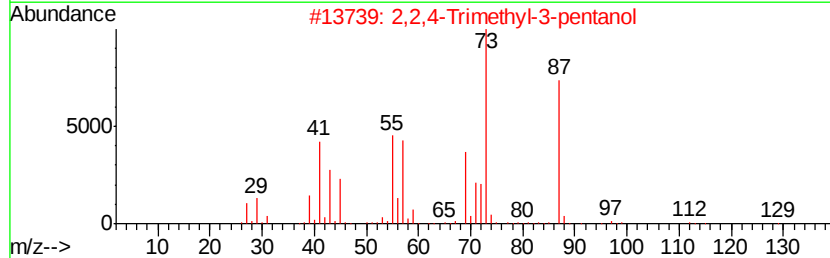
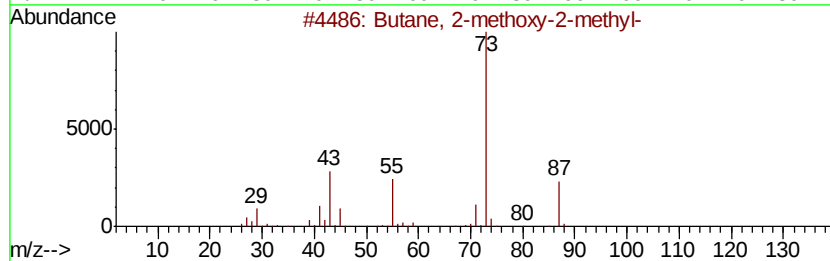
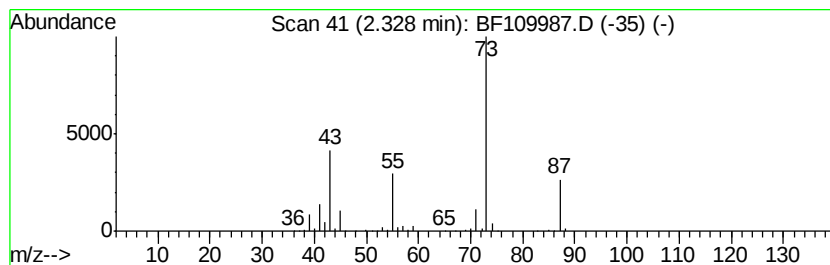
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	12.77 ng	694738	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	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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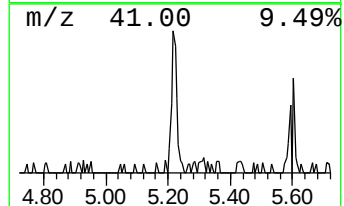
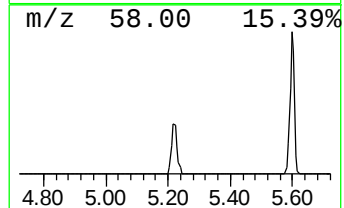
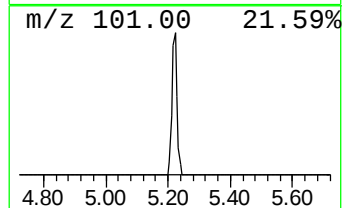
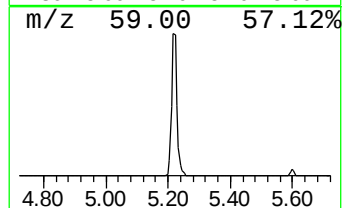
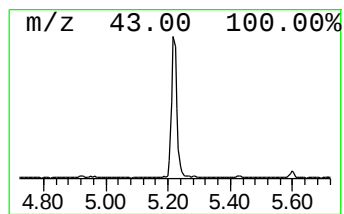
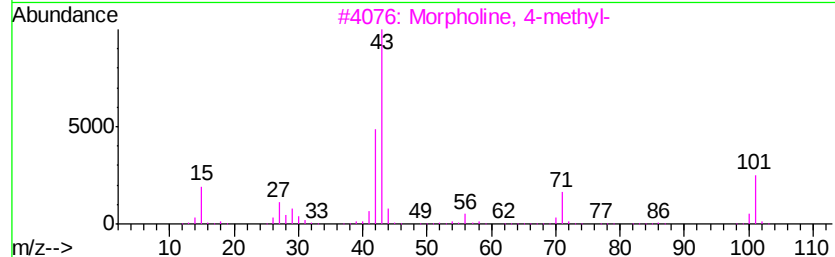
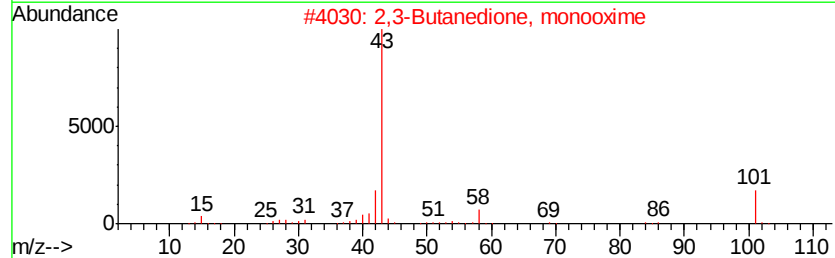
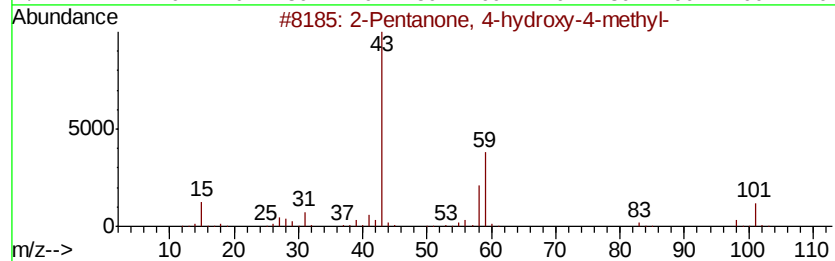
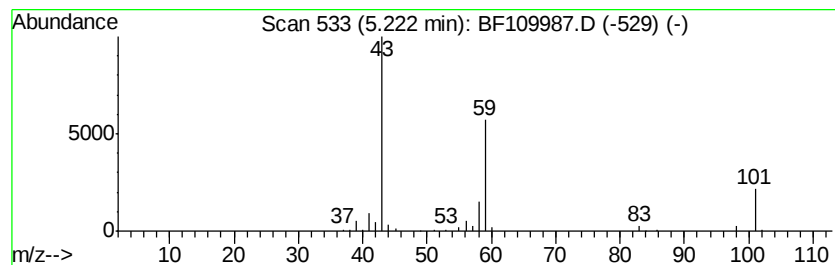
