

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110718\
 Data File : BF110570.D
 Acq On : 7 Nov 2018 21:55
 Operator : JU/SJ
 Sample : J5813-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-K

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-BF102318.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	2.257	24	29	39	rVB	303548	416859	30.21%	3.026%
2	5.186	524	527	534	rBV	42075	55166	4.00%	0.400%
3	5.575	589	593	614	rBV	1398539	1300261	94.24%	9.439%
4	6.575	759	763	778	rBV	1335415	1379767	100.00%	10.017%
5	6.722	784	788	791	rBV	1600868	1345827	97.54%	9.770%
6	6.951	824	827	834	rBV	426531	354809	25.72%	2.576%
7	7.110	850	854	868	rBV	1071884	995953	72.18%	7.230%
8	7.516	919	923	934	rBV	807623	789874	57.25%	5.734%
9	8.233	1042	1045	1066	rBV	369400	412333	29.88%	2.993%
10	9.304	1224	1227	1238	rBV	1112697	1098768	79.63%	7.977%
11	9.698	1291	1294	1303	rBV	162161	151701	10.99%	1.101%
12	9.992	1341	1344	1353	rBV	412729	408160	29.58%	2.963%
13	10.786	1475	1479	1492	rBV	704948	687526	49.83%	4.991%
14	11.486	1595	1598	1601	rBV	408611	405712	29.40%	2.945%
15	11.510	1601	1602	1607	rVB	122095	105132	7.62%	0.763%
16	11.992	1681	1684	1688	rBV	90562	85296	6.18%	0.619%
17	12.110	1700	1704	1706	rBV2	16396	19241	1.39%	0.140%
18	12.321	1737	1740	1745	rBV	19811	19930	1.44%	0.145%
19	12.704	1802	1805	1809	rBV	261668	240371	17.42%	1.745%
20	12.939	1842	1845	1849	rVB	213827	193491	14.02%	1.405%
21	13.068	1863	1867	1871	rBV	1314622	1086376	78.74%	7.887%
22	13.151	1878	1881	1885	rVB3	11145	18303	1.33%	0.133%
