

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101818\
 Data File : BF109981.D
 Acq On : 19 Oct 2018 1:29
 Operator : JU/SJ
 Sample : J5570-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-08

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	534234	702895	16.66%	1.721%
2	3.604	255	258	271	rBV	32098	68928	1.63%	0.169%
3	5.216	524	532	539	rBV	138993	179770	4.26%	0.440%
4	5.598	592	597	600	rBV	3782827	3735141	88.53%	9.143%
5	6.598	761	767	771	rBV2	3700850	4218972	100.00%	10.327%
6	6.745	787	792	795	rBV	4333269	3888349	92.16%	9.518%
7	6.975	827	831	834	rBV	1635047	1255535	29.76%	3.073%
8	7.134	854	858	861	rVB	3482539	3036108	71.96%	7.432%
9	7.539	921	927	930	rBV	2548072	2487660	58.96%	6.089%
10	8.257	1045	1049	1053	rBV	1974776	1609267	38.14%	3.939%
11	9.333	1227	1232	1235	rBV	4684791	3887849	92.15%	9.517%
12	9.722	1294	1298	1302	rBV	623626	477289	11.31%	1.168%
13	10.016	1344	1348	1352	rBV	1912187	1706413	40.45%	4.177%
14	10.804	1478	1482	1486	rBV	2409119	2231229	52.89%	5.462%
15	11.510	1598	1602	1604	rBV	1719710	1480331	35.09%	3.624%
16	11.527	1604	1605	1610	rVB	126957	99762	2.36%	0.244%
17	12.016	1684	1688	1691	rBV2	158967	144735	3.43%	0.354%
18	12.721	1804	1808	1812	rBV	290073	235560	5.58%	0.577%
19	12.951	1840	1847	1850	rBV	218078	221915	5.26%	0.543%
20	13.092	1867	1871	1874	rVB	3072376	2602488	61.69%	6.370%