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.58 ng	140531	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	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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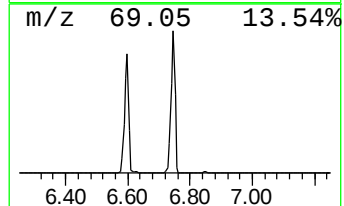
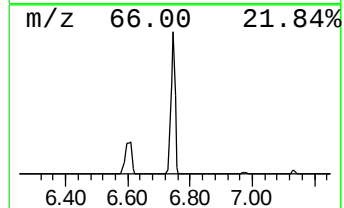
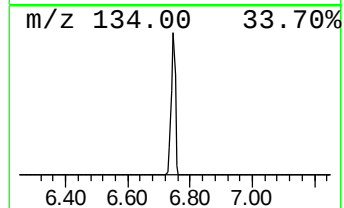
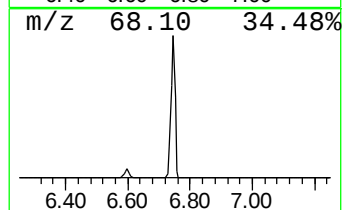
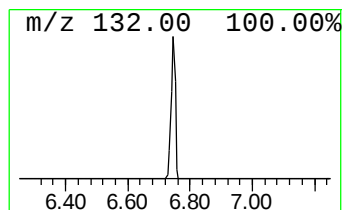
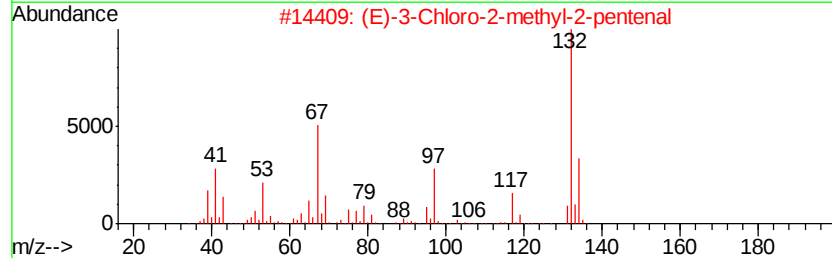
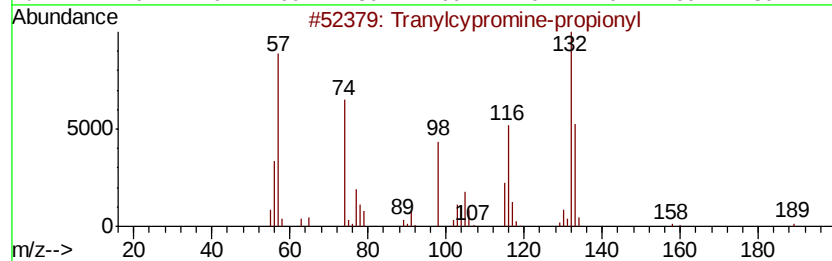
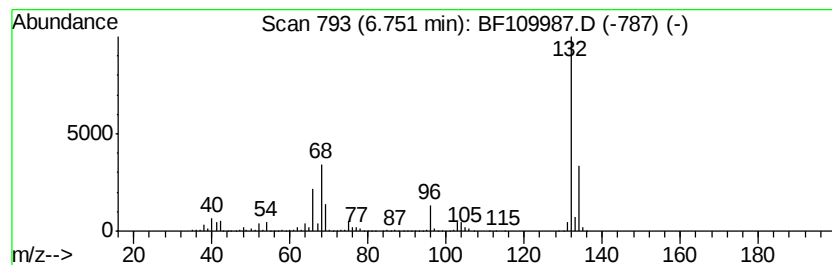
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	62.19 ng	3383140	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicvclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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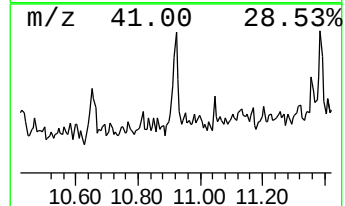