23	13.262	1894	1900	1906	rBV2	29263	52775	3.82%	0.383%
24	13.368	1915	1918	1926	rBV5	11437	22247	1.61%	0.162%
25	13.498	1937	1940	1943	rBV4	18909	20856	1.51%	0.151%
26	13.615	1957	1960	1963	rBV2	15815	17424	1.26%	0.126%
27	13.780	1985	1988	1991	rBV	18182	19471	1.41%	0.141%
28	13.886	2003	2006	2008	rBV	25822	23705	1.72%	0.172%
29	13.945	2013	2016	2021	rVV3	141436	171373	12.42%	1.244%
30	13.986	2021	2023	2028	rVB	26559	38164	2.77%	0.277%
31	14.139	2044	2049	2052	rBV2	492072	569597	41.28%	4.135%
32	14.162	2052	2053	2060	rVB	111786	97001	7.03%	0.704%
33	14.262	2068	2070	2073	rVB	27124	22015	1.60%	0.160%
34	14.568	2119	2122	2130	rBV4	53930	92541	6.71%	0.672%

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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

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35	14.886	2173	2176	2181	rVB	61178	63826	4.63%	0.463%
36	14.962	2187	2189	2194	rVB	38284	41030	2.97%	0.298%
37	15.045	2199	2203	2207	rBV2	83990	93351	6.77%	0.678%
38	15.209	2228	2231	2234	rBV	67468	104863	7.60%	0.761%
39	15.239	2234	2236	2239	rVV	117550	114004	8.26%	0.828%
40	15.274	2239	2242	2248	rVB4	50644	77140	5.59%	0.560%
41	15.603	2295	2298	2300	rBV	40884	43795	3.17%	0.318%
42	15.639	2300	2304	2306	rVV	52368	76696	5.56%	0.557%
43	15.668	2306	2309	2313	rVB	197487	240897	17.46%	1.749%
44	16.092	2377	2381	2388	rVB	88090	136154	9.87%	0.988%
45	16.627	2468	2472	2478	rVB3	37193	65026	4.71%	0.472%

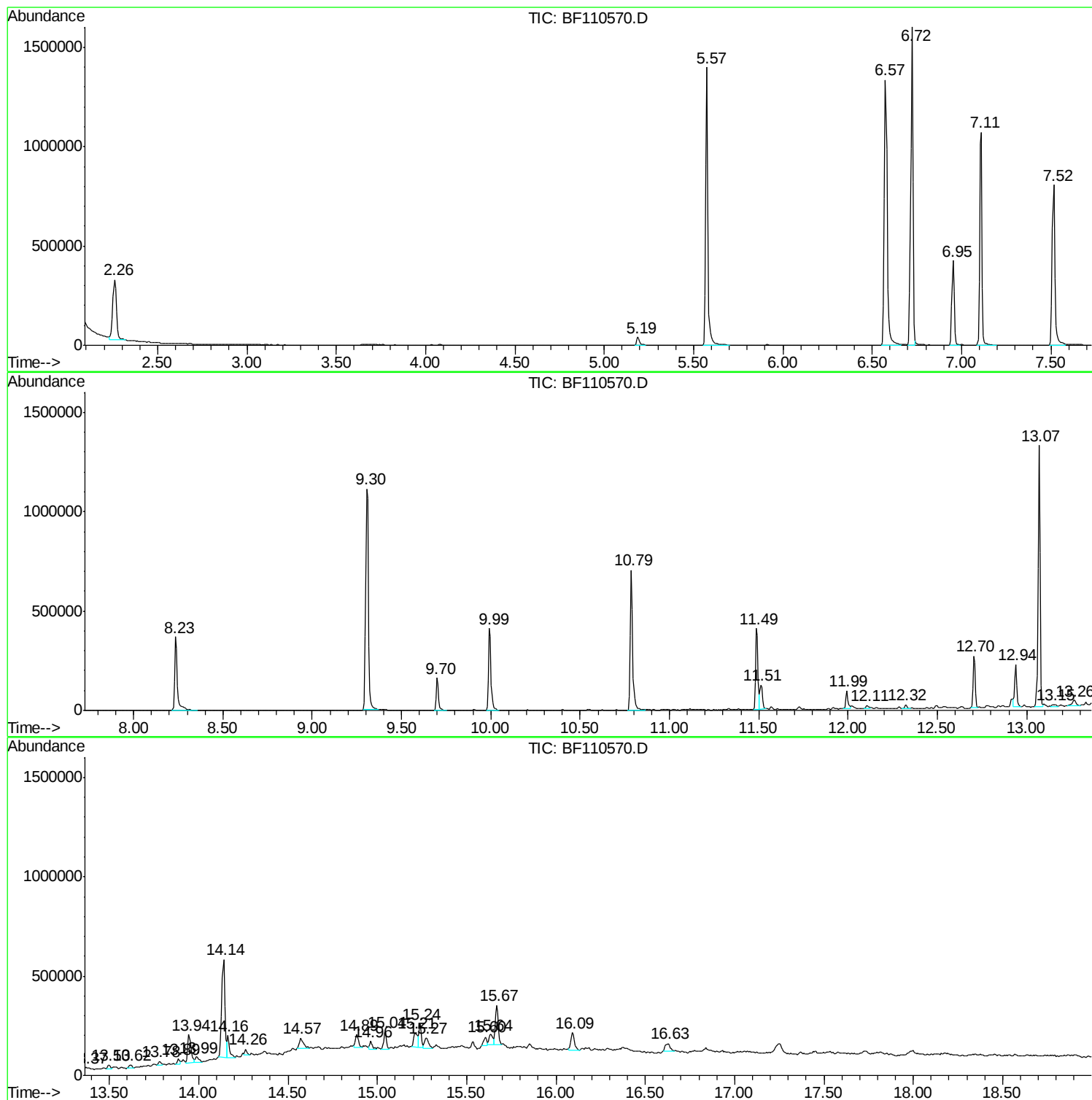
