

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
 Data File : BF109989.D
 Acq On : 19 Oct 2018 5:06
 Operator : JU/SJ
 Sample : J5573-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 0692-KM-CA-AMD-COMP

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	2.334	37	42	49	rVB	502491	660200	22.18%	2.540%
2	5.210	527	531	538	rVB	470263	488449	16.41%	1.879%
3	5.598	593	597	600	rBV	2366873	2016220	67.74%	7.757%
4	6.593	761	766	777	rBV2	2577908	2976465	100.00%	11.451%
5	6.745	787	792	795	rBV	2730543	2383541	80.08%	9.170%
6	6.975	828	831	835	rBV	1205959	1024275	34.41%	3.941%
7	7.134	854	858	861	rBV	2787699	2235600	75.11%	8.601%
8	7.540	922	927	930	rBV	1847866	1718184	57.73%	6.610%
9	7.704	951	955	958	rVB3	30563	33588	1.13%	0.129%
10	8.257	1046	1049	1053	rBV	1286073	1177466	39.56%	4.530%
11	9.334	1228	1232	1235	rBV	3029836	2407999	80.90%	9.264%
12	9.722	1295	1298	1303	rBV	330935	266271	8.95%	1.024%
13	10.016	1345	1348	1352	rBV	1133735	1065594	35.80%	4.100%
14	10.804	1479	1482	1489	rBV	941537	859711	28.88%	3.307%
15	10.939	1502	1505	1508	rVB2	39950	35907	1.21%	0.138%
16	11.386	1578	1581	1585	rVB	44119	38207	1.28%	0.147%
17	11.510	1598	1602	1605	rBV	1234257	1033082	34.71%	3.974%