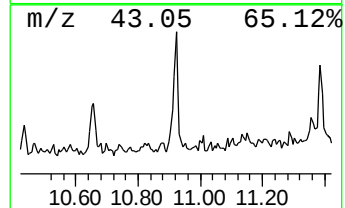
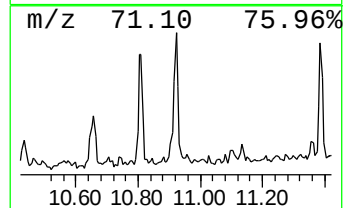
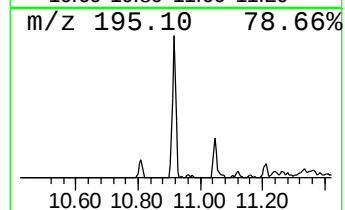
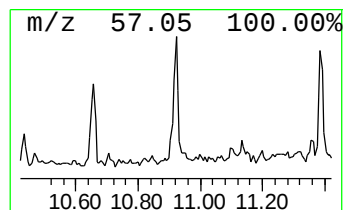
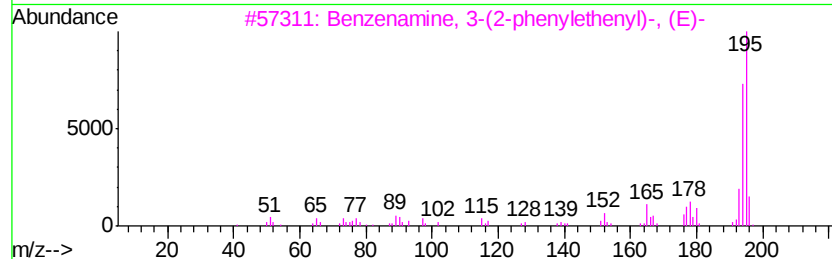
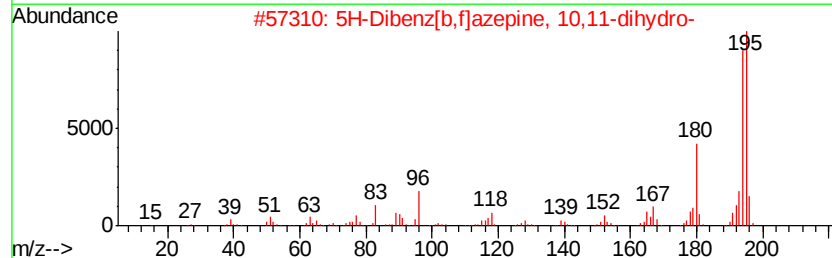
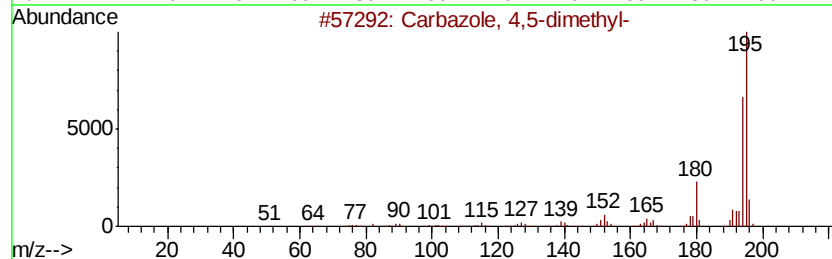
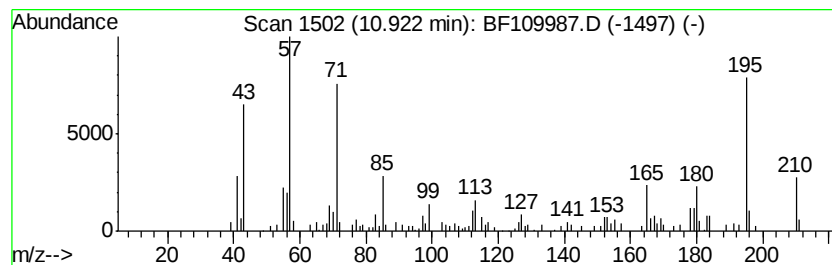
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Carbazole, 4,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.92	3.02 ng	173193	Phenanthrene-d10	11.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbazole, 4,5-dimethyl-	195	C14H13N	018992-66-0	62
2	5H-Dibenz[b,f]azepine, 10,11-dih...	195	C14H13N	000494-19-9	53
3	Benzenamine, 3-(2-phenylethenyl)...	195	C14H13N	014064-82-5	49
4	Carbazole, 3,5-dimethyl-	195	C14H13N	078787-81-2	49