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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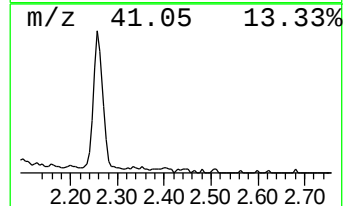
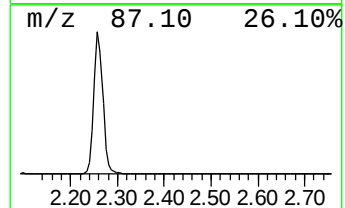
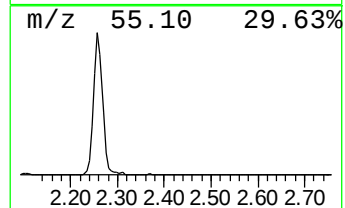
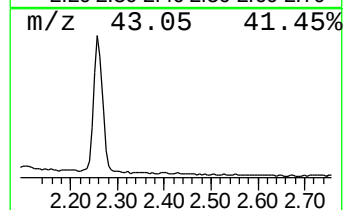
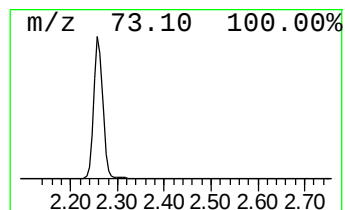
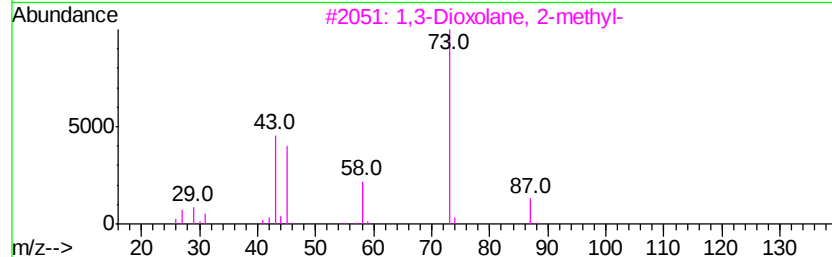
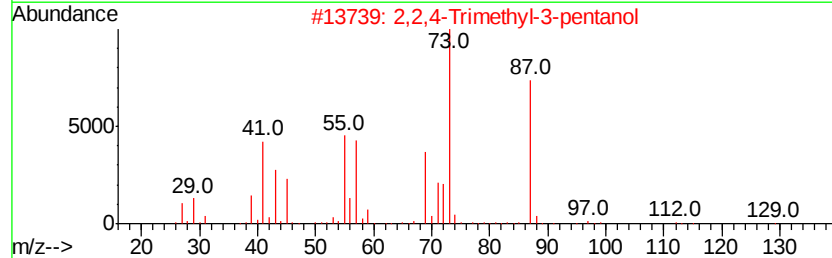
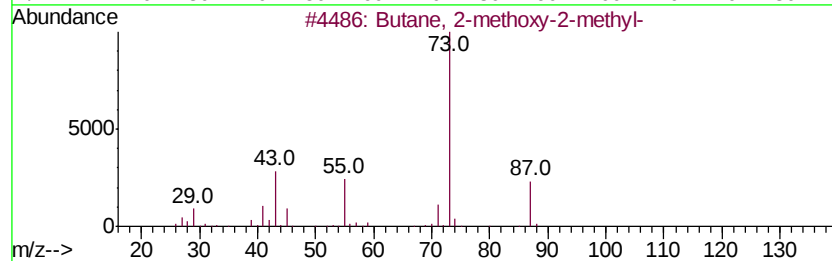
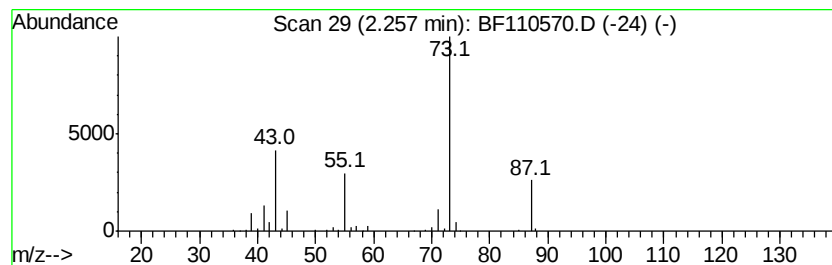
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.26	23.50 ng	416859	1,4-Dichlorobenzene-d4	6.95

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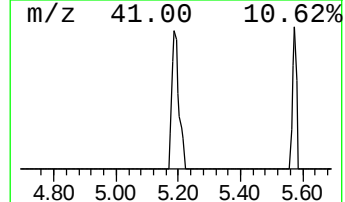
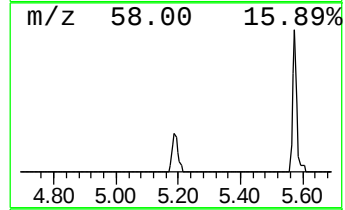
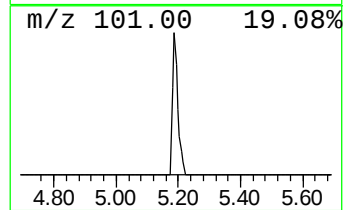
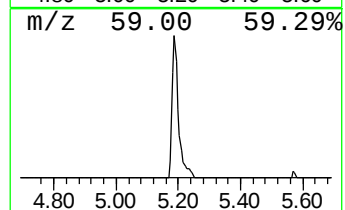
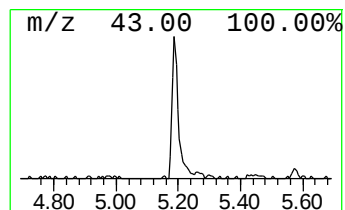
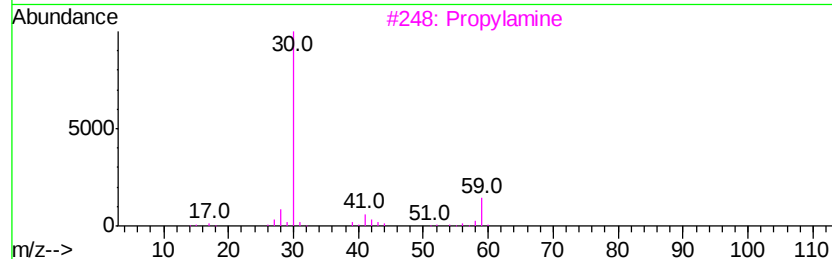
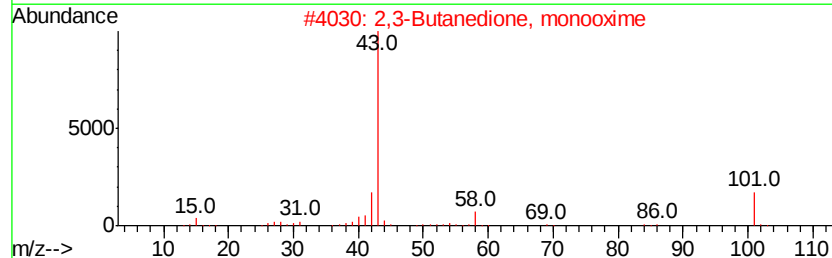
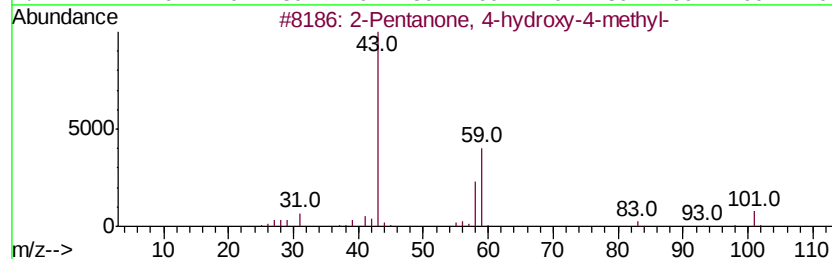
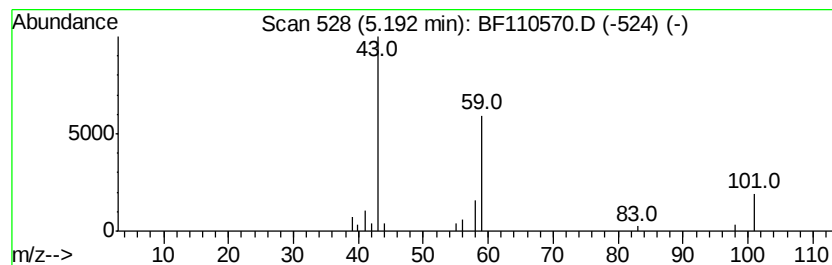
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.11 ng	55166	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3			Propylamine	59	C3H9N	000107-10-8	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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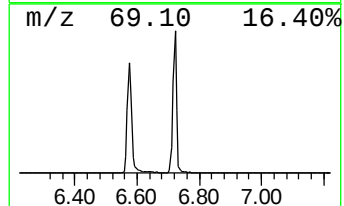
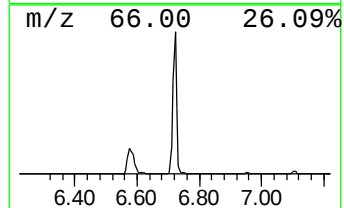
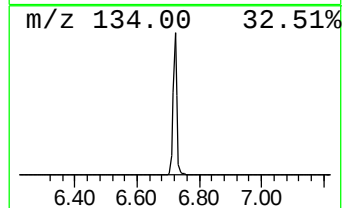
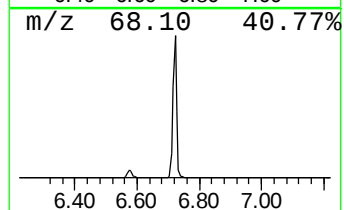
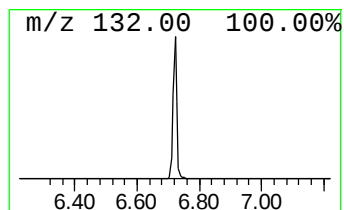
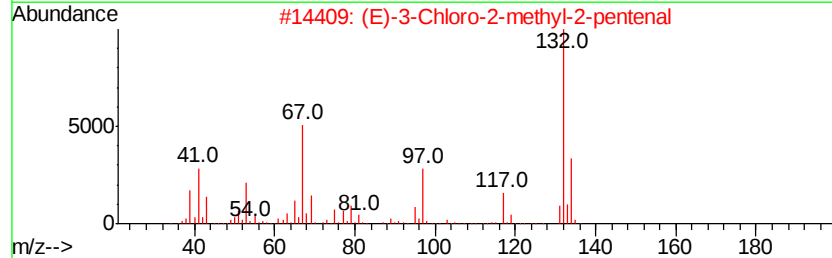
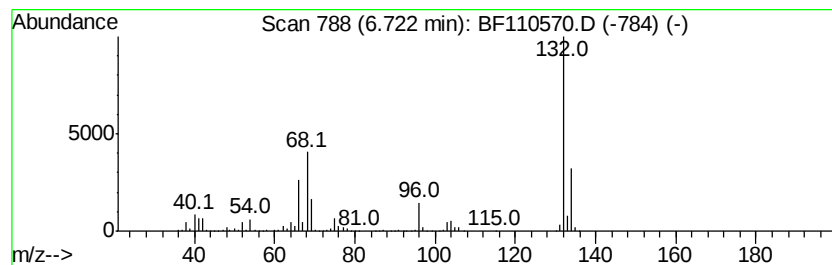