18	12.727	1806	1809	1812	rBV	75180	67120	2.26%	0.258%
19	12.898	1836	1838	1842	rBV2	32281	30561	1.03%	0.118%
20	12.957	1842	1848	1854	rVV	79411	98655	3.31%	0.380%
21	13.092	1867	1871	1875	rBV	2332693	2190464	73.59%	8.427%
22	13.974	2018	2021	2027	rBV2	87164	104855	3.52%	0.403%
23	14.157	2048	2052	2055	rBV	1151581	1024368	34.42%	3.941%
24	14.298	2074	2076	2080	rVB	57593	46161	1.55%	0.178%
25	14.604	2125	2128	2137	rVB	111477	128449	4.32%	0.494%
26	14.927	2180	2183	2189	rVB	147148	151552	5.09%	0.583%
27	15.010	2194	2197	2202	rVB	90911	98729	3.32%	0.380%
28	15.286	2240	2244	2249	rVB	178103	225509	7.58%	0.868%
29	15.686	2307	2312	2320	rBV2	711829	967630	32.51%	3.723%
30	16.151	2387	2391	2397	rVB	173976	266267	8.95%	1.024%
31	16.698	2480	2484	2489	rVB2	109448	172145	5.78%	0.662%

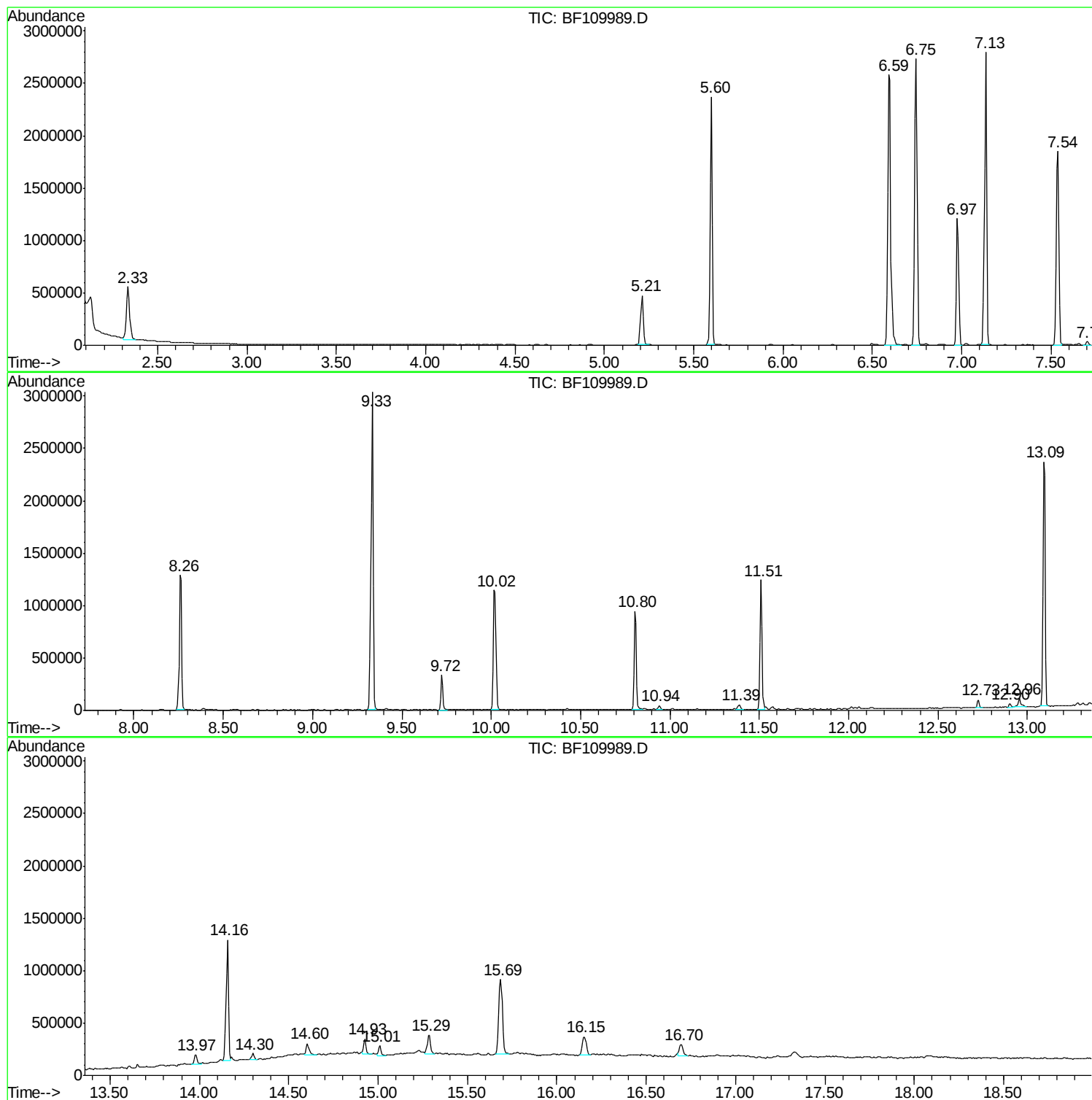
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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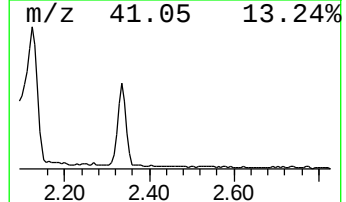
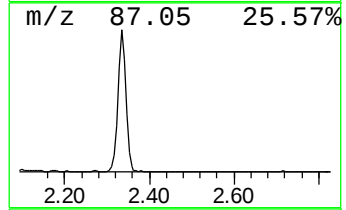
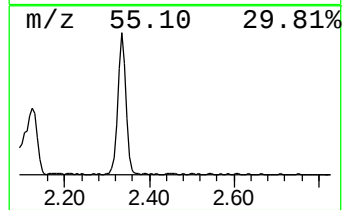
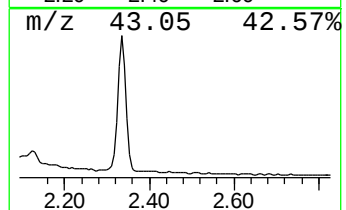
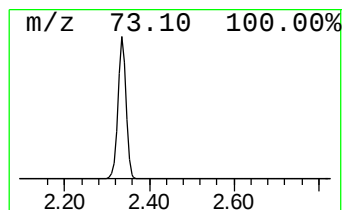
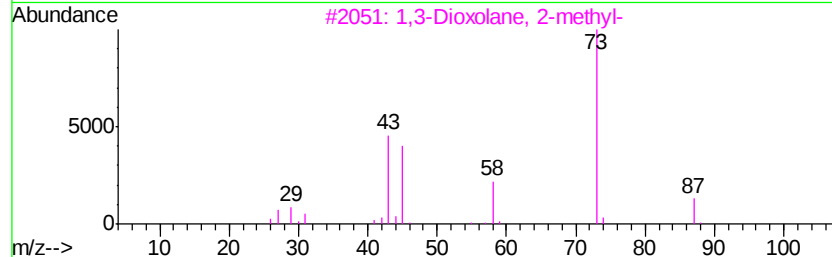
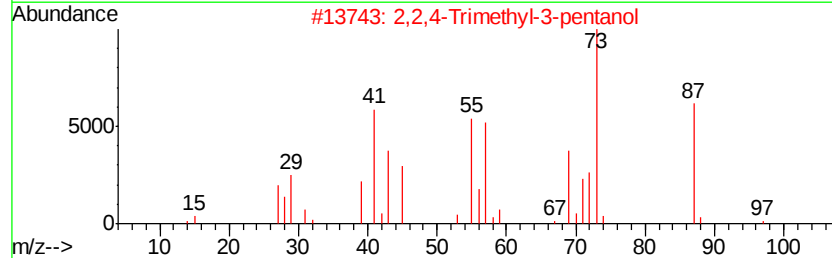
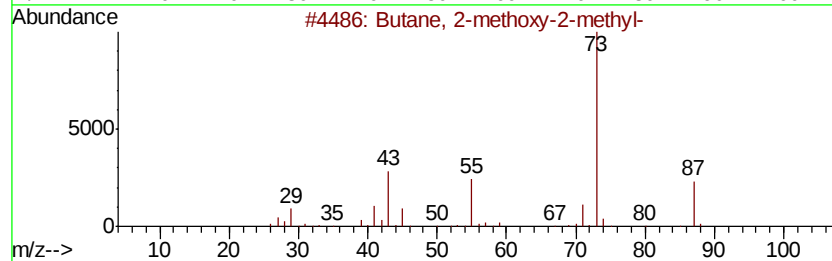