5	Naphthalene, 1,2,3-trimethyl-4-p...	210	C16H18	026137-53-1	46



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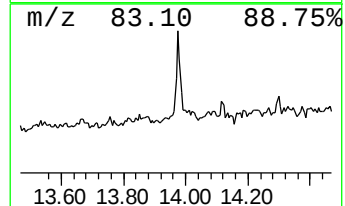
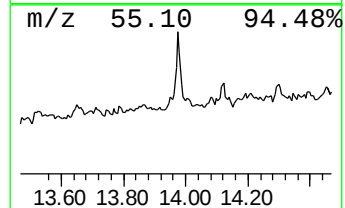
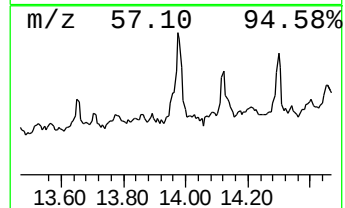
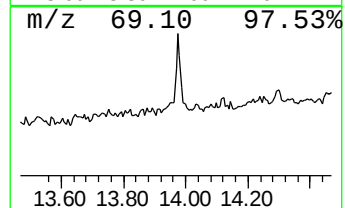
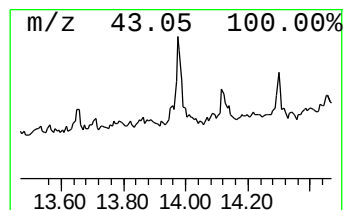
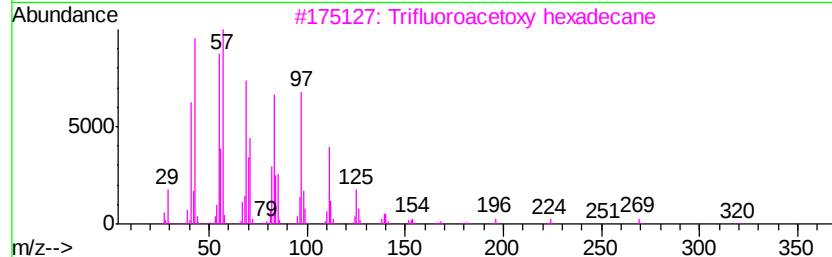
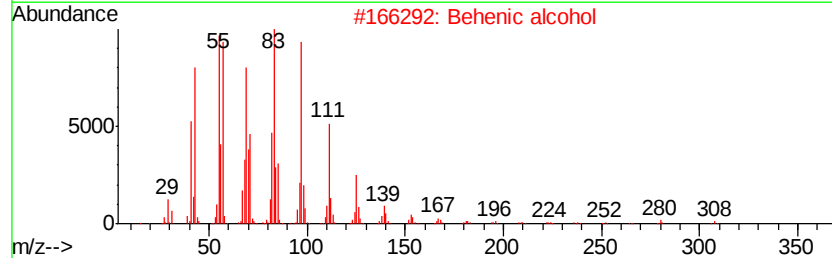
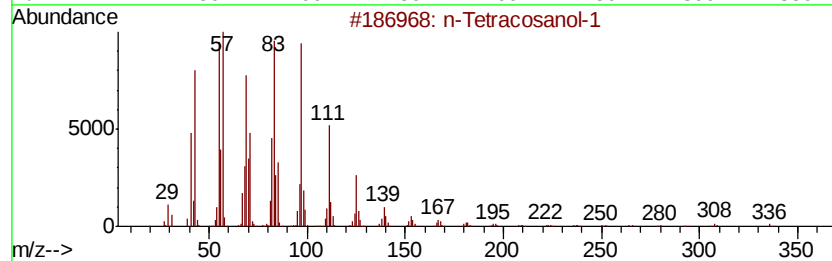
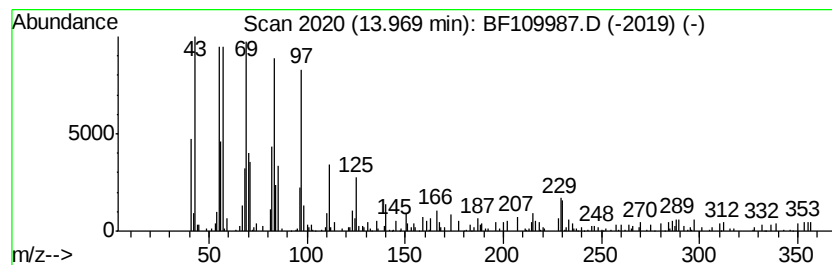
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.62 ng	247270	Chrysene-d12	14.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
4		1-Hexacosanol	382	C26H54O	000506-52-5	87
5		1-Heneicosanol	312	C21H44O	015594-90-8	87



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Acq On : 19 Oct 2018 4:12