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	75.86 ng	1345830	1,4-Dichlorobenzene-d4	6.95

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	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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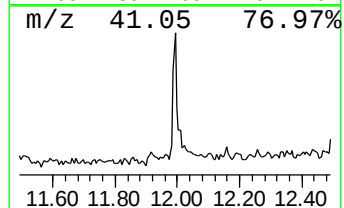
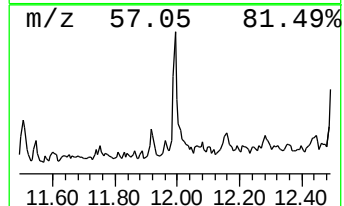
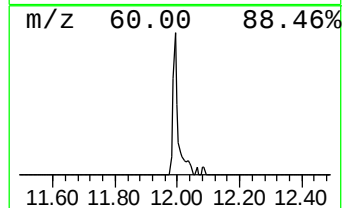
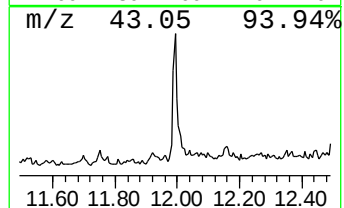
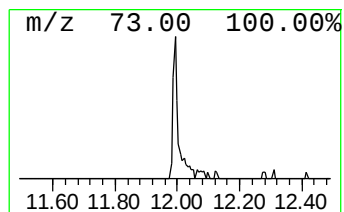
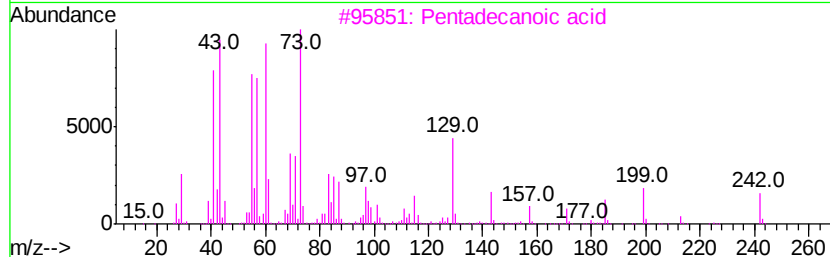
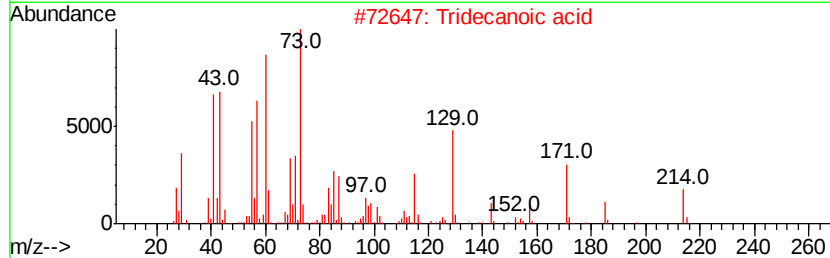
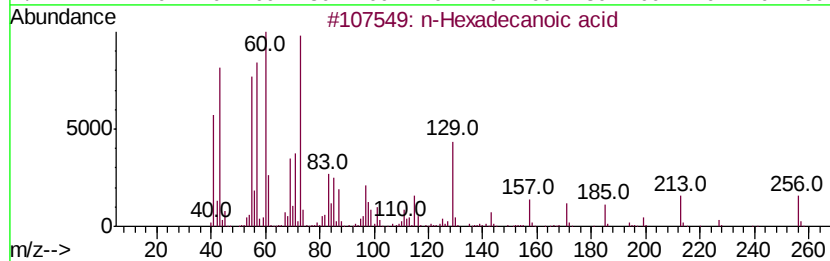
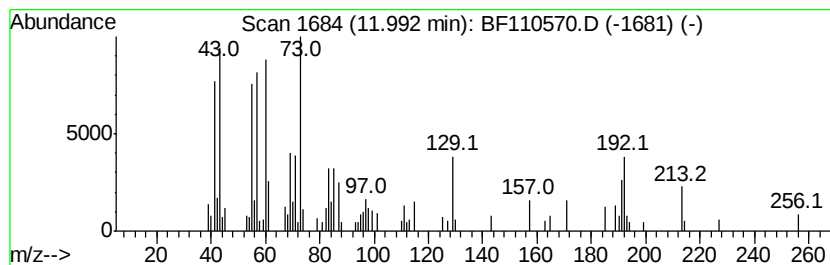
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	4.20 ng	85296	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		D-Glucopyranoside, 4-O-decyl-	320	C16H32O6	1000158-00-4	27



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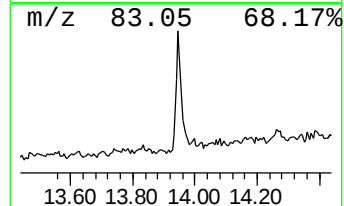
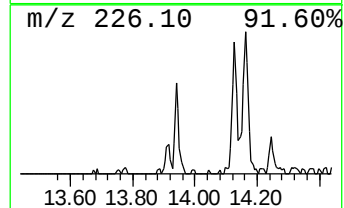
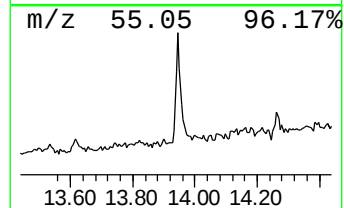
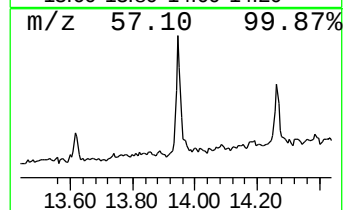
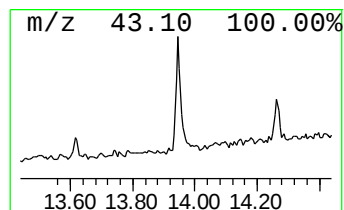
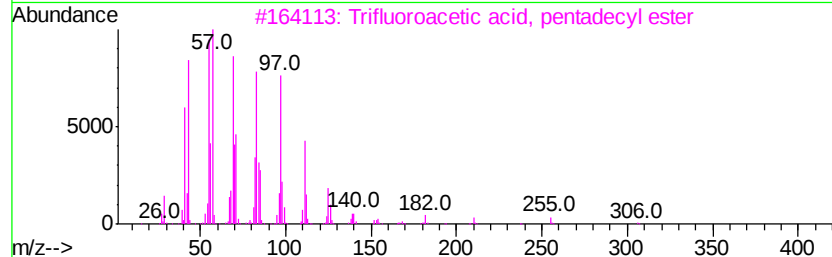
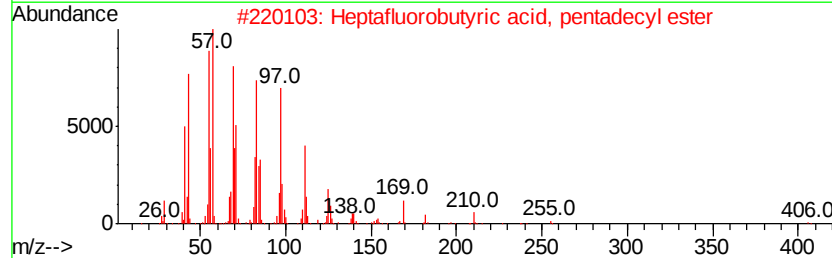
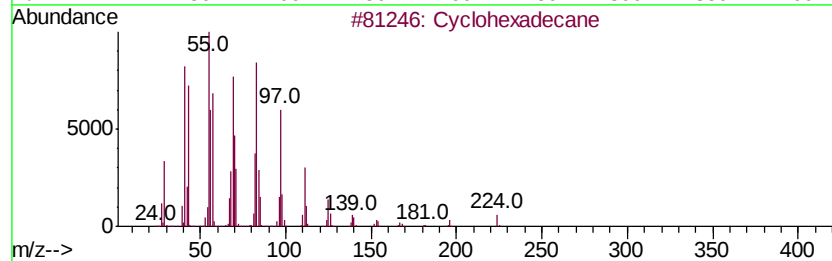
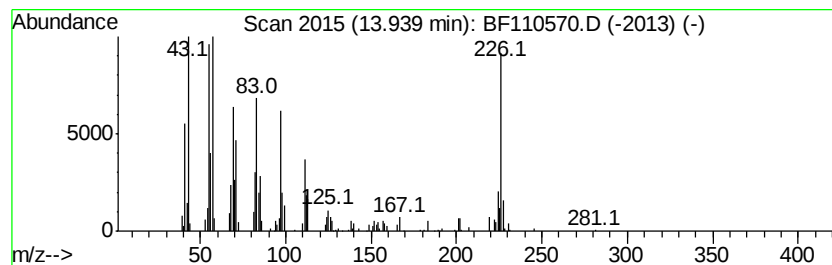
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	6.02 ng	171373	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 98
2		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 93
3		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 91
4		Carbonic acid, hexadecyl isobuty...	342 C21H42O3	1000314-61-3 87