21	13.651	1961	1966	1969	rBV2	60783	57339	1.36%	0.140%
22	13.974	2015	2021	2033	rBV4	254106	341319	8.09%	0.835%
23	14.151	2047	2051	2054	rBV	1335682	1237525	29.33%	3.029%
24	14.174	2054	2055	2060	rVB	103103	79081	1.87%	0.194%
25	14.298	2072	2076	2080	rBV	116576	111122	2.63%	0.272%
26	14.604	2125	2128	2136	rVB	229251	234428	5.56%	0.574%
27	14.921	2178	2182	2192	rBV	239468	295313	7.00%	0.723%
28	15.004	2193	2196	2200	rVB	111214	113659	2.69%	0.278%
29	15.080	2205	2209	2213	rVB3	53691	59366	1.41%	0.145%
30	15.221	2229	2233	2236	rBV	100419	142784	3.38%	0.350%
31	15.280	2239	2243	2246	rVV	351499	401252	9.51%	0.982%
32	15.304	2246	2247	2251	rVB2	61504	57615	1.37%	0.141%
33	15.539	2284	2287	2295	rVB	64945	98071	2.32%	0.240%
34	15.609	2295	2299	2305	rVB	68943	97609	2.31%	0.239%

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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	15.680	2305	2311	2324	rBV2	1212739	1716591	40.69%	4.202%
36	16.151	2385	2391	2396	rBV	358780	573489	13.59%	1.404%
37	16.204	2396	2400	2405	rVB4	42530	72771	1.72%	0.178%
38	16.686	2477	2482	2489	rBV	185881	333449	7.90%	0.816%
39	17.227	2570	2574	2582	rVB2	37970	88323	2.09%	0.216%
40	17.327	2585	2591	2598	rVB2	94087	197982	4.69%	0.485%
41	17.415	2602	2606	2613	rVB9	35170	65074	1.54%	0.159%