Operator : JU/SJ
Sample : J5579-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
7-1-ROLLOFFS

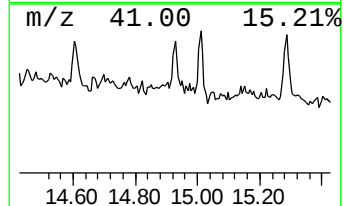
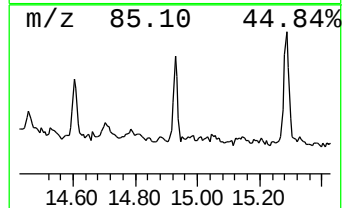
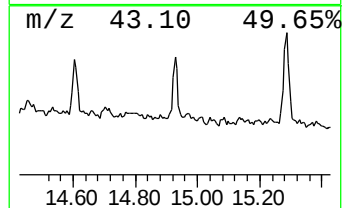
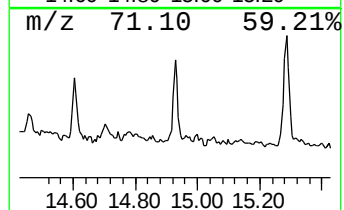
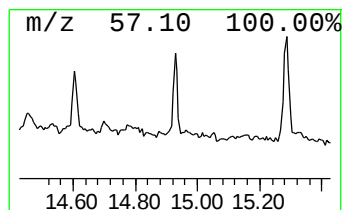
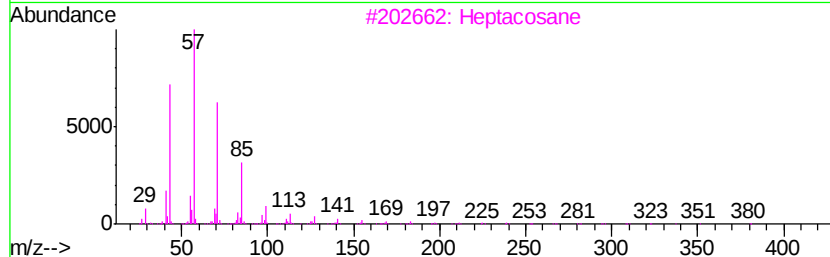
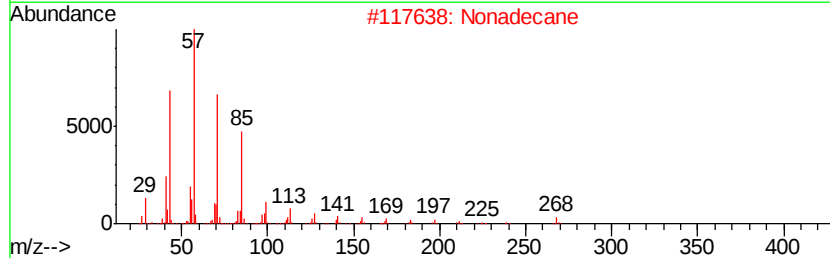
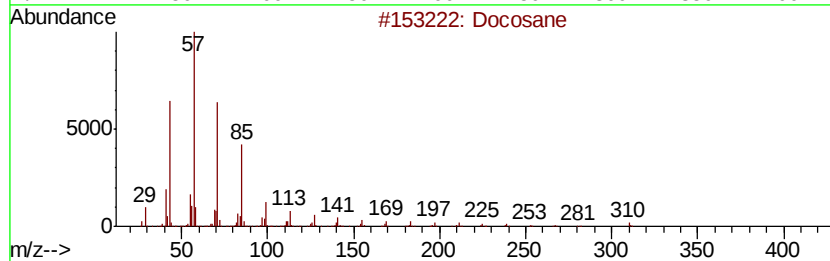
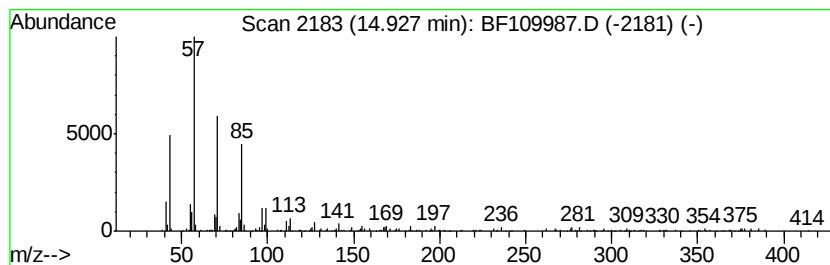
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.59 ng	140571	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	87
2		Nonadecane	268	C19H40	000629-92-5	83
3		Heptacosane	380	C27H56	000593-49-7	83
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5		Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109987.D