5		Trichloroacetic acid, 4-hexadecy...	386 C18H33Cl3O2	1000282-92-4 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110570.D
Acq On : 7 Nov 2018 21:55
Operator : JU/SJ
Sample : J5813-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-K

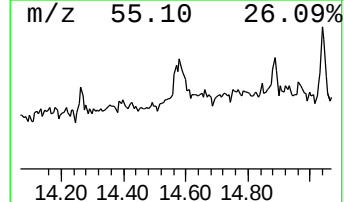
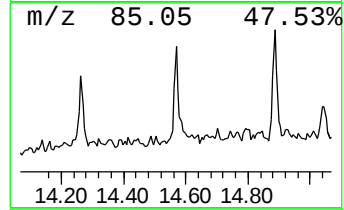
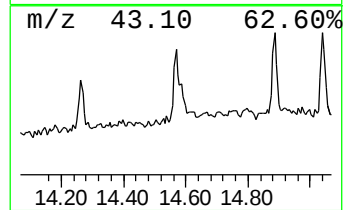
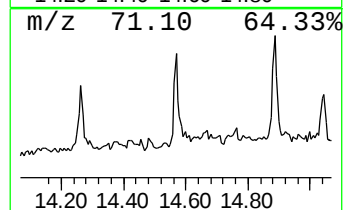
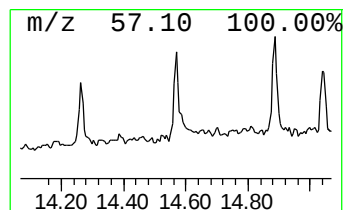
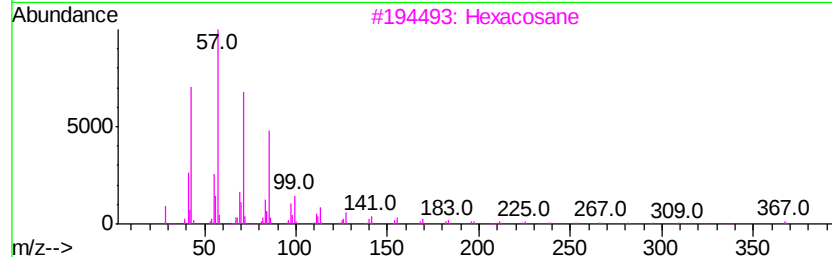
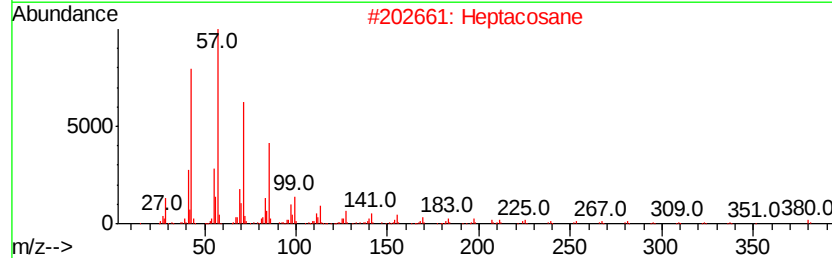
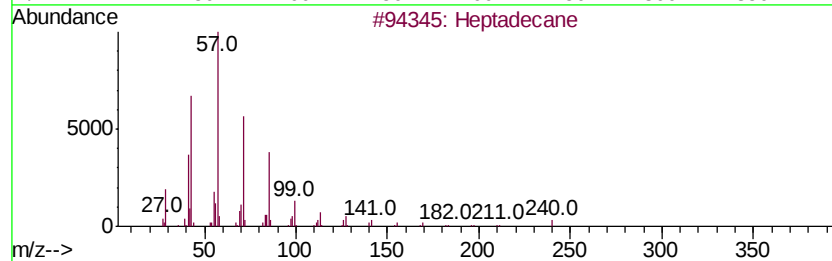
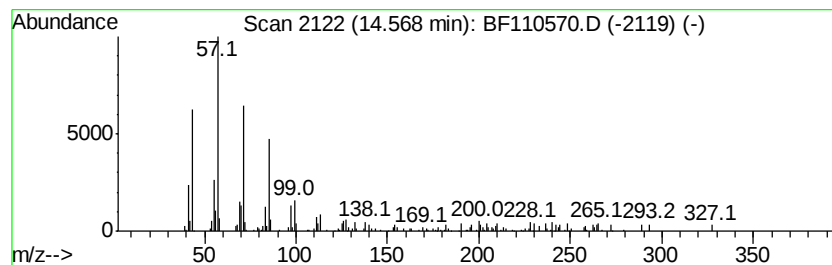
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.25 ng	92541	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	89
2		Heptacosane	380	C27H56	000593-49-7	62
3		Hexacosane	366	C26H54	000630-01-3	62
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110570.D
Acq On : 7 Nov 2018 21:55
Operator : JU/SJ
Sample : J5813-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-K

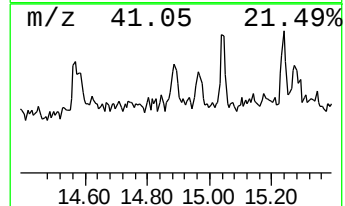
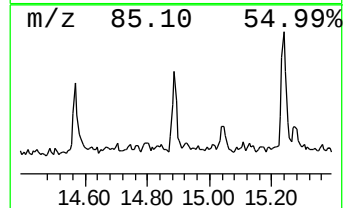
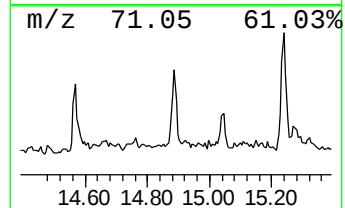
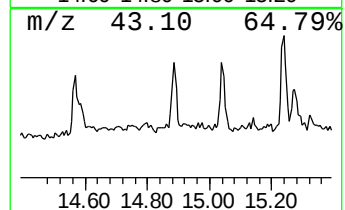
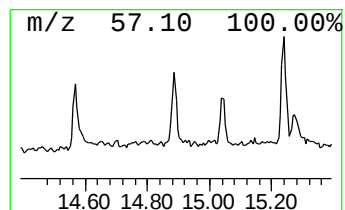
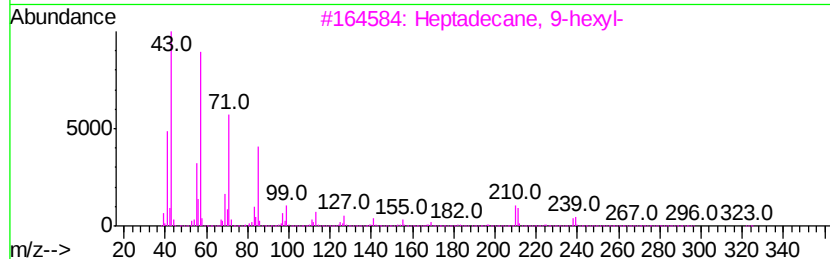
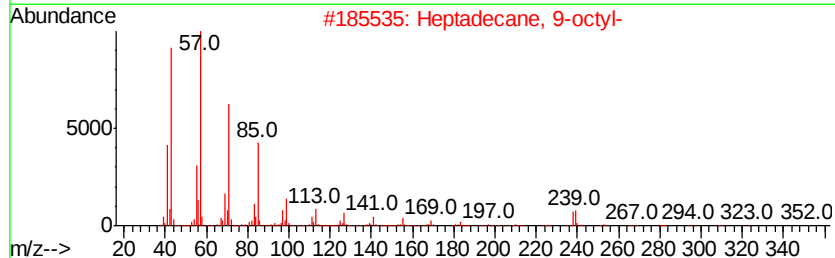
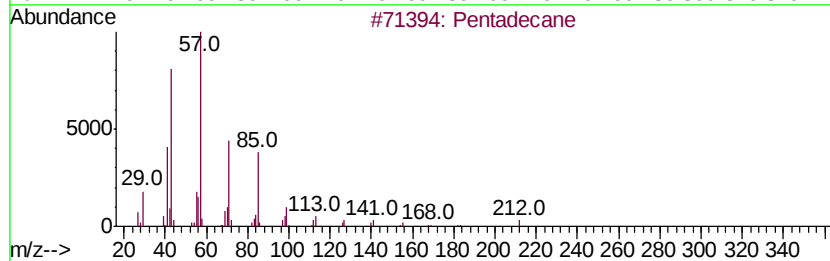
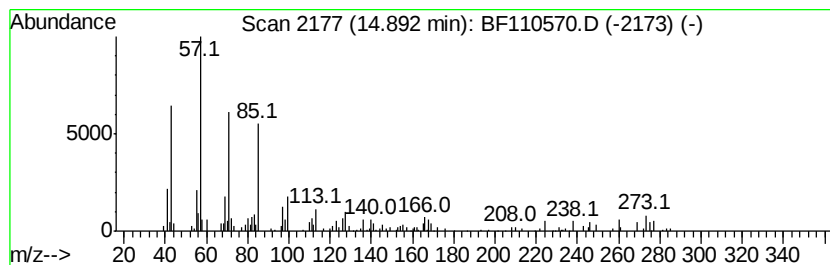
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.24 ng	63826	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	58
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	58