42	17.851	2676	2680	2688	rVB9	52117	108961	2.58%	0.267%
43	18.074	2713	2718	2727	rVB5	37169	99307	2.35%	0.243%

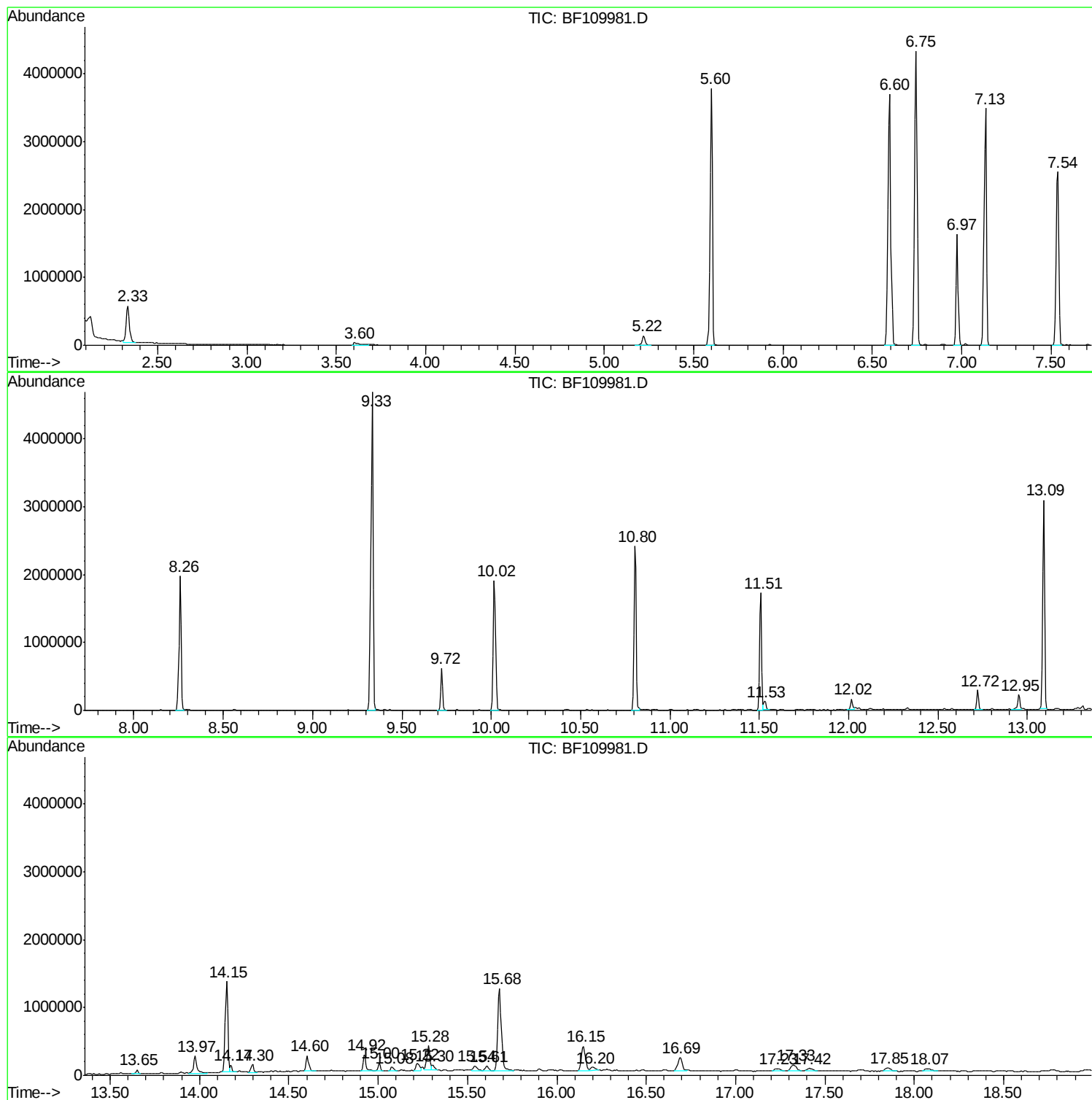
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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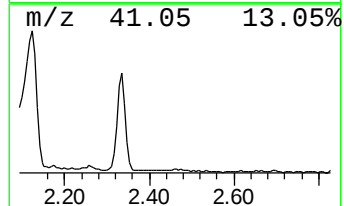
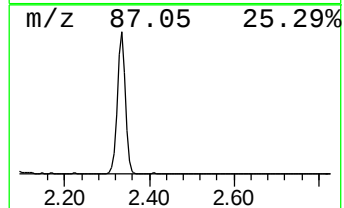
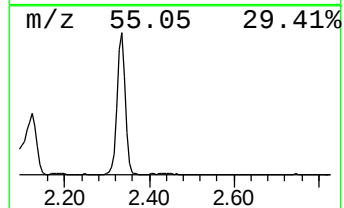
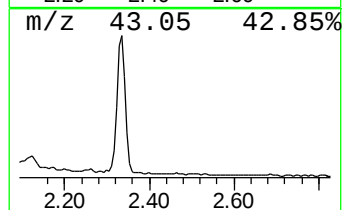
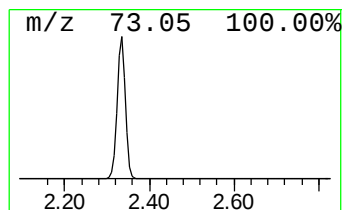
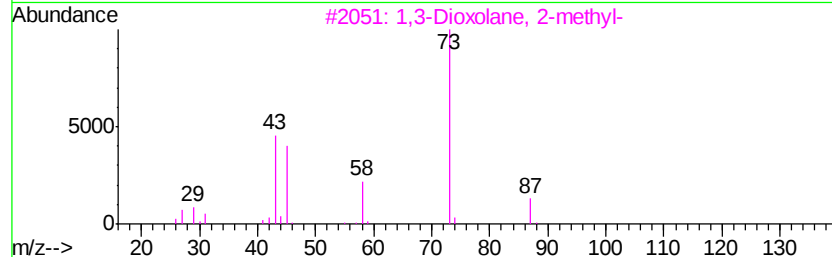
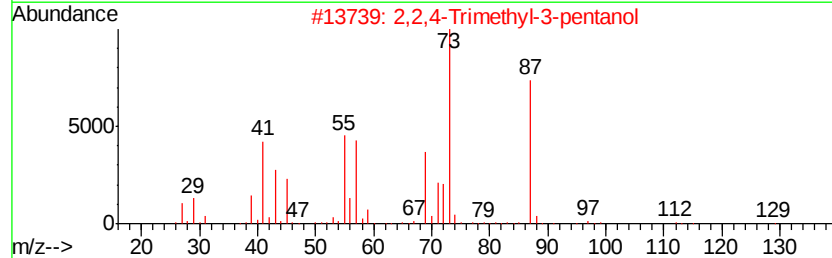
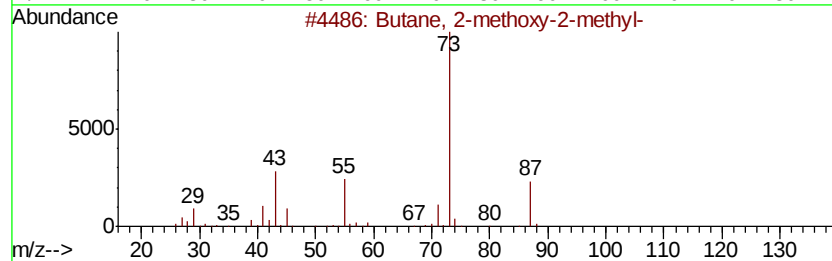
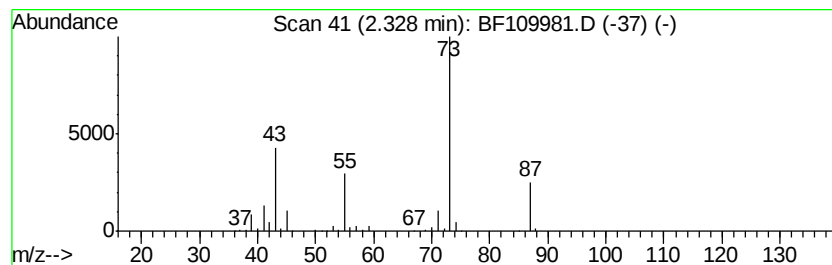
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	11.20 ng	702895	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	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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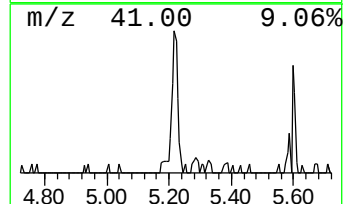
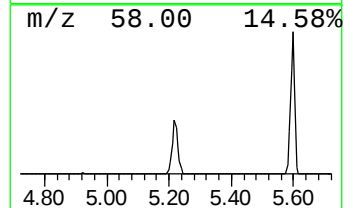
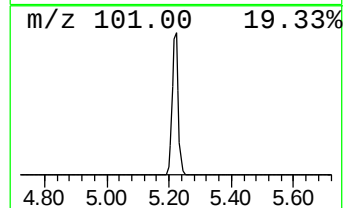
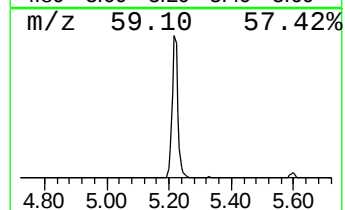
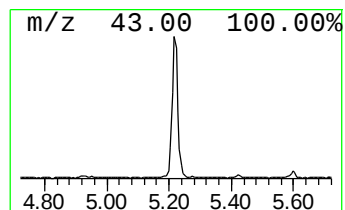
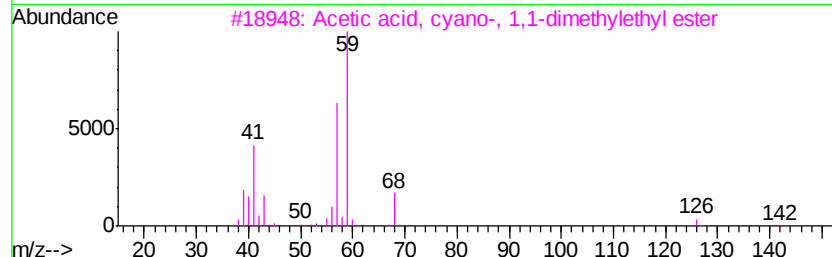
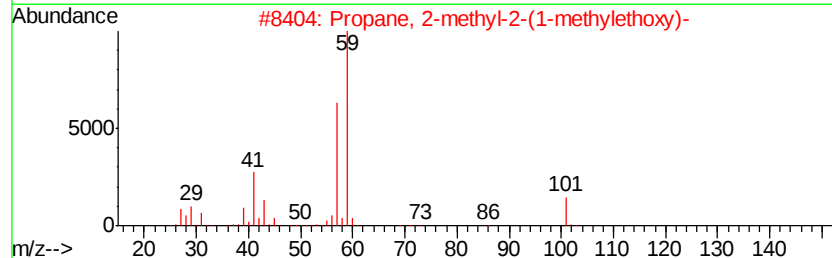
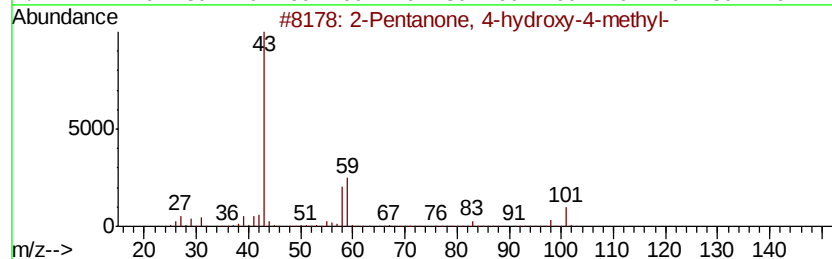
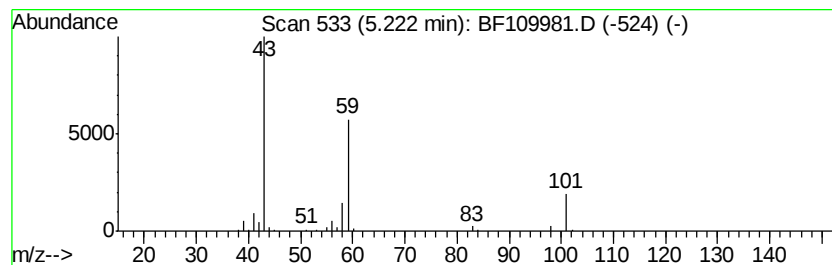
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.86 ng	179770	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		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	53