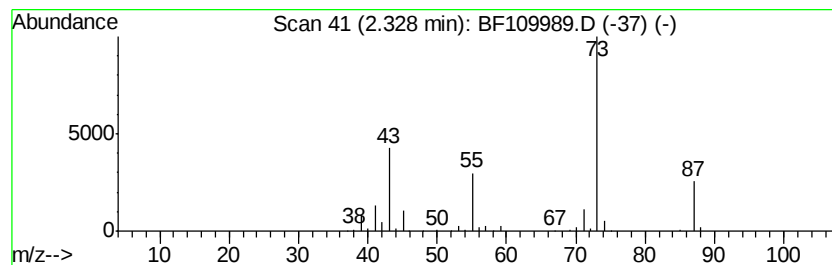
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	12.89 ng	660200	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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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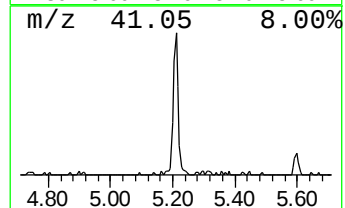
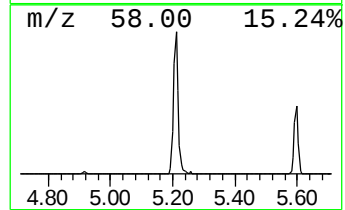
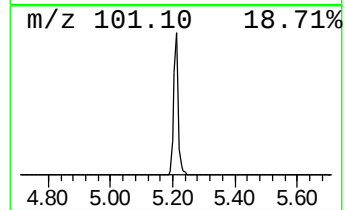
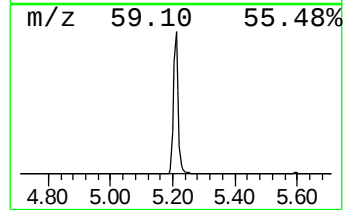
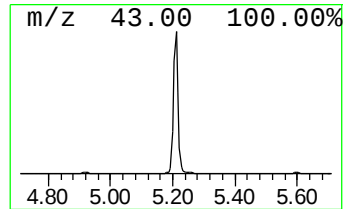
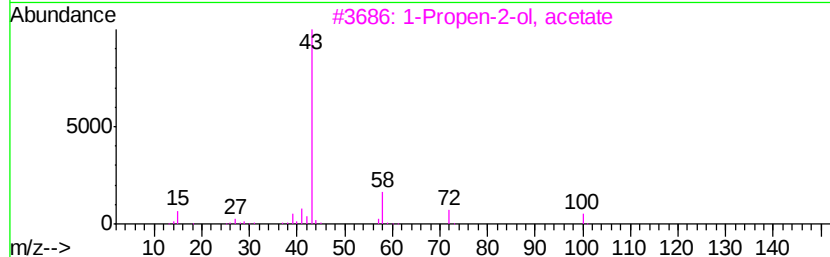
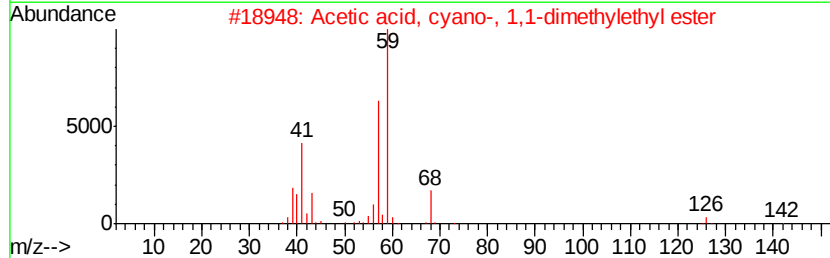
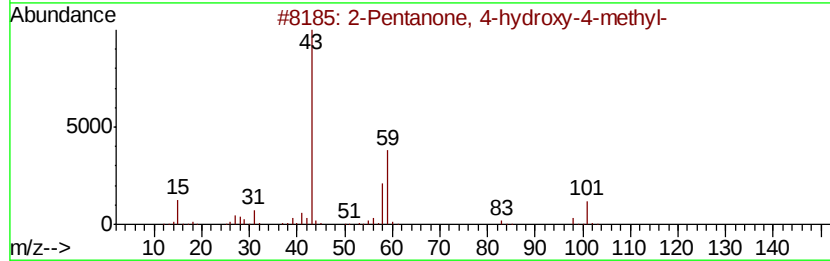
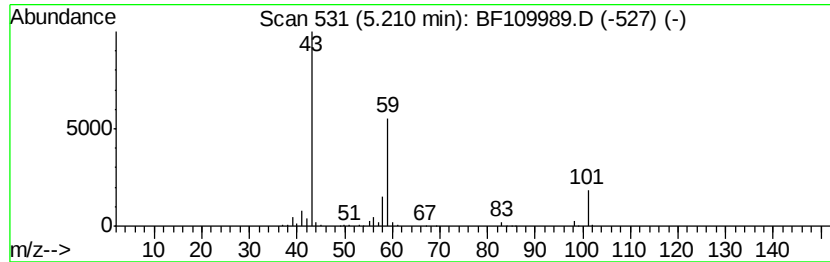
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	9.54 ng	488449	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		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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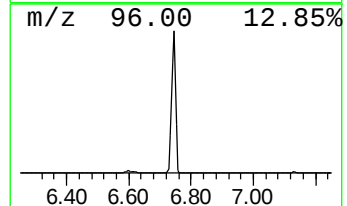
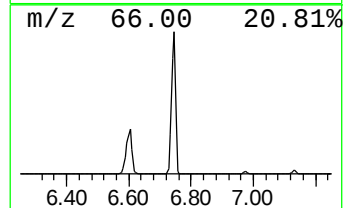
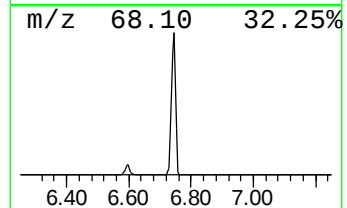
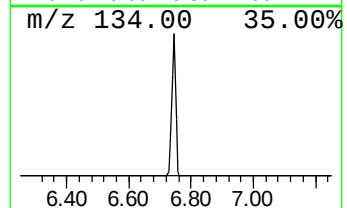
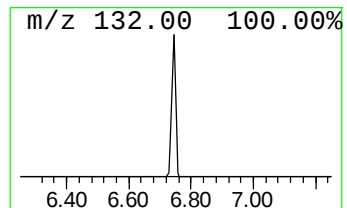
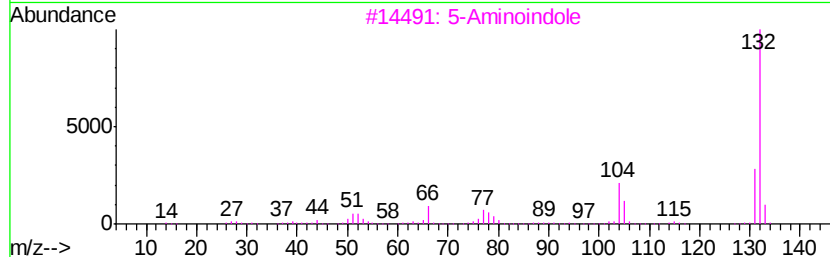
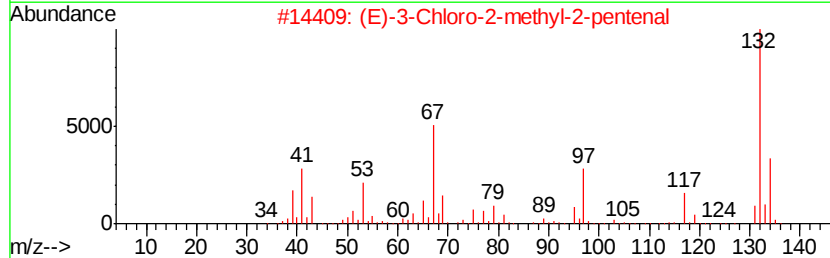
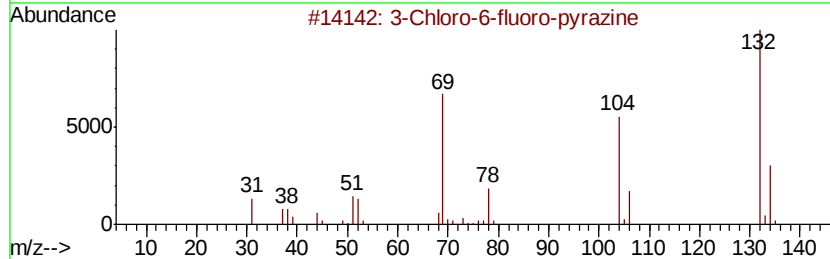