3		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	53
4		Hexacosane	366	C26H54	000630-01-3	52
5		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110570.D
Acq On : 7 Nov 2018 21:55
Operator : JU/SJ
Sample : J5813-11
Misc :
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ClientSampleId :
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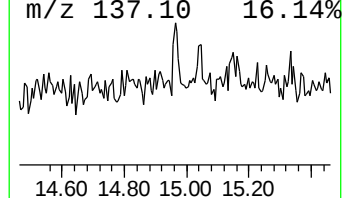
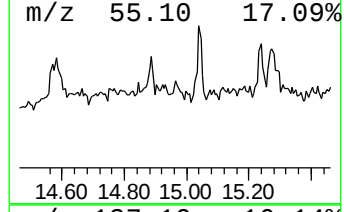
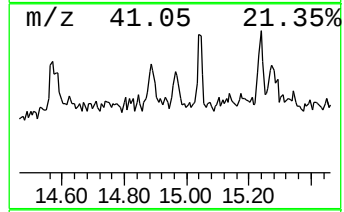
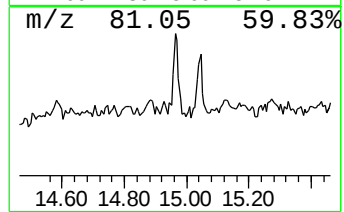
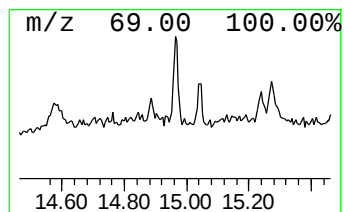
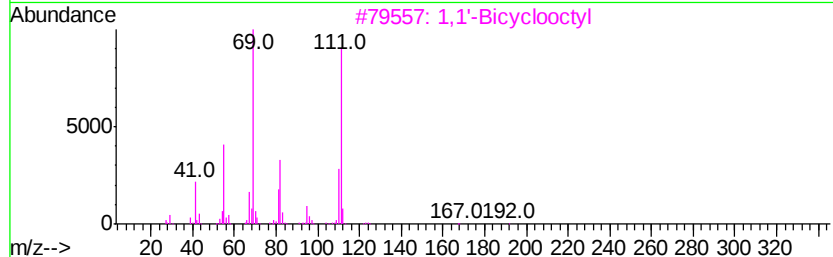
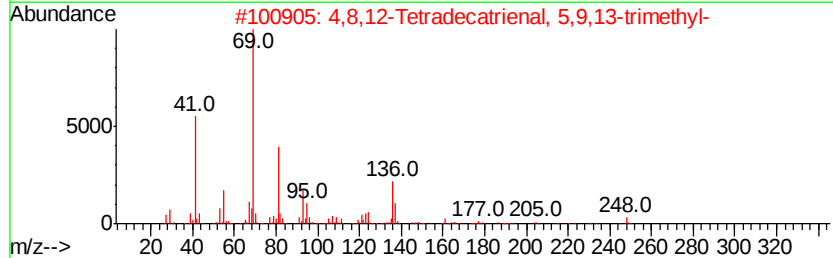
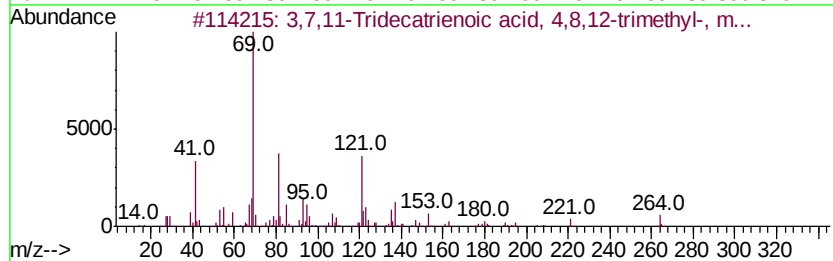
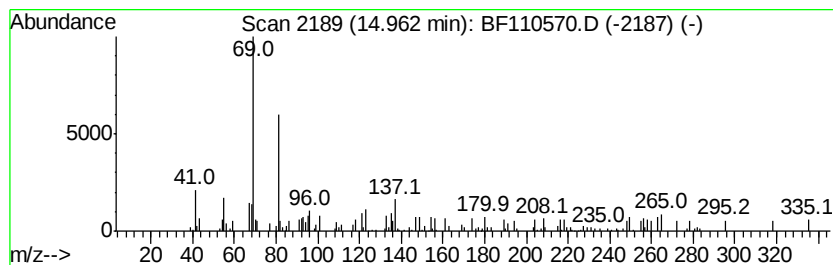
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3,7,11-Tridecatrienoic acid... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.41 ng	41030	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	50
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	49
3			1,1'-Bicyclooctyl	222	C16H30	006708-17-4	47
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	47
5			1,3-Butylene glycol dimethacrylate	226	C12H18O4	001189-08-8	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110570.D
Acq On : 7 Nov 2018 21:55
Operator : JU/SJ
Sample : J5813-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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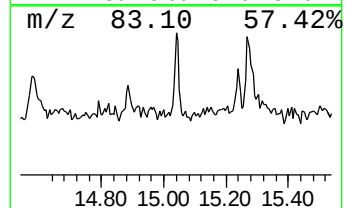
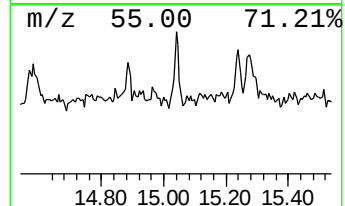
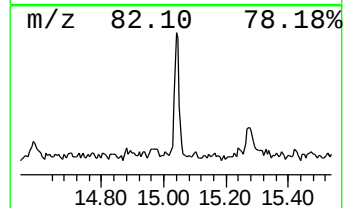
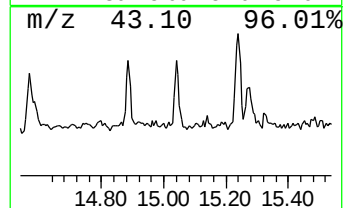