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	37
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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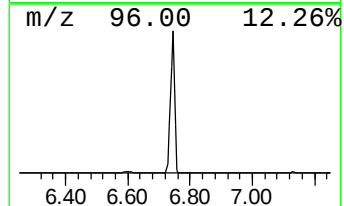
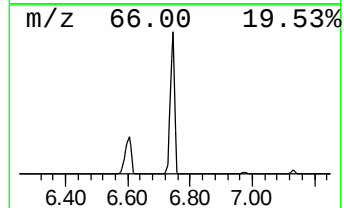
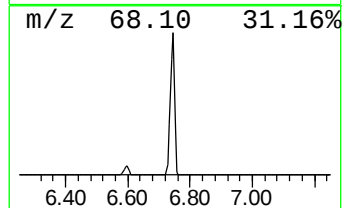
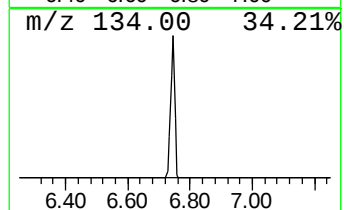
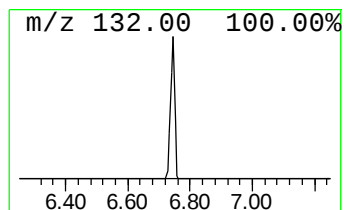
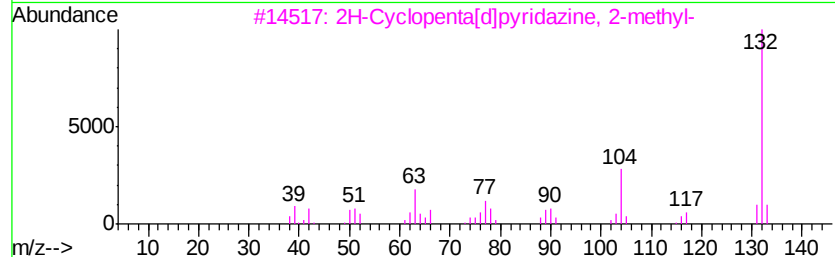
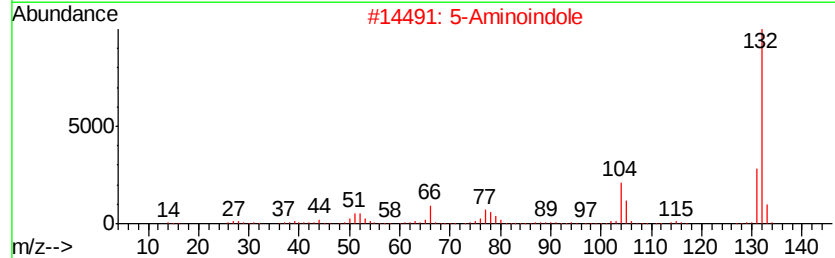
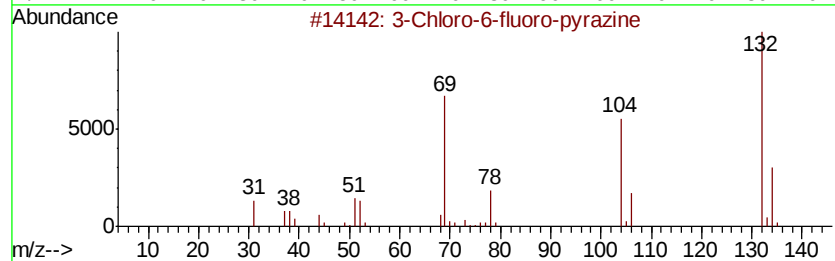
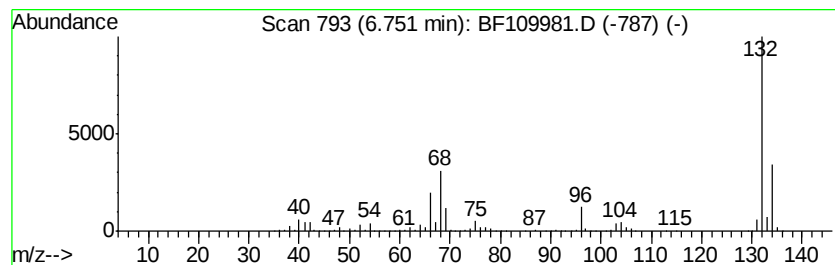
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	61.94 ng	3888350	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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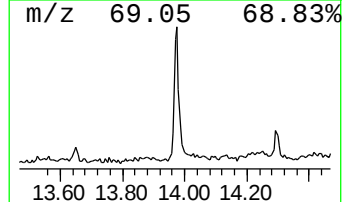
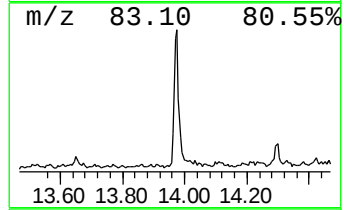
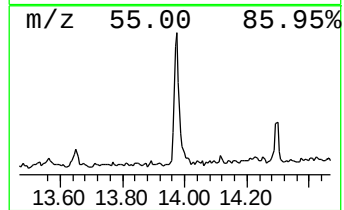
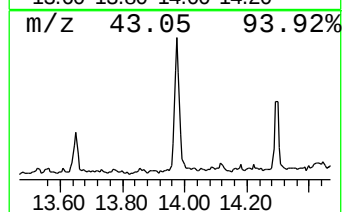
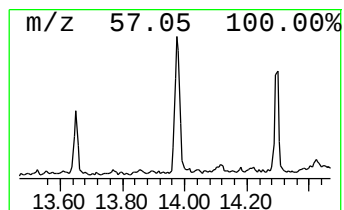
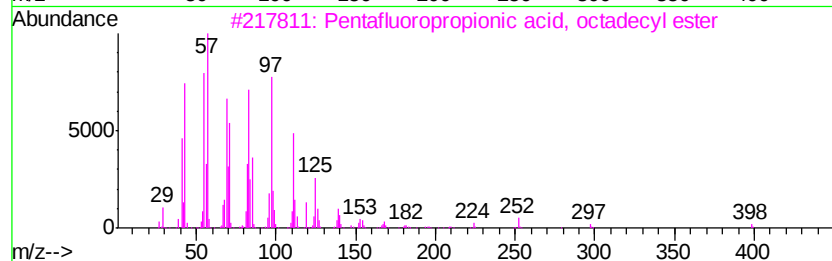
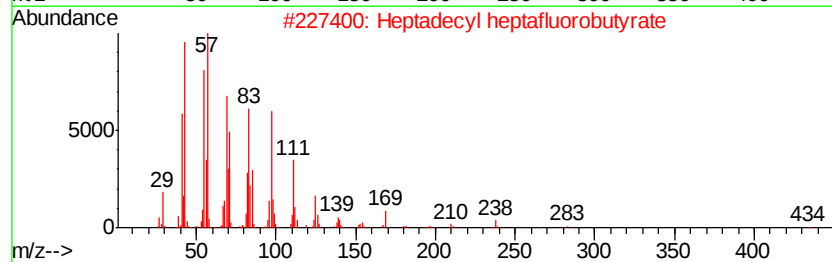
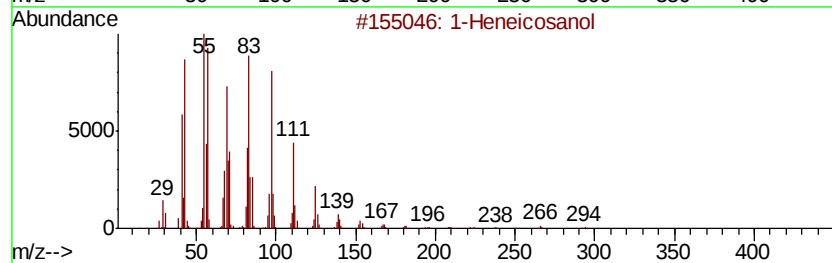
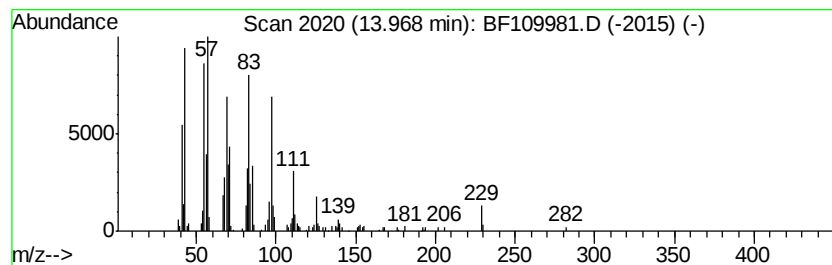
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.52 ng	341319	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	92
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	90