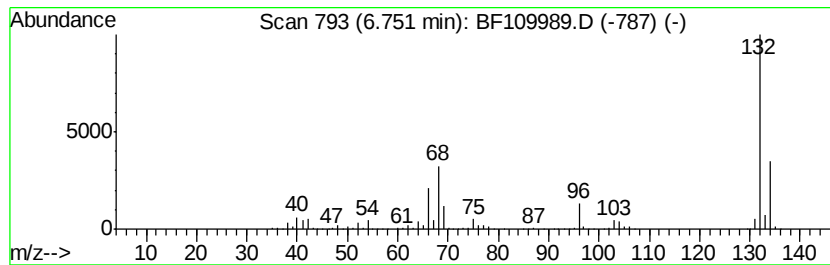
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	46.54 ng	2383540	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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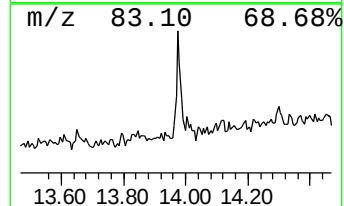
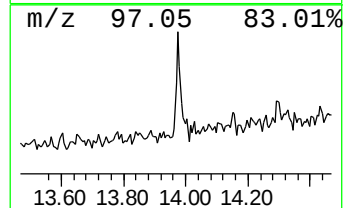
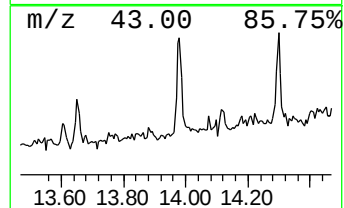
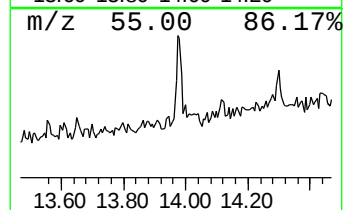
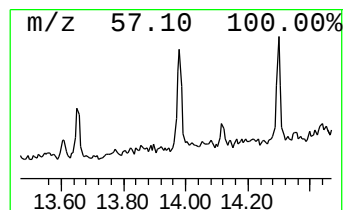
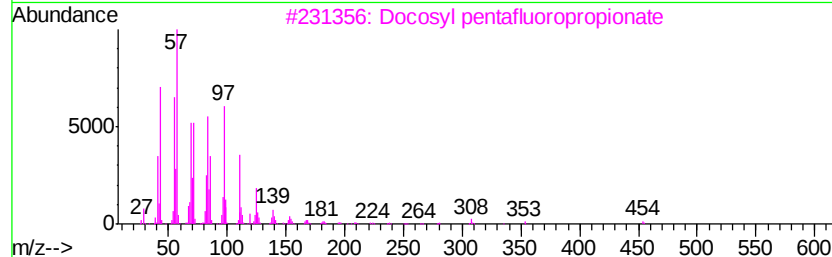
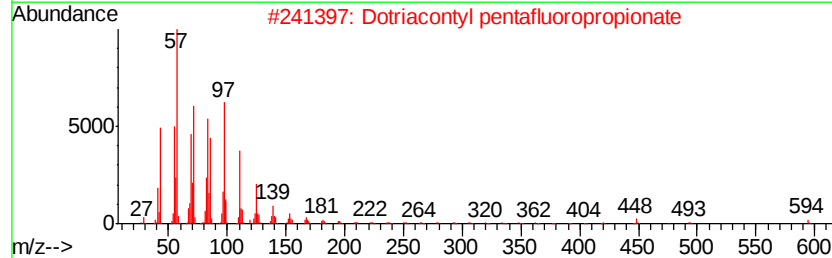
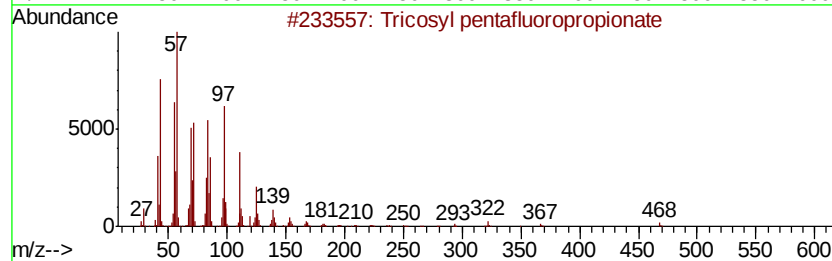
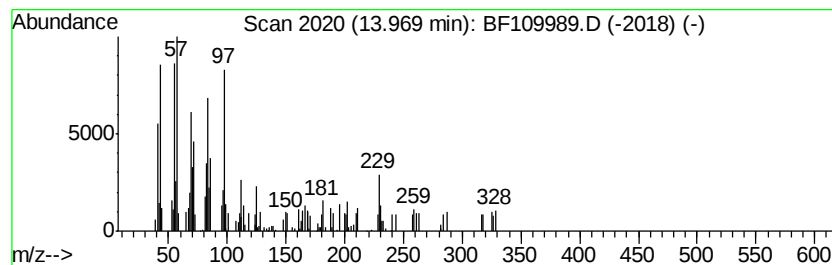
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Peak Number 5 Tricosyl pentafluoropropionate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.97	2.05 ng	104855	Chrysene-d12		14.16	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	83
2		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	83
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	83
4		Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	83
5		Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	83



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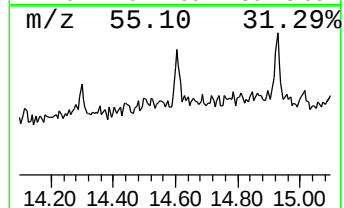
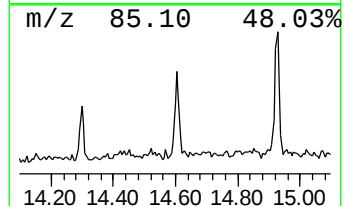