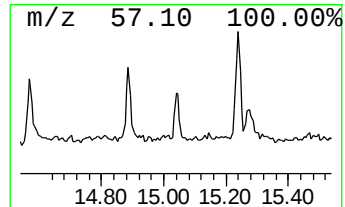
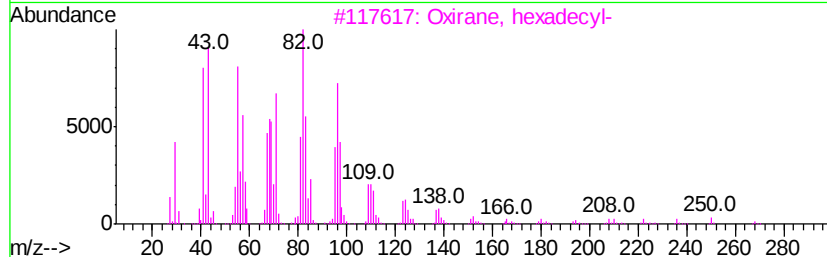
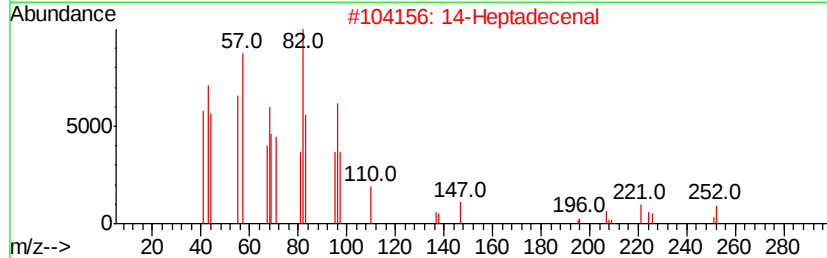
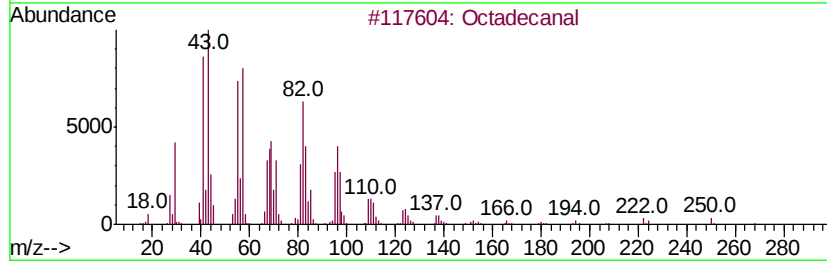
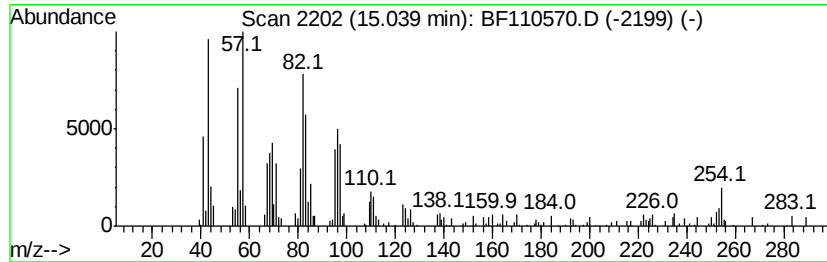
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	7.75 ng	93351	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	87
2			14-Heptadecenal	252	C17H32O	1000144-58-0	86
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
4			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	68
5			1,19-Eicosadiene	278	C20H38	014811-95-1	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110570.D
Acq On : 7 Nov 2018 21:55
Operator : JU/SJ
Sample : J5813-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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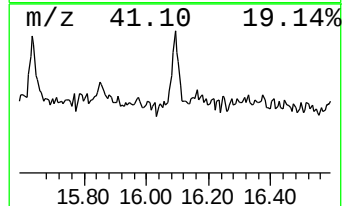
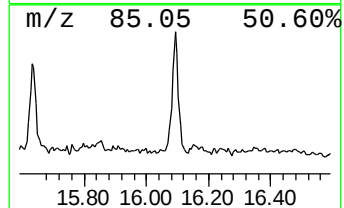
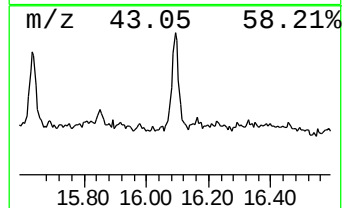
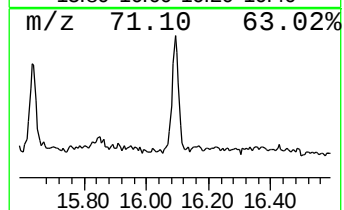
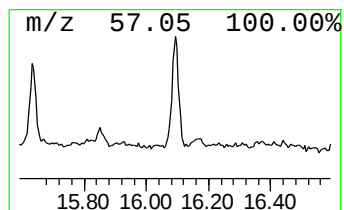
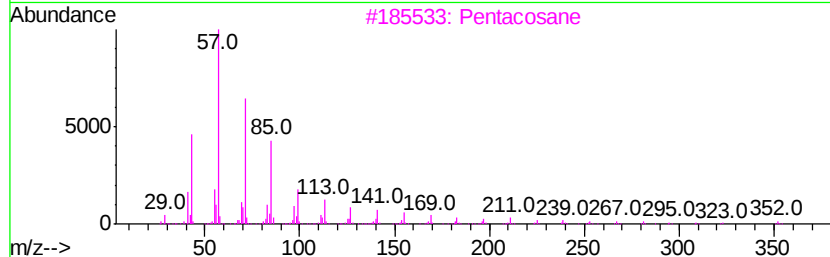
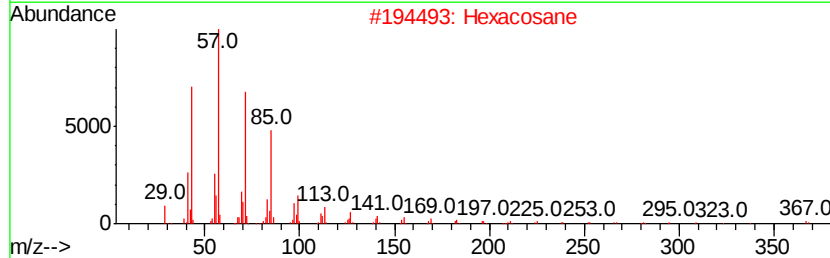
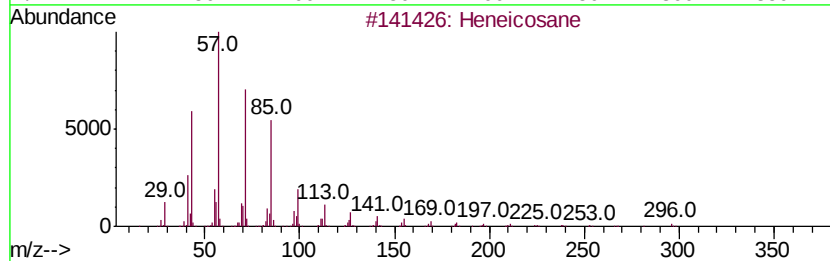
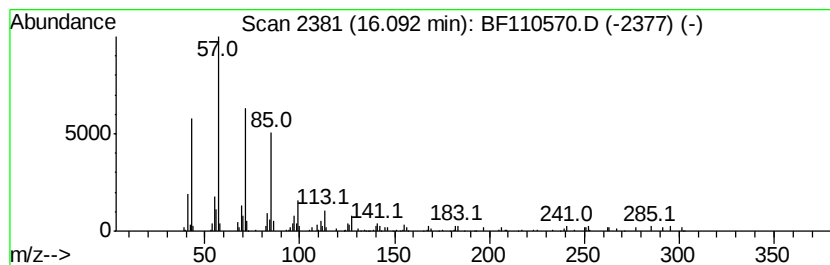
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	11.30 ng	136154	Perylene-d12	15.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Pentacosane		352	C25H52	000629-99-2	87
4	triacontane		422	C30H62	000638-68-6	87
5	Octadecane		254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
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Acq On : 7 Nov 2018 21:55
Operator : JU/SJ