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
5		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	87



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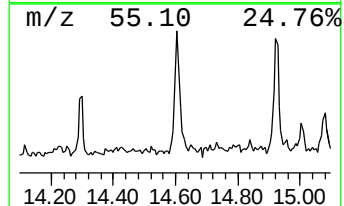
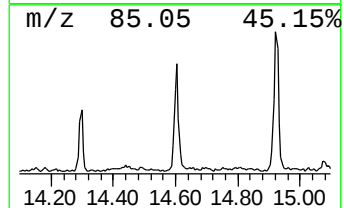
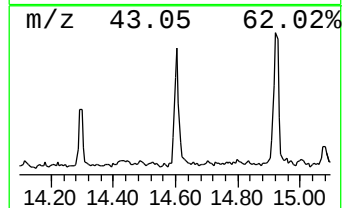
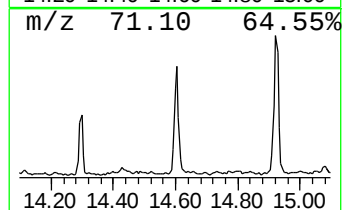
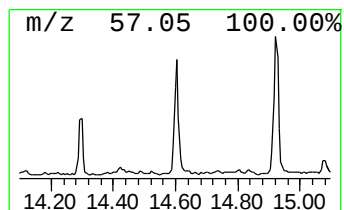
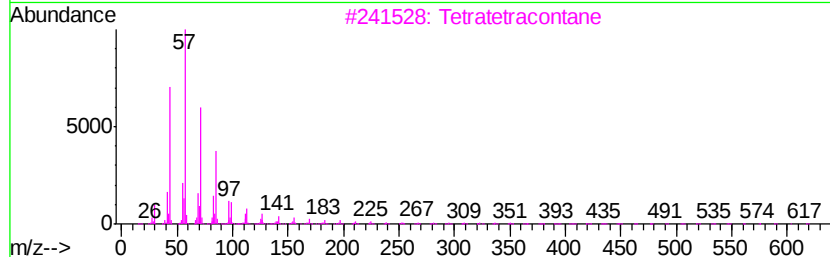
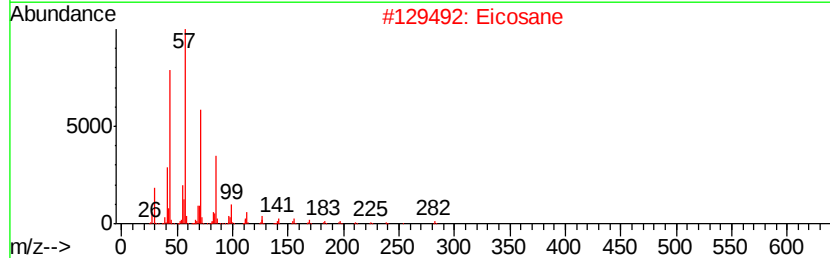
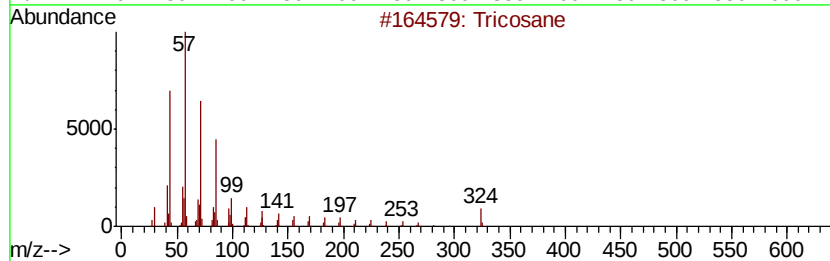
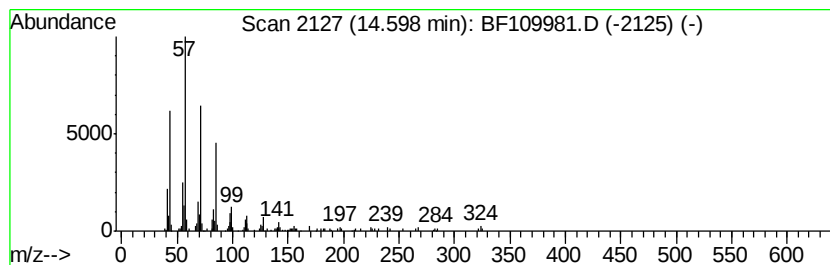
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.79 ng	234428	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	94
2	Eicosane		282	C20H42	000112-95-8	92
3	Tetratetracontane		619	C44H90	007098-22-8	90
4	Tritetracontane		605	C43H88	007098-21-7	90
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109981.D
Acq On : 19 Oct 2018 1:29
Operator : JU/SJ
Sample : J5570-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-08

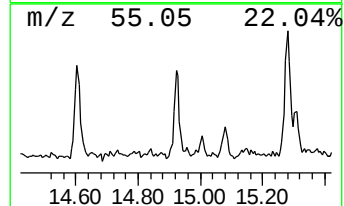
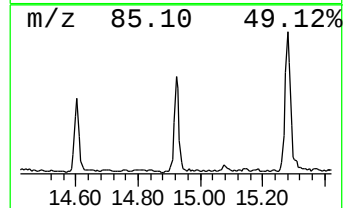
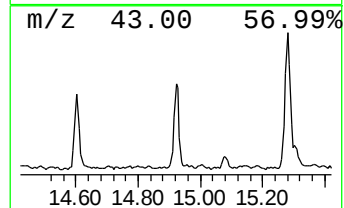
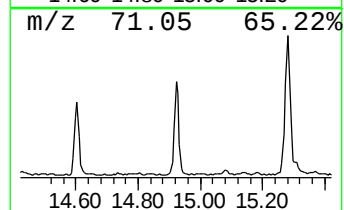
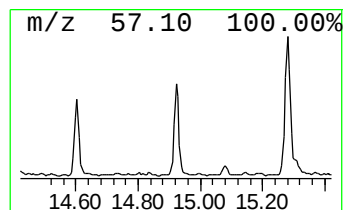
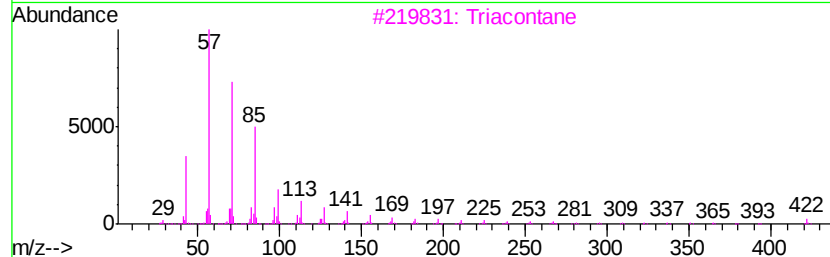
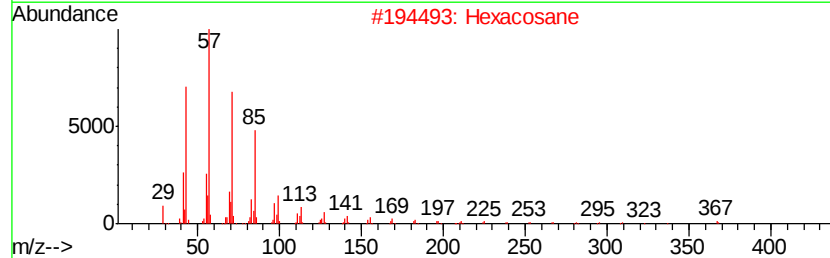
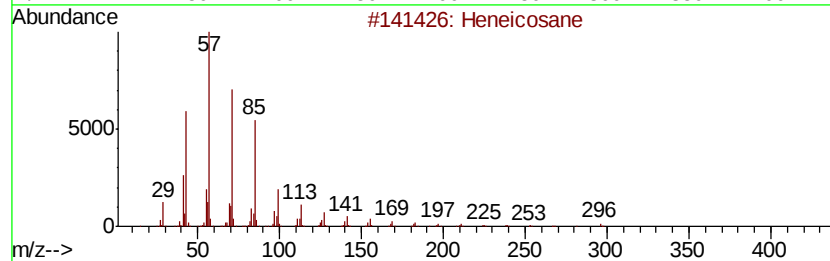