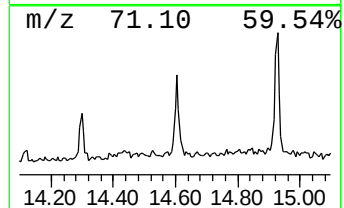
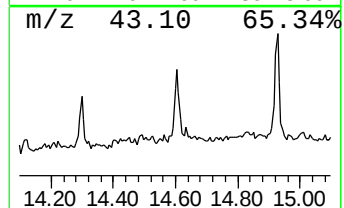
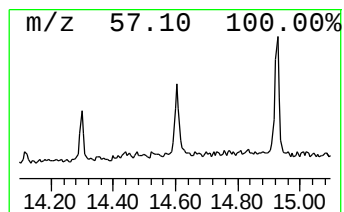
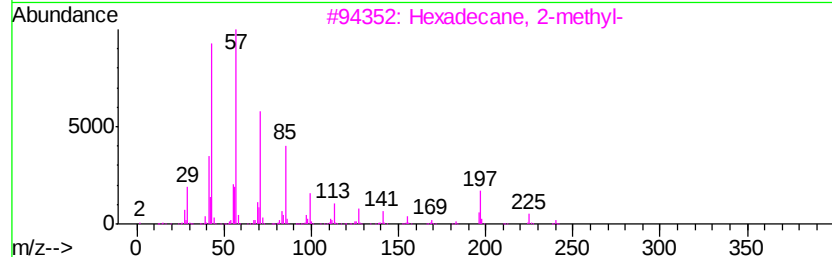
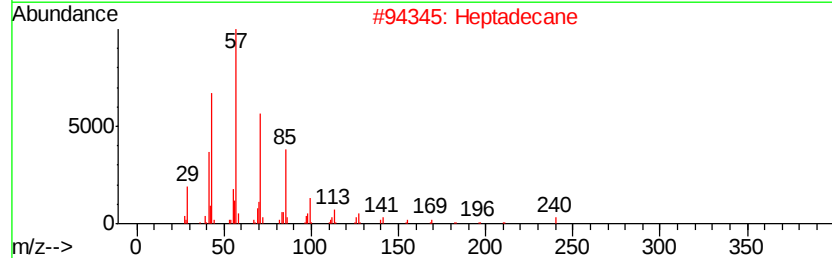
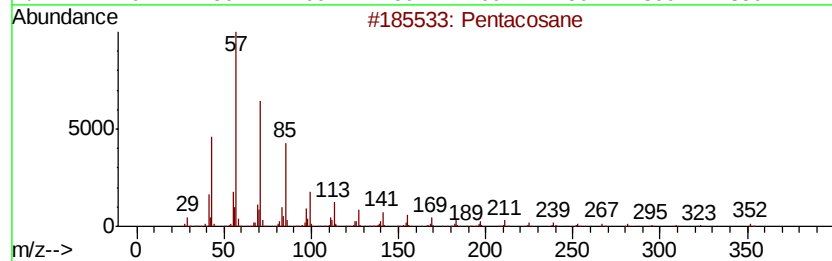
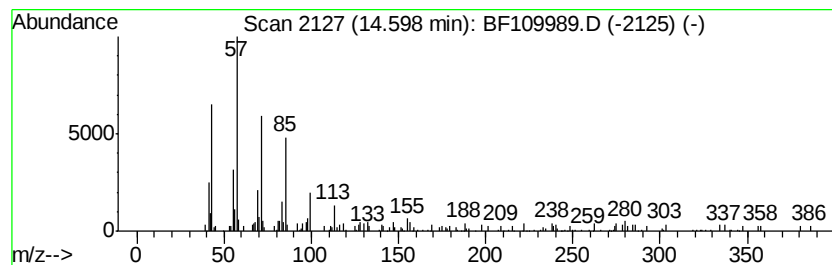
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.51 ng	128449	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	90
2		Heptadecane	240	C17H36	000629-78-7	90
3		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	81
4		Hexacosane	366	C26H54	000630-01-3	74
5		Tetratetracontane	619	C44H90	007098-22-8	72



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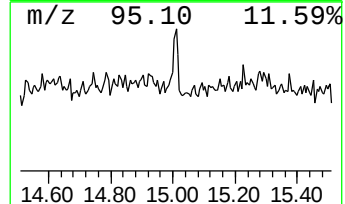
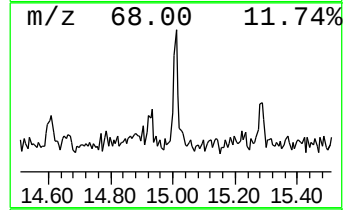
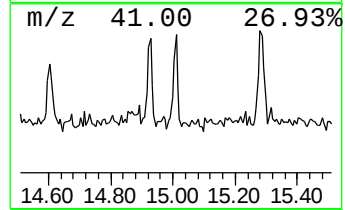
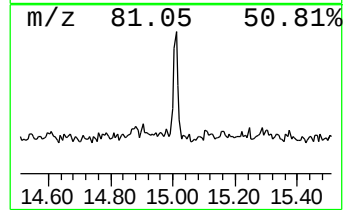
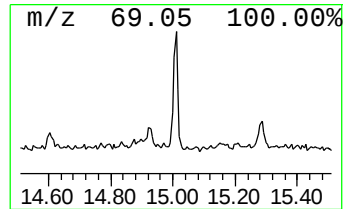
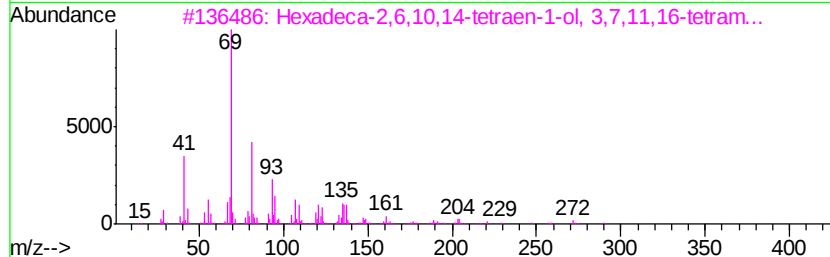
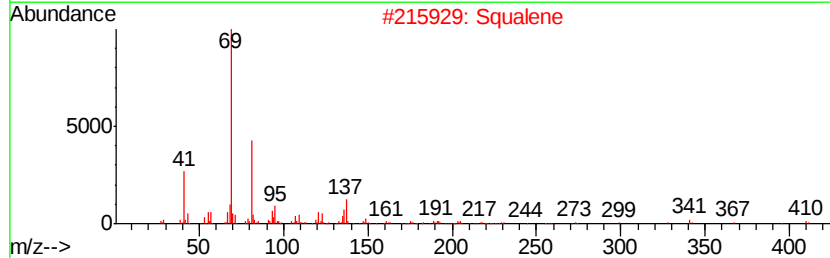
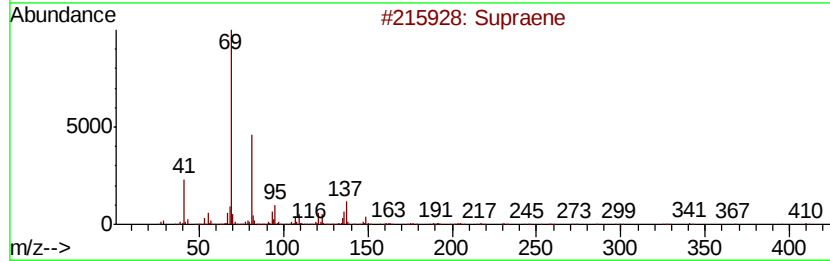
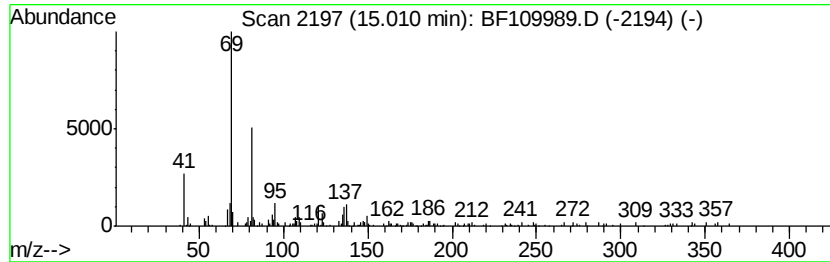
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ClientSampleId :
0692-KM-CA-AMD-COMP

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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 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