Acq On : 19 Oct 2018 4:12
Operator : JU/SJ
Sample : J5579-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-1-ROLLOFFS

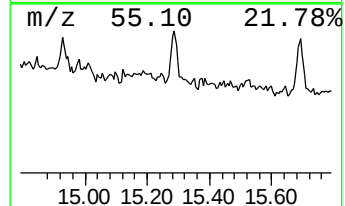
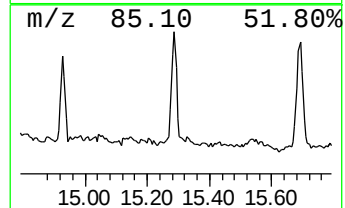
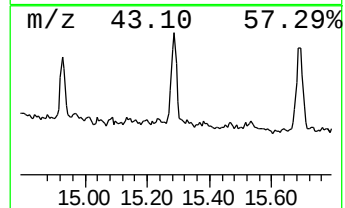
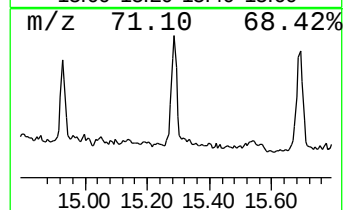
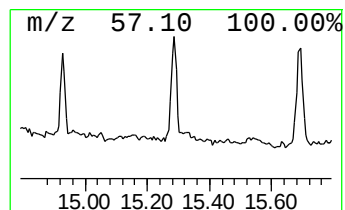
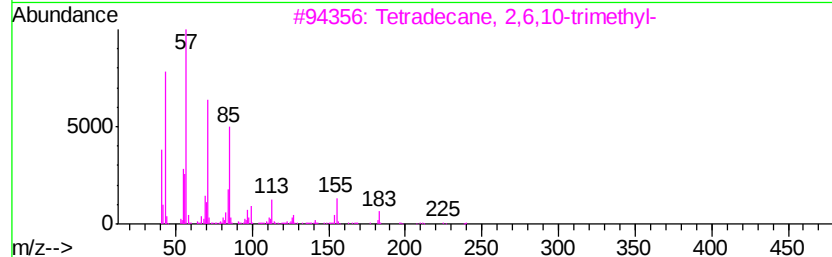
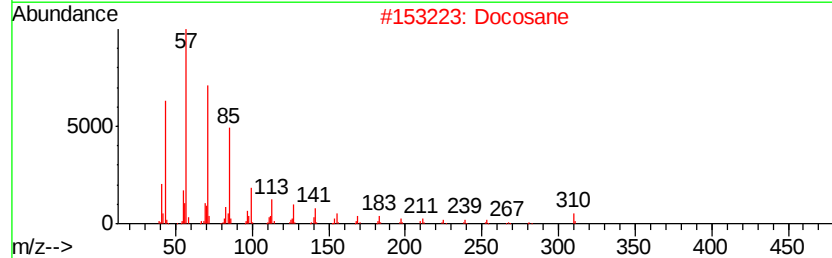
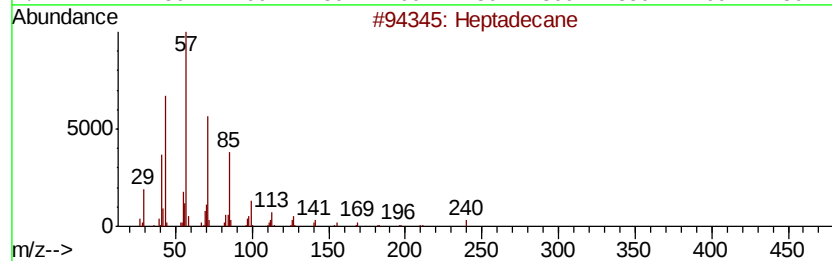
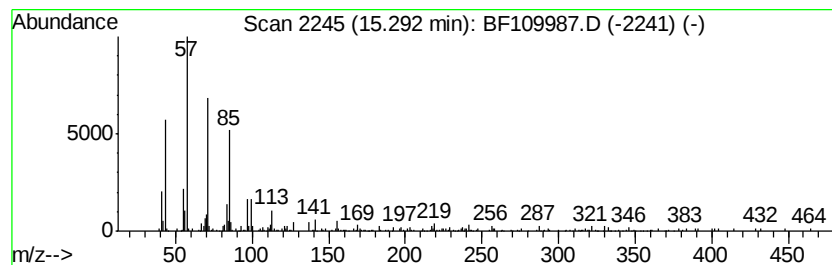
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	4.96 ng	268937	Perylene-d12	15.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Docosane		310	C22H46	000629-97-0	87
3	Tetradecane, 2,6,10-trimethyl-		240	C17H36	014905-56-7	87
4	Tridecane, 6-propyl-		226	C16H34	055045-10-8	87