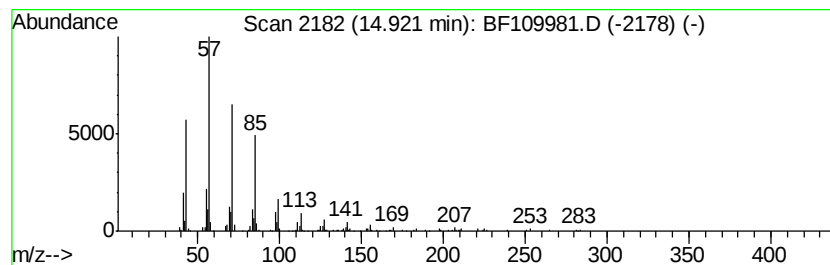
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	3.44 ng	295313	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	triacontane		422	C30H62	000638-68-6	91
4	Nonadecane		268	C19H40	000629-92-5	87
5	Eicosane		282	C20H42	000112-95-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109981.D
Acq On : 19 Oct 2018 1:29
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Instrument :
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ClientSampleId :
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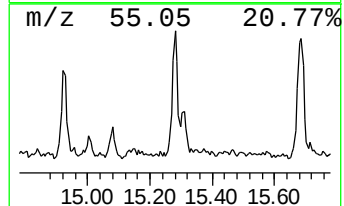
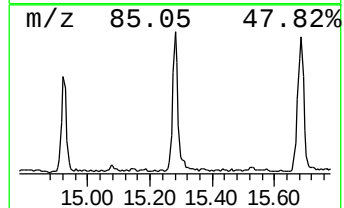
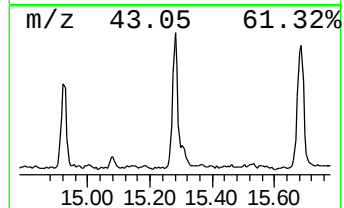
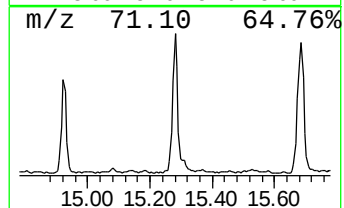
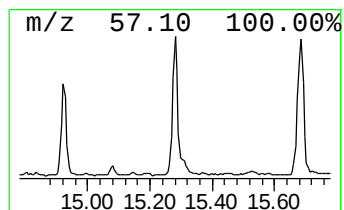
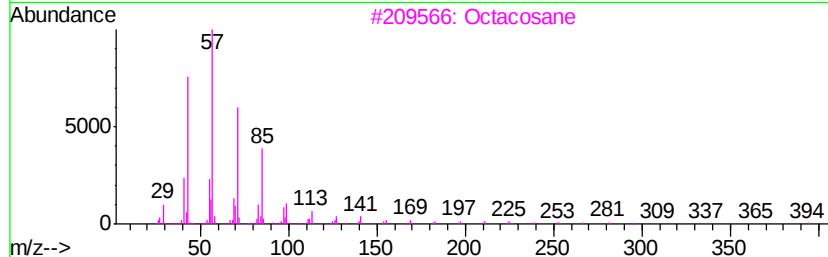
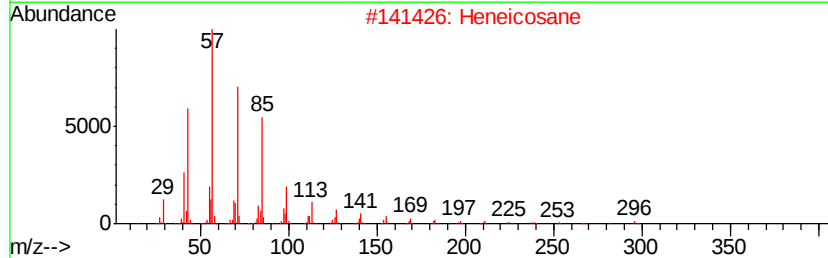
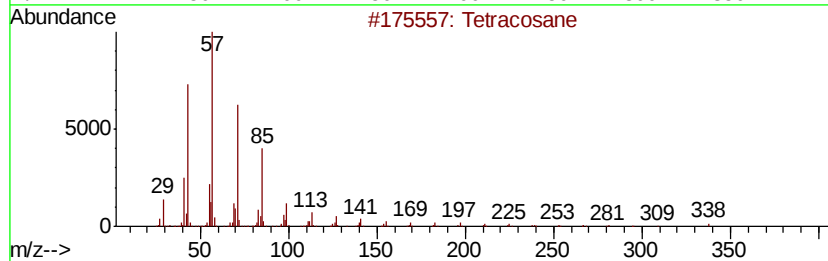
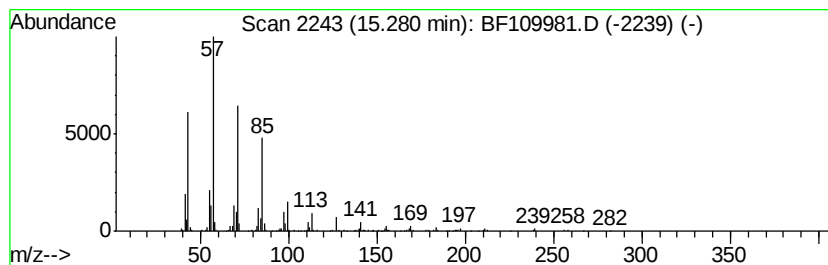
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	4.67 ng	401252	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109981.D
Acq On : 19 Oct 2018 1:29
Operator : JU/SJ
Sample : J5570-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

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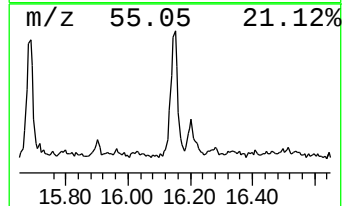
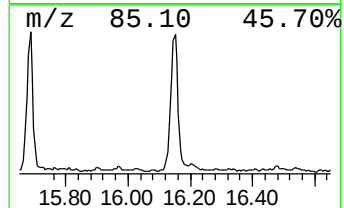
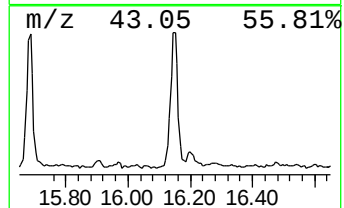