15.01	2.04 ng	98729	Perylene-d12		15.69		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			Squalene	410	C30H50	000111-02-4	86
3			Hexadeca-2,6,10,14-tetraen-1-ol, ...	290	C20H34O	007614-21-3	80
4			Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	72
5			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109989.D
Acq On : 19 Oct 2018 5:06
Operator : JU/SJ
Sample : J5573-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0692-KM-CA-AMD-COMP

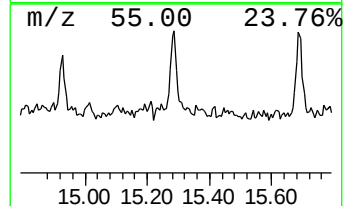
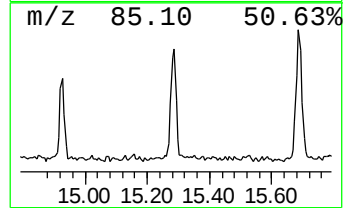
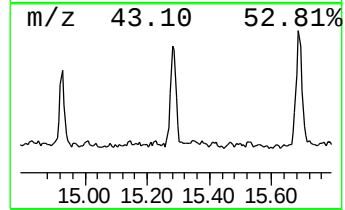
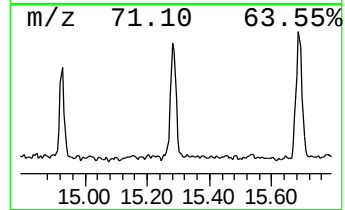
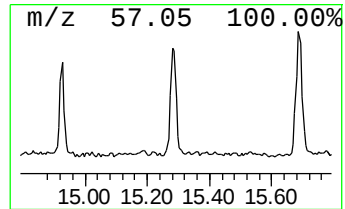
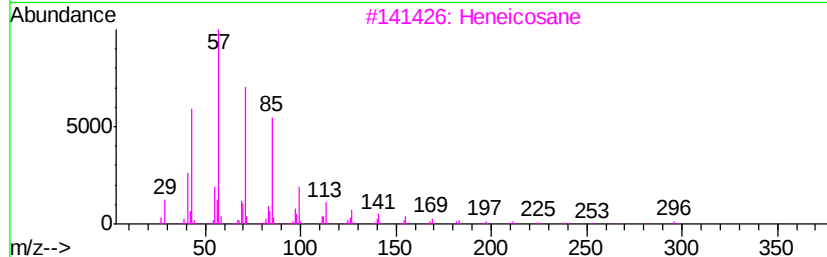
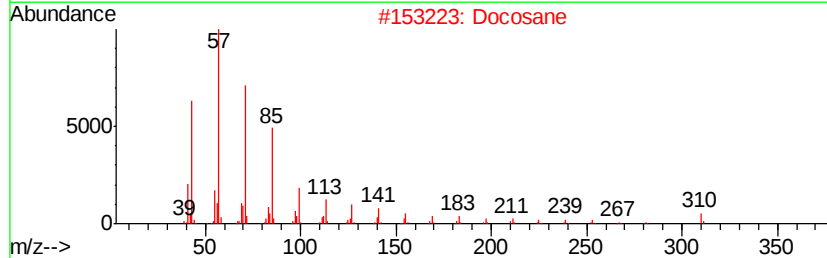
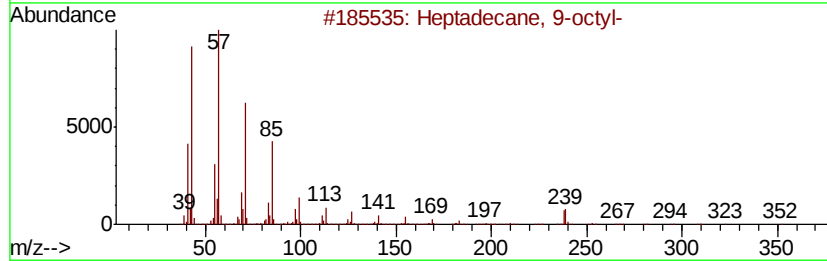
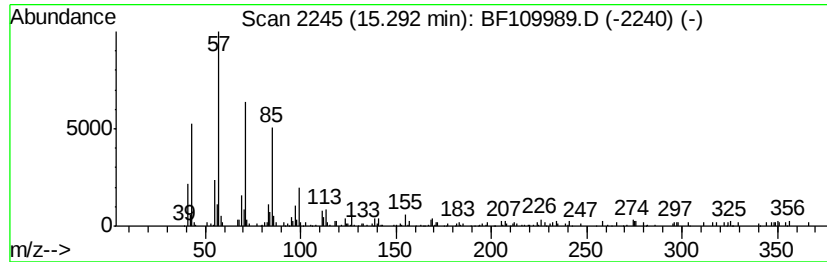
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	4.66 ng	225509	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2		Docosane	310	C22H46	000629-97-0	86
3		Heneicosane	296	C21H44	000629-94-7	81
4		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	81
5		Tricosane	324	C23H48	000638-67-5	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109989.D