Sample : J5813-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TS-K

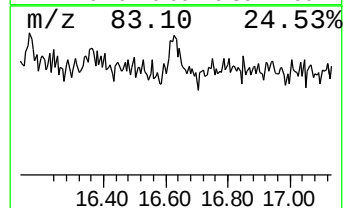
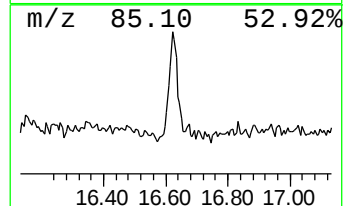
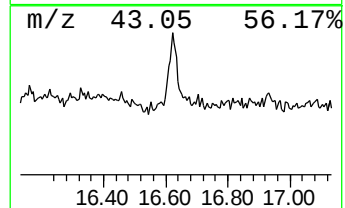
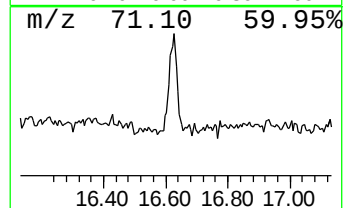
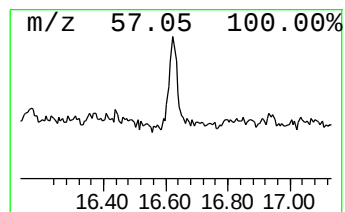
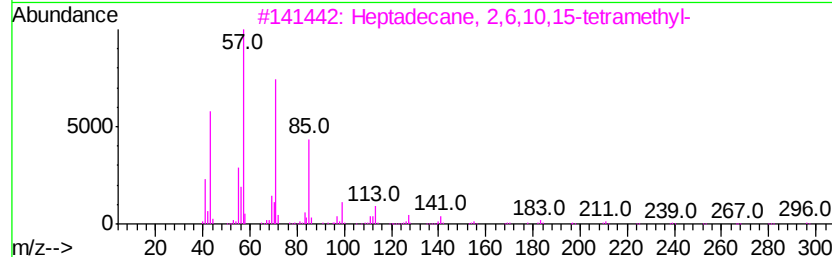
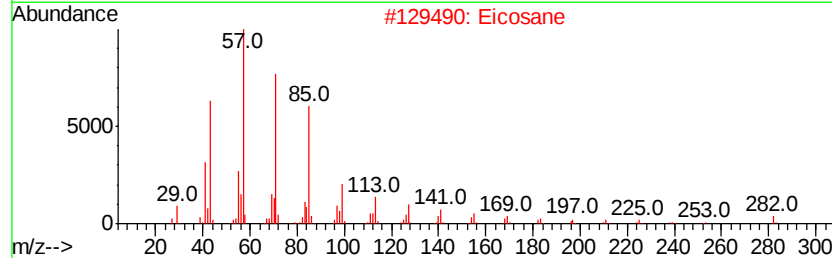
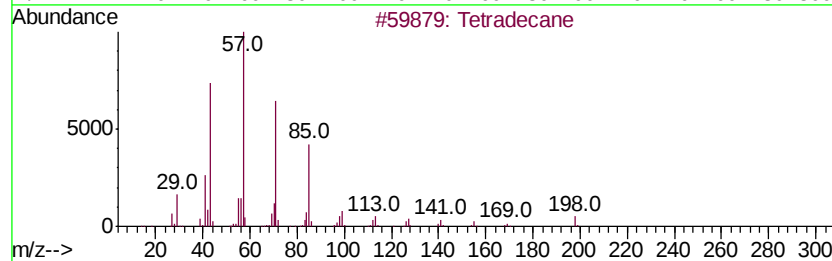
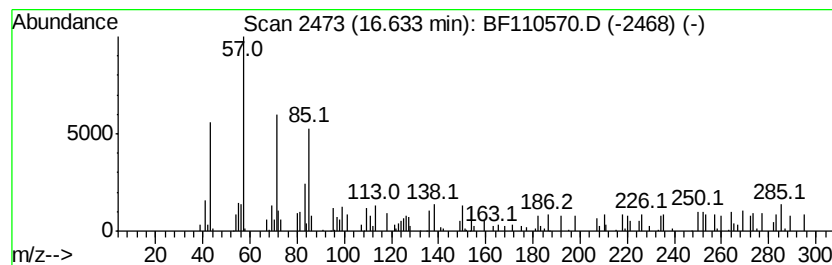
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	5.40 ng	65026	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	70
2			Eicosane	282	C20H42	000112-95-8	62
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58
4			Heptadecane	240	C17H36	000629-78-7	58
5			Tetratetracontane	619	C44H90	007098-22-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110718\
Data File : BF110570.D
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Operator : JU/SJ
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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...	5.19	3.1	ng	55166	1	6.95	354809	20.0
unknown6.72	6.72	75.9	ng	1345830	1	6.95	354809	20.0
n-Hexadecanoic acid	11.99	4.2	ng	85296	4	11.49	405712	20.0
Cyclohexadecane	13.94	6.0	ng	171373	5	14.14	569597	20.0
Heptadecane	14.57	3.3	ng	92541	5	14.14	569597	20.0
Pentadecane	14.89	2.2	ng	63826	5	14.14	569597	20.0
3,7,11-Tridecatri...	14.96	3.4	ng	41030	6	15.67	240897	20.0
Octadecanal	15.04	7.8	ng	93351	6	15.67	240897	20.0
Heneicosane	16.09	11.3	ng	136154	6	15.67	240897	20.0
Tetradecane	16.63	5.4	ng	65026	6	15.67	240897	20.0