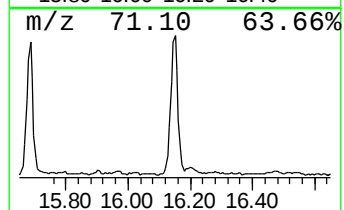
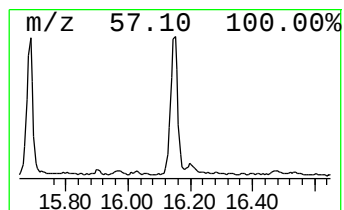
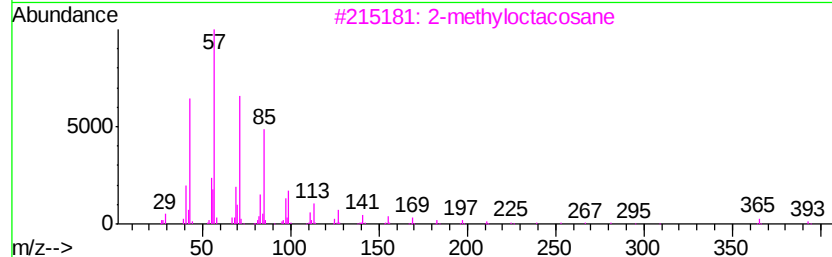
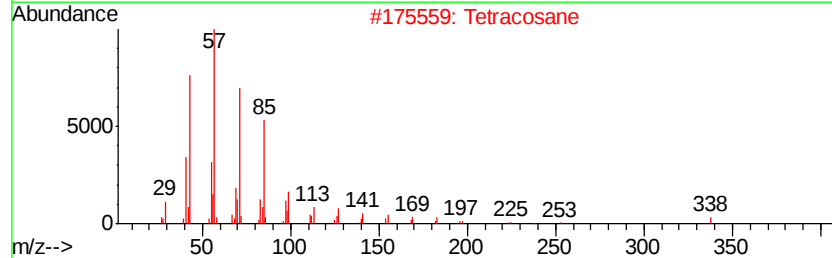
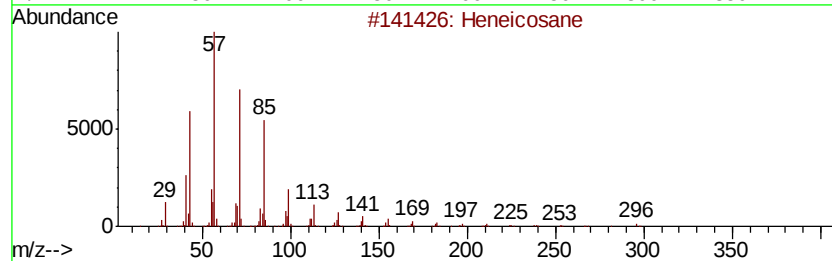
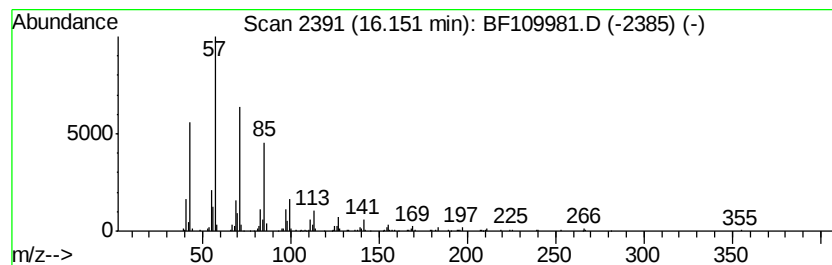
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	6.68 ng	573489	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109981.D
Acq On : 19 Oct 2018 1:29
Operator : JU/SJ
Sample : J5570-03
Misc :
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Instrument :
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ClientSampleId :
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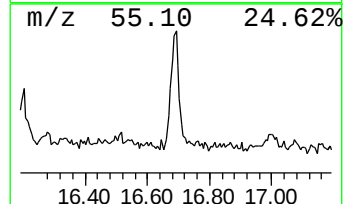
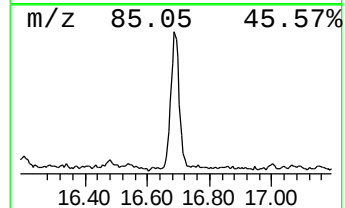
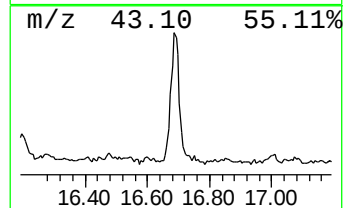
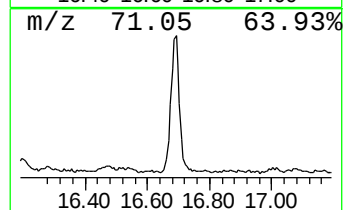
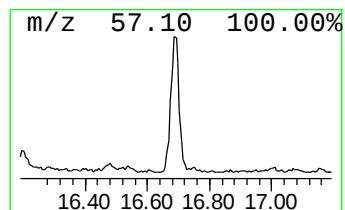
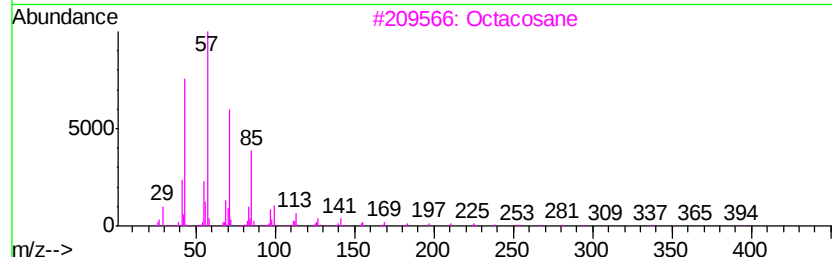
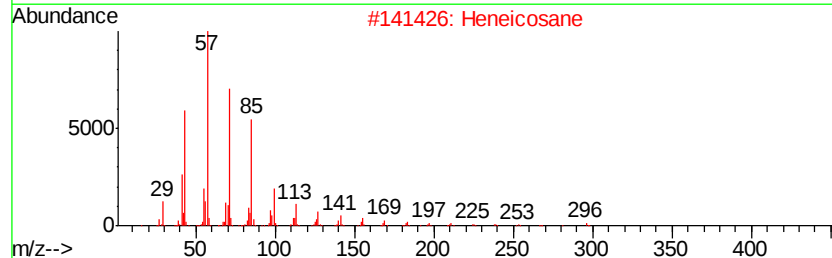
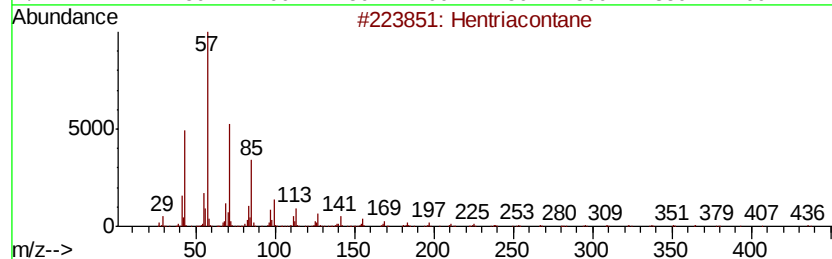
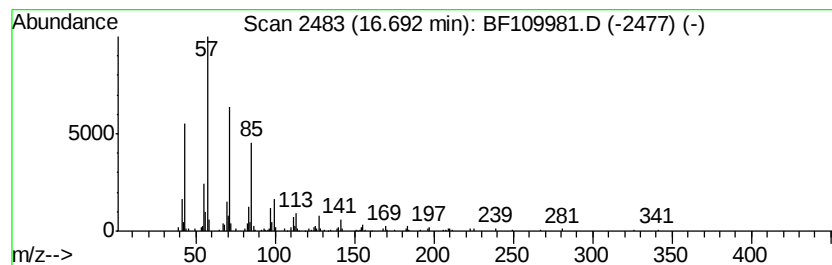
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	3.89 ng	333449	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101818\
Data File : BF109981.D
Acq On : 19 Oct 2018 1:29
Operator : JU/SJ
Sample : J5570-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