Acq On : 19 Oct 2018 5:06
Operator : JU/SJ
Sample : J5573-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0692-KM-CA-AMD-COMP

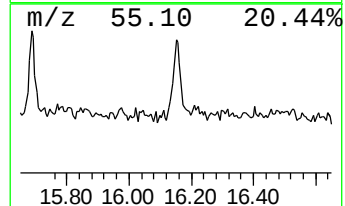
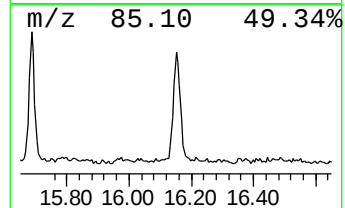
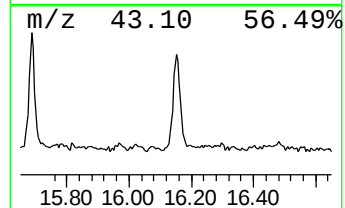
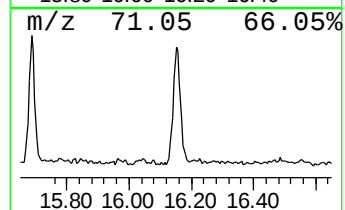
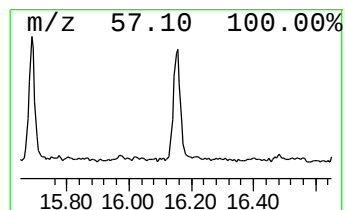
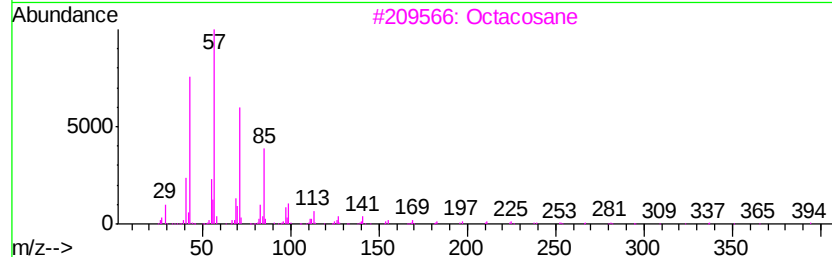
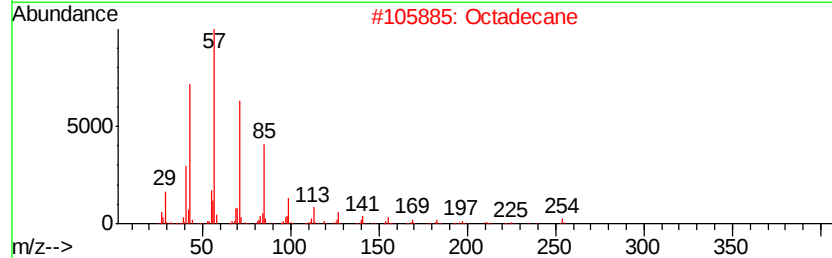
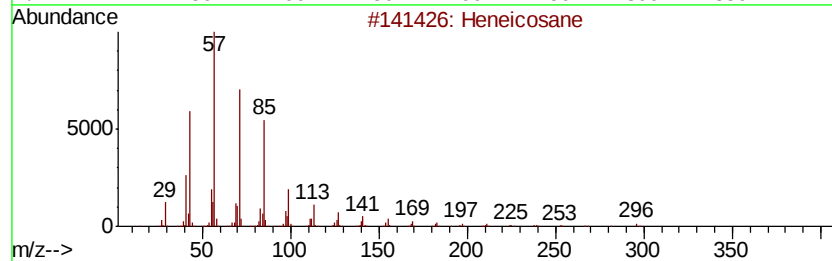
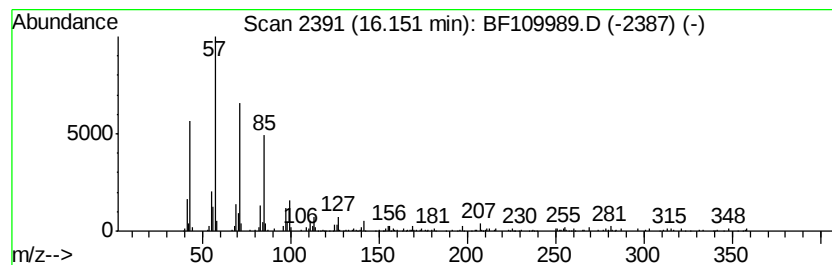
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	5.50 ng	266267	Perylene-d12	15.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	98
2	Octadecane		254	C18H38	000593-45-3	95
3	Octacosane		394	C28H58	000630-02-4	90
4	Tetracosane		338	C24H50	000646-31-1	87
5	Tridecane, 6-propyl-		226	C16H34	055045-10-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109989.D
Acq On : 19 Oct 2018 5:06
Operator : JU/SJ
Sample : J5573-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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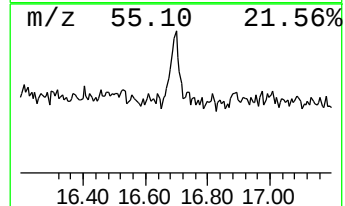
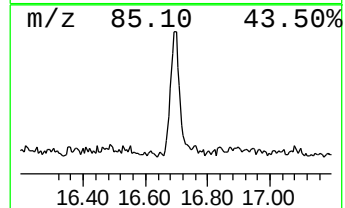
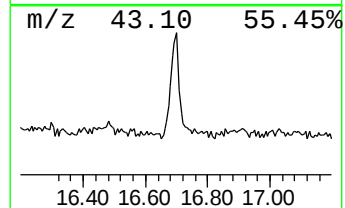
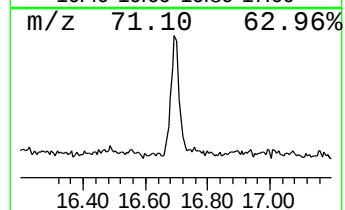
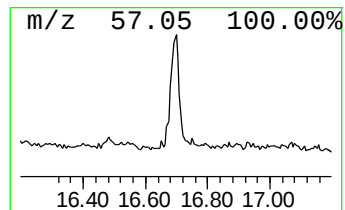
