

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
 Data File : BF110617.D
 Acq On : 9 Nov 2018 10:31
 Operator : JU/SJ
 Sample : J5813-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-D

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-BF110818.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	2.269	25	31	42	rVB	314726	436772	21.32%	2.264%
2	5.192	524	528	538	rBV	32552	48679	2.38%	0.252%
3	5.569	587	592	595	rBV	1923695	1801812	87.95%	9.340%
4	6.575	757	763	777	rBV	1764486	2035429	99.35%	10.551%
5	6.716	782	787	790	rBV	2227315	1965354	95.93%	10.188%
6	6.945	822	826	832	rBV	561657	477659	23.31%	2.476%
7	7.098	848	852	856	rBV	1606004	1503663	73.39%	7.794%
8	7.510	917	922	925	rBV	1293873	1205926	58.86%	6.251%
9	8.227	1040	1044	1056	rBV	654184	612783	29.91%	3.176%
10	9.298	1221	1226	1229	rBV	2386673	2048775	100.00%	10.620%
11	9.692	1289	1293	1297	rBV	241863	211739	10.33%	1.098%
12	9.986	1339	1343	1352	rVB	680816	604297	29.50%	3.132%
13	10.774	1474	1477	1491	rBV	764262	758241	37.01%	3.930%
14	11.480	1593	1597	1599	rBV	529694	479957	23.43%	2.488%
15	11.504	1599	1601	1604	rVB	63301	55311	2.70%	0.287%
16	11.986	1678	1683	1699	rBV	447818	664190	32.42%	3.443%
17	12.639	1789	1794	1798	rBV6	16641	31140	1.52%	0.161%
18	12.698	1798	1804	1807	rBV	139245	140728	6.87%	0.729%
19	12.774	1811	1817	1825	rBV	481039	596046	29.09%	3.090%
20	12.927	1837	1843	1848	rVB	110381	123670	6.04%	0.641%
21	13.062	1861	1866	1869	rBV	1454098	1292377	63.08%	6.699%
22	13.486	1935	1938	1942	rBV5	21477	37495	1.83%	0.194%
23	13.939	2012	2015	2021	rBV2	131355	191579	9.35%	0.993%
24	14.127	2043	2047	2050	rBV	492576	498026	24.31%	2.582%
25	14.157	2050	2052	2059	rVB	51993	46997	2.29%	0.244%
26	14.257	2066	2069	2072	rVB	45371	40217	1.96%	0.208%
27	14.562	2117	2121	2124	rBV	104176	117426	5.73%	0.609%
28	14.874	2171	2174	2178	rVB	149780	154661	7.55%	0.802%
29	15.204	2227	2230	2231	rBV	46050	57525	2.81%	0.298%
30	15.227	2231	2234	2238	rVB	230184	261709	12.77%	1.357%
31	15.627	2298	2302	2304	rBV	157199	211308	10.31%	1.095%
32	15.656	2304	2307	2311	rVB	250874	297189	14.51%	1.541%
33	16.074	2375	2378	2384	rVB	128893	192248	9.38%	0.997%
34	16.609	2465	2469	2474	rVB	60089	90582	4.42%	0.470%

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ALS Vial : 4 Sample Multiplier: 1

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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-BF110818.M
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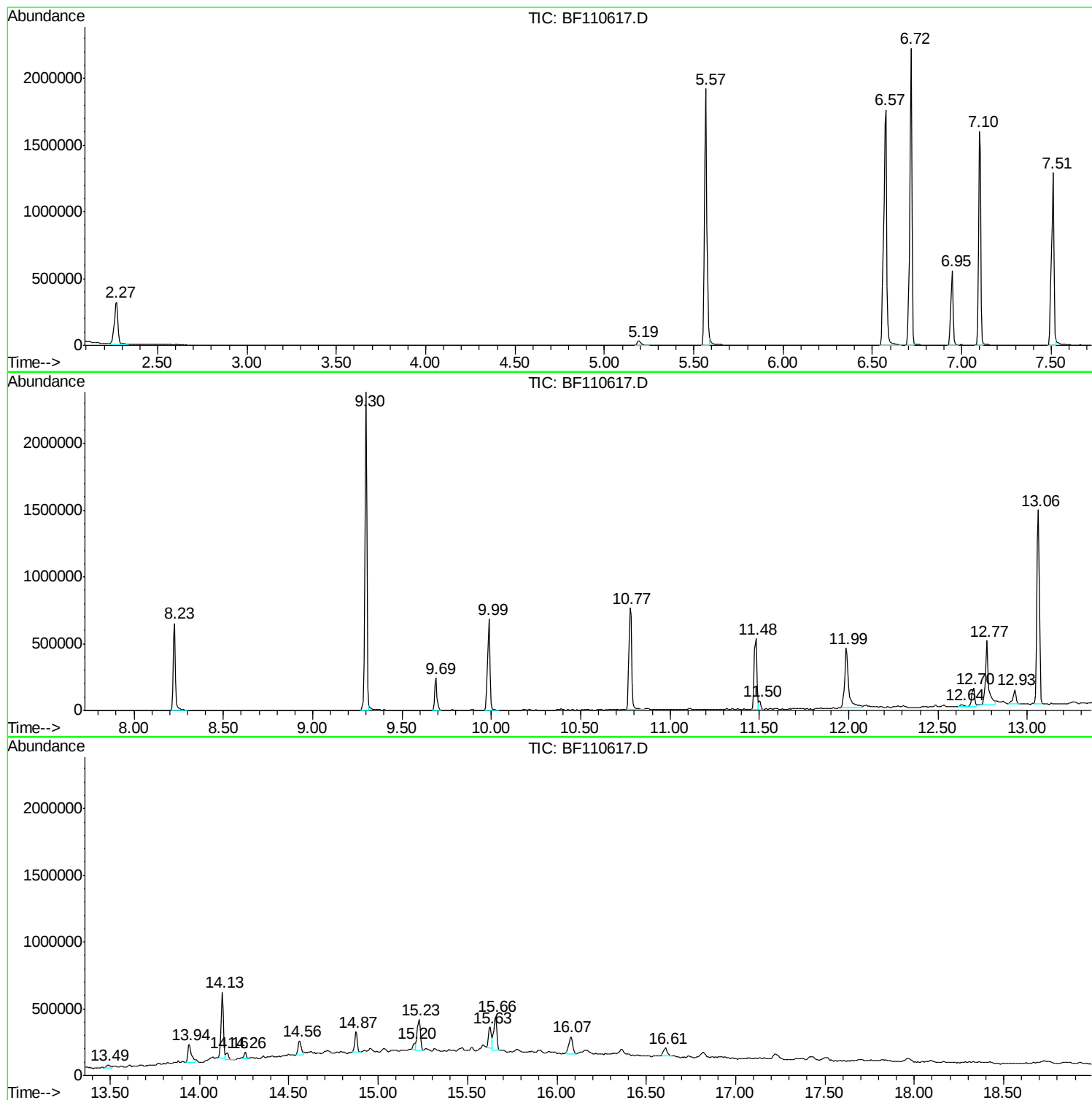
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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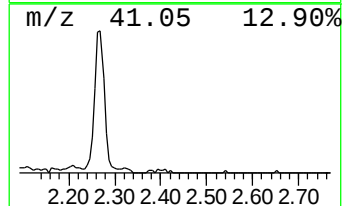
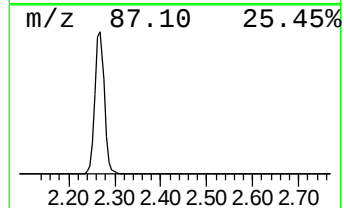
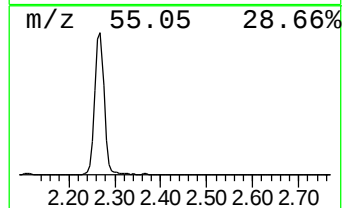
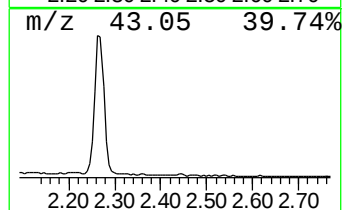
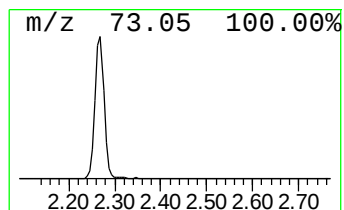
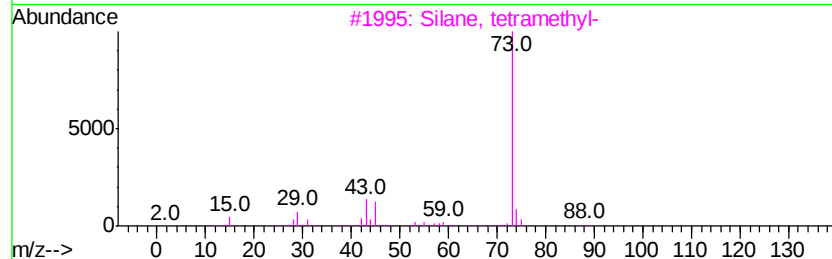
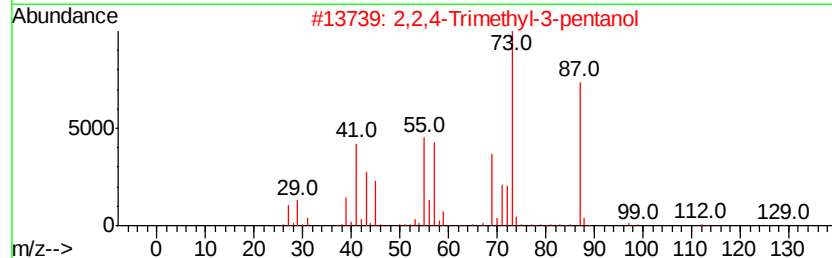
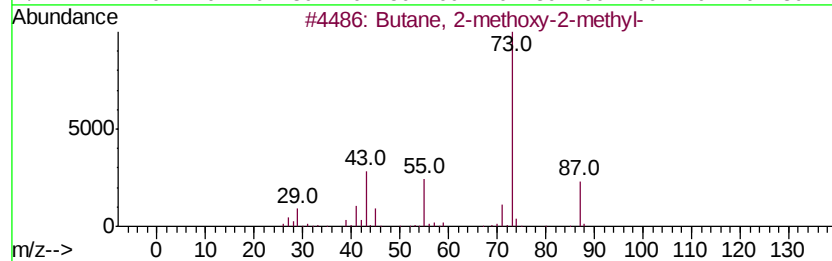
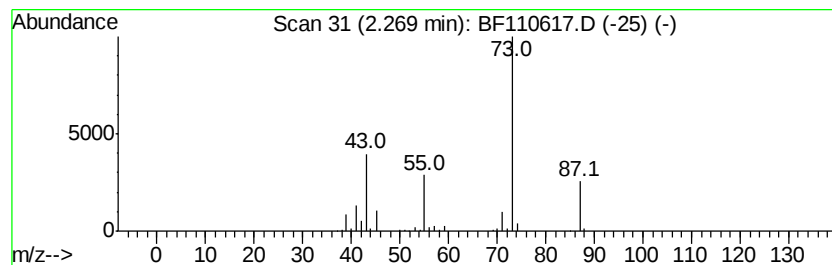
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	18.29 ng	436772	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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17



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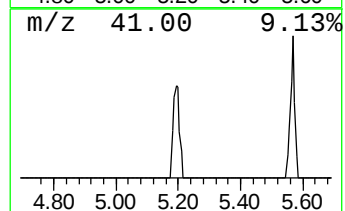
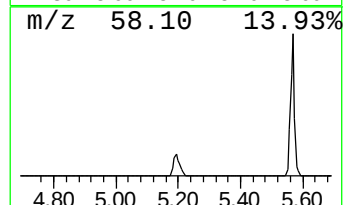
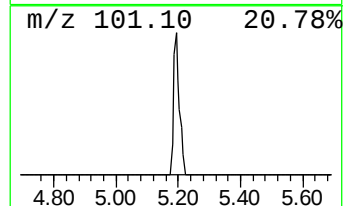
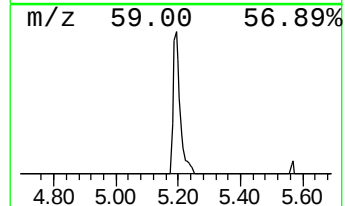
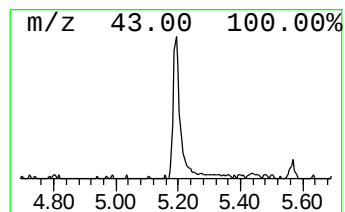
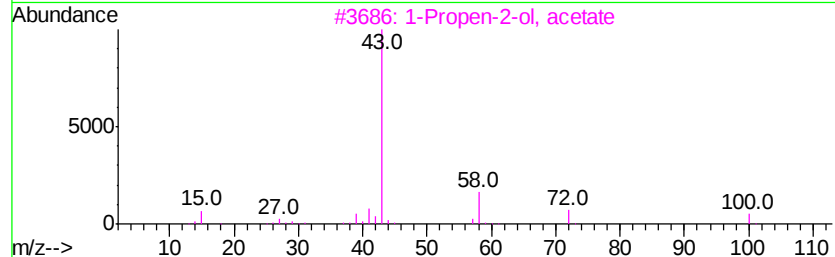
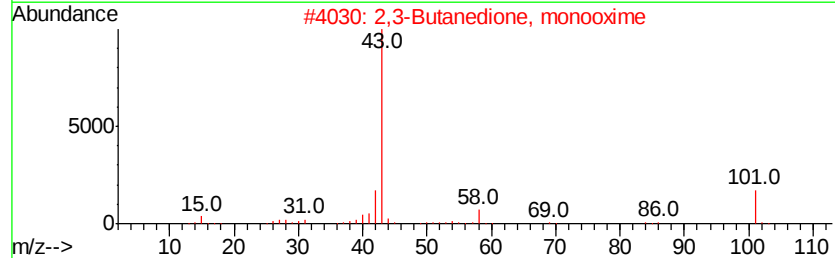
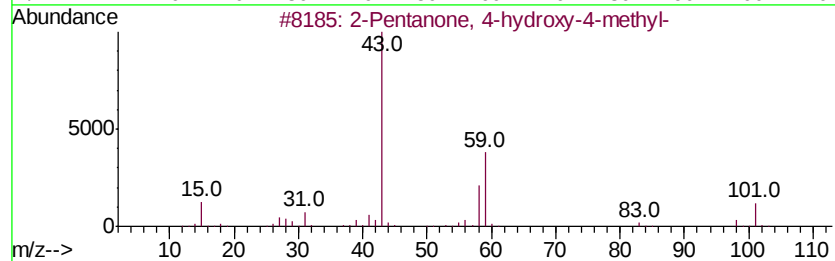
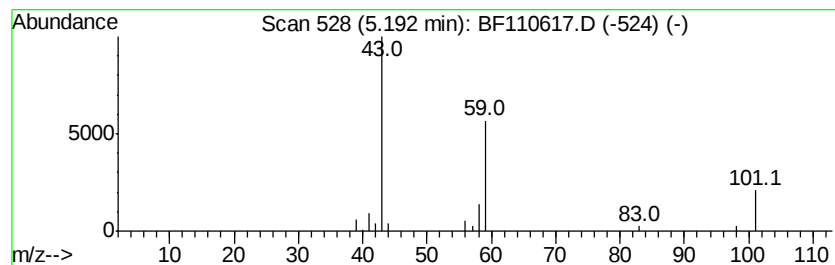
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.04 ng	48679	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4		3-Hexanol	102	C6H14O	000623-37-0	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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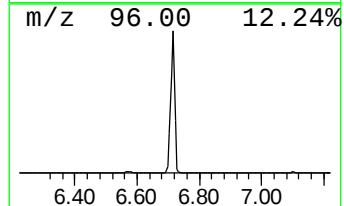
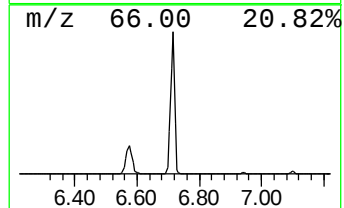
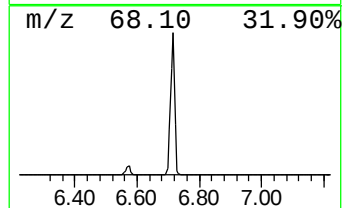
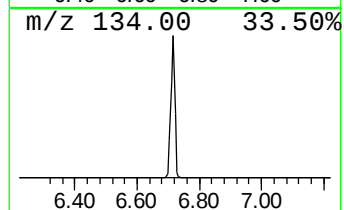
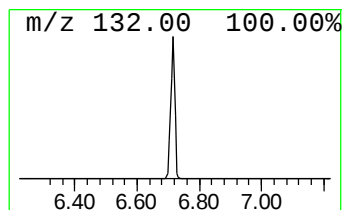
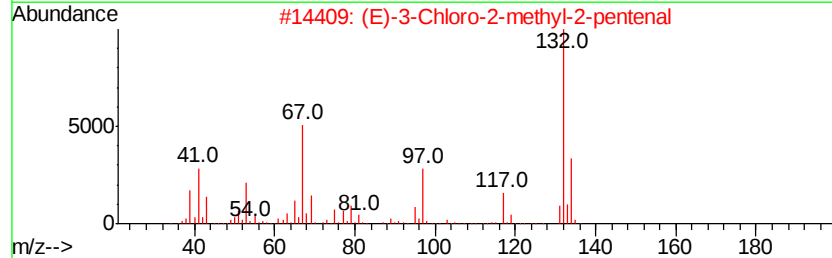
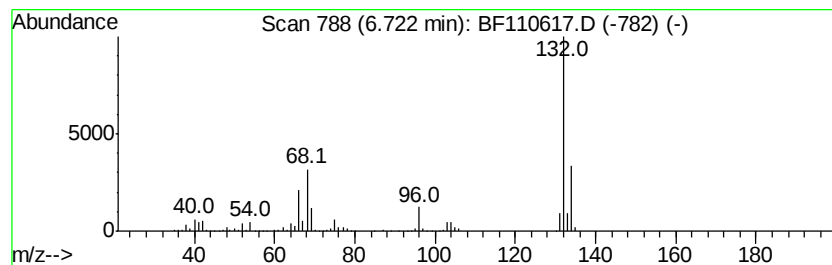
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	82.29 ng	1965350	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	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
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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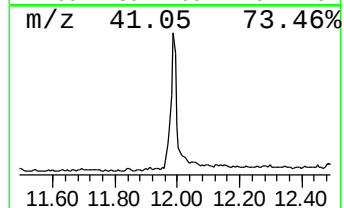
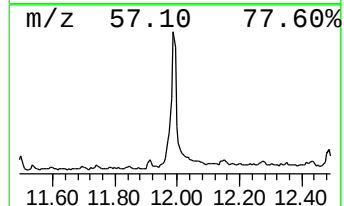
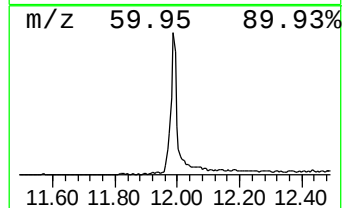
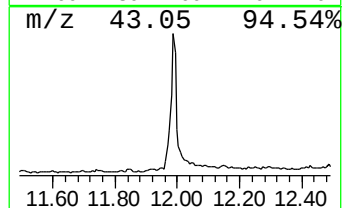
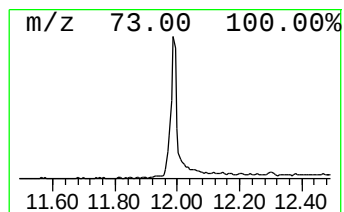
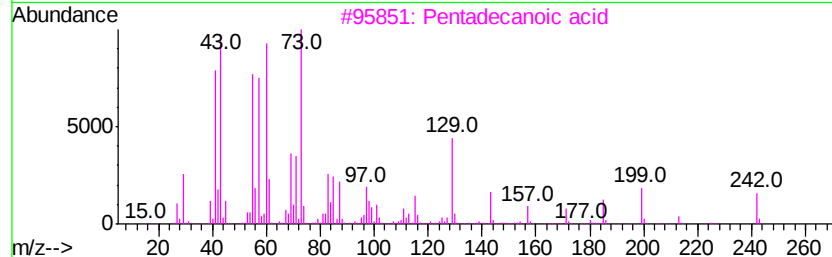
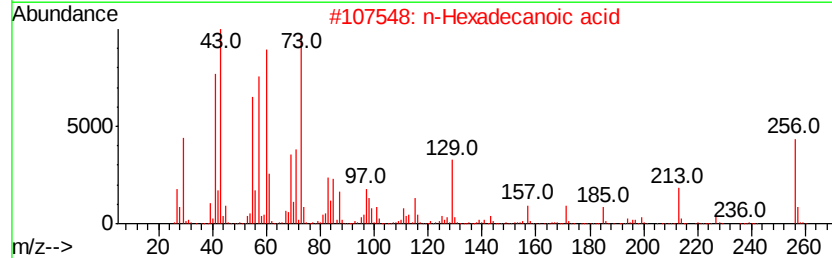
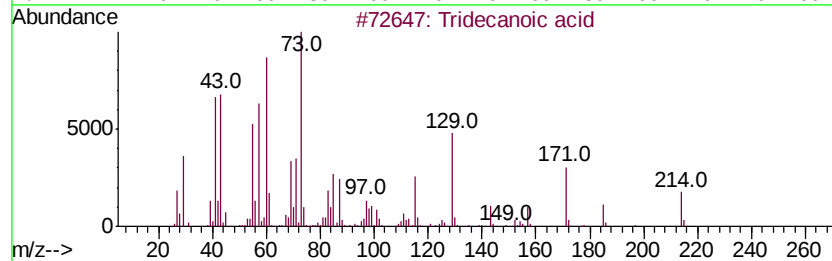
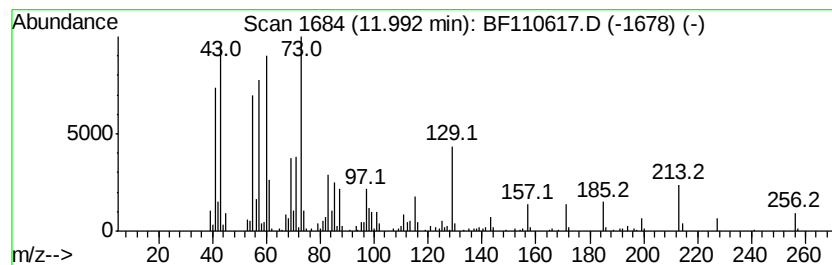
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	27.68 ng	664190	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	80



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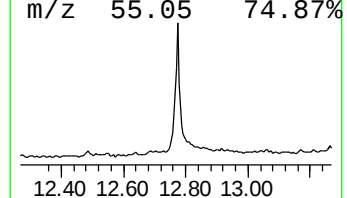
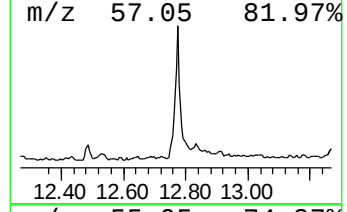
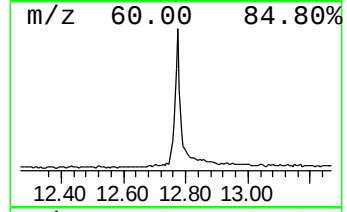
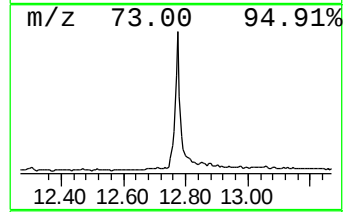