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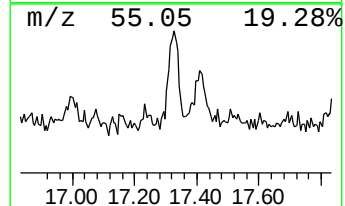
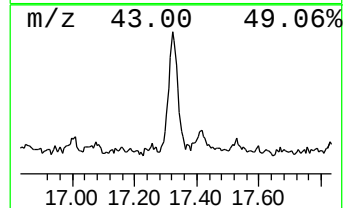
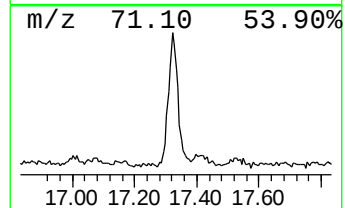
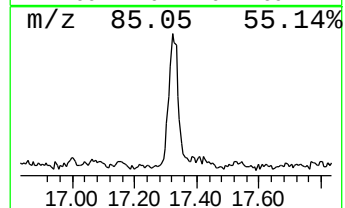
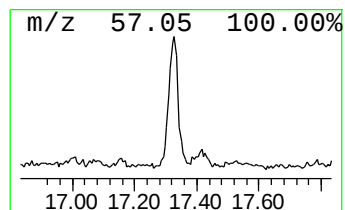
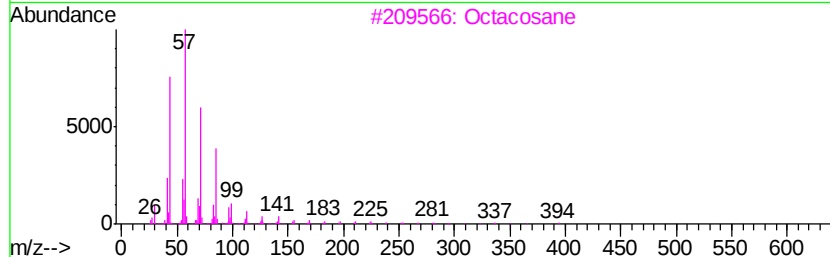
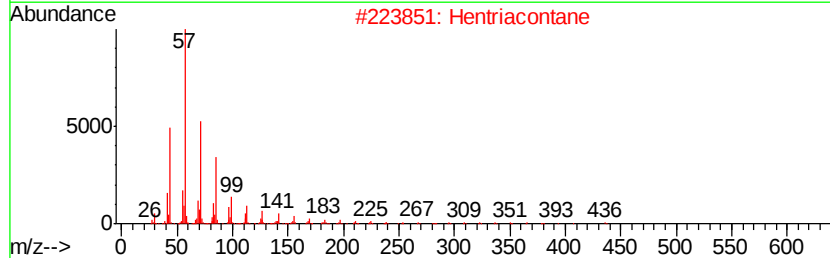
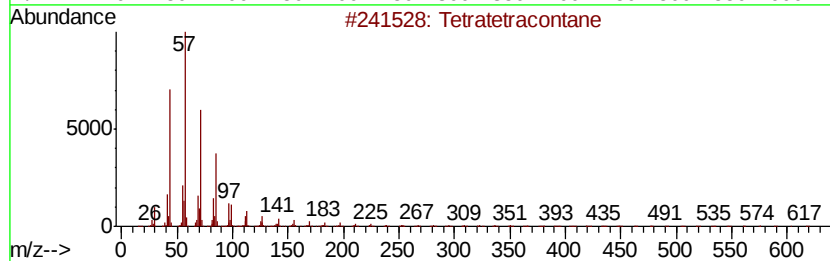
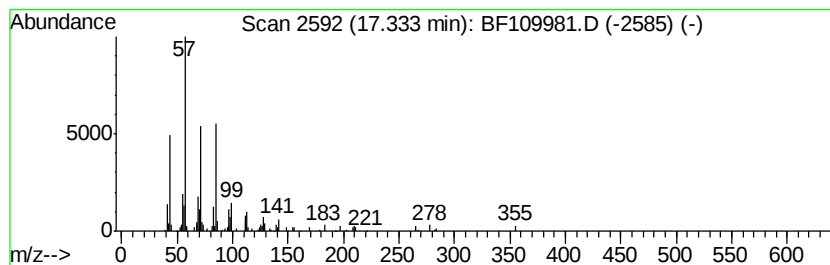
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	2.31 ng	197982	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	87
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Octacosane	394	C28H58	000630-02-4	87
4		triacontane	422	C30H62	000638-68-6	86
5		Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101818\
Data File : BF109981.D
Acq On : 19 Oct 2018 1:29
Operator : JU/SJ
Sample : J5570-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.22	2.9	ng	179770	1	6.97	1255540	20.0
unknown6.75	6.75	61.9	ng	3888350	1	6.97	1255540	20.0
1-Heneicosanol	13.97	5.5	ng	341319	5	14.15	1237530	20.0
Tricosane	14.60	3.8	ng	234428	5	14.15	1237530	20.0
Heneicosane	14.92	3.4	ng	295313	6	15.68	1716590	20.0
Tetracosane	15.28	4.7	ng	401252	6	15.68	1716590	20.0
2-methyloctacosane	16.15	6.7	ng	573489	6	15.68	1716590	20.0
Hentriacontane	16.69	3.9	ng	333449	6	15.68	1716590	20.0
Tetratetracontane	17.33	2.3	ng	197982	6	15.68	1716590	20.0