5	2-Bromotetradecane		276	C14H29Br	074036-95-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
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Sample : J5579-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-1-ROLLOFFS

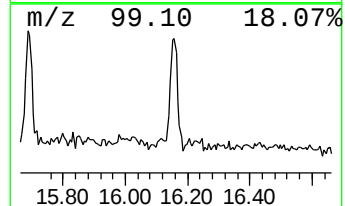
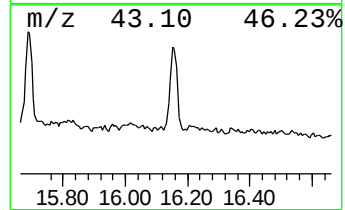
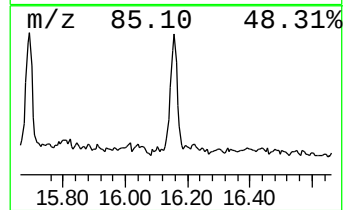
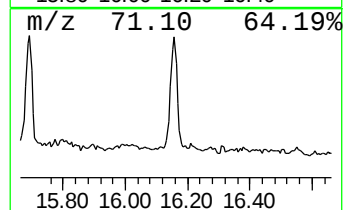
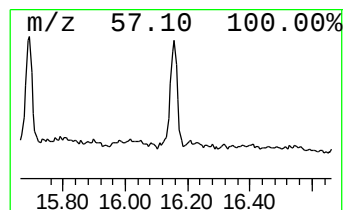
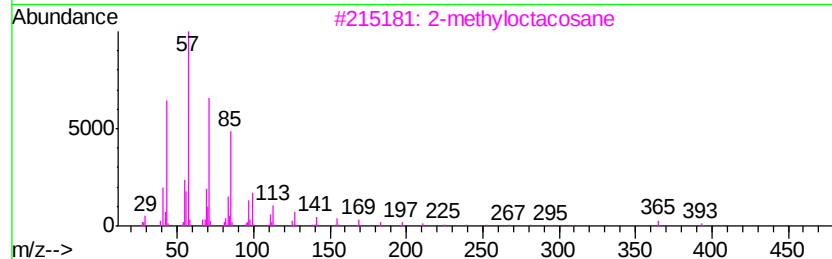
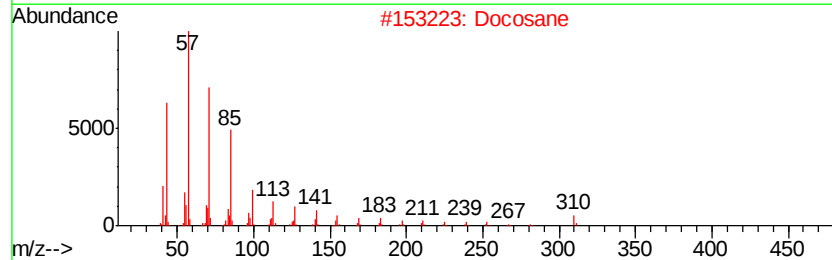
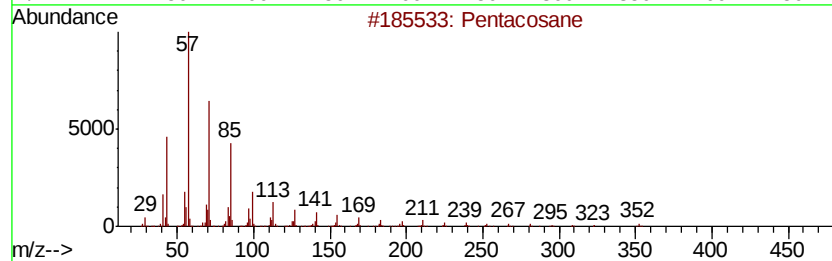
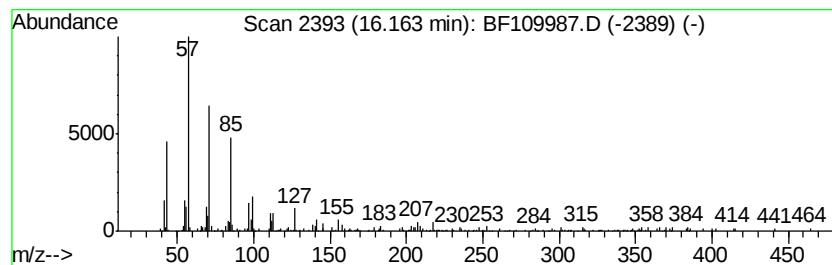
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	5.75 ng	311806	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	93
2		Docosane	310	C22H46	000629-97-0	87
3		2-methyloctacosane	408	C29H60	1000376-72-8	86
4		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101818\
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Sample : J5579-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-1-ROLLOFFS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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
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2-Pentanone, 4-hy...	5.22	2.6	ng	140531	1	6.97	1088020	20.0
unknown6.75	6.75	62.2	ng	3383140	1	6.97	1088020	20.0
Carbazole, 4,5-di...	10.92	3.0	ng	173193	4	11.51	1147280	20.0
n-Tetracosanol-1	13.97	4.6	ng	247270	5	14.16	1071210	20.0
Docosane	14.93	2.6	ng	140571	6	15.69	1083720	20.0
Heptadecane	15.29	5.0	ng	268937	6	15.69	1083720	20.0
Pentacosane	16.16	5.8	ng	311806	6	15.69	1083720	20.0