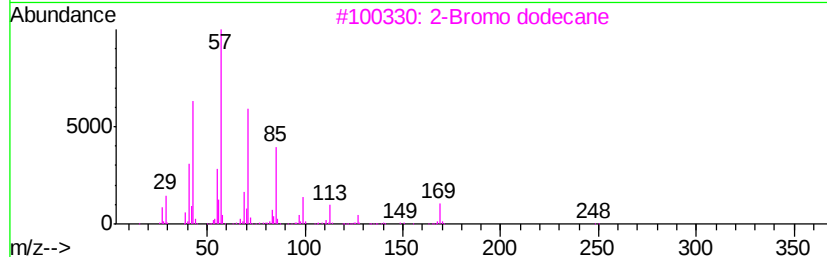
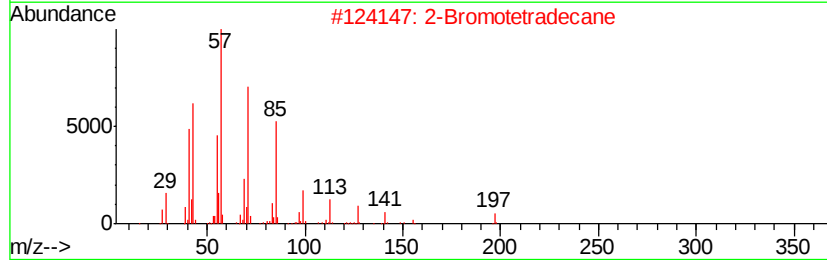
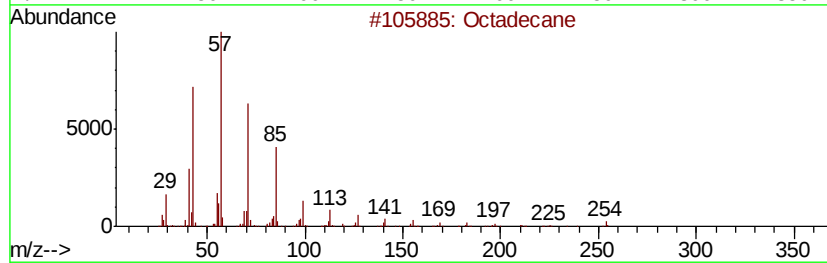
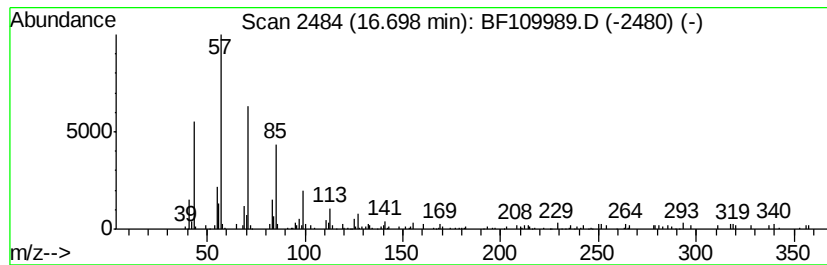
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	3.56 ng	172145	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		2-Bromotetradecane	276	C14H29Br	074036-95-6	86
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4		Heptadecane	240	C17H36	000629-78-7	80
5		Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101818\
Data File : BF109989.D
Acq On : 19 Oct 2018 5:06
Operator : JU/SJ
Sample : J5573-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0692-KM-CA-AMD-COMP

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
Butane, 2-methoxy...	2.33	12.9	ng	660200	1	6.97	1024280	20.0
2-Pentanone, 4-hy...	5.21	9.5	ng	488449	1	6.97	1024280	20.0
unknown6.75	6.75	46.5	ng	2383540	1	6.97	1024280	20.0
Tricosyl pentaflu...	13.97	2.0	ng	104855	5	14.16	1024370	20.0
Pentacosane	14.60	2.5	ng	128449	5	14.16	1024370	20.0
Supraene	15.01	2.0	ng	98729	6	15.69	967630	20.0
Heptadecane, 9-oc...	15.29	4.7	ng	225509	6	15.69	967630	20.0
Heneicosane	16.15	5.5	ng	266267	6	15.69	967630	20.0
Octadecane	16.70	3.6	ng	172145	6	15.69	967630	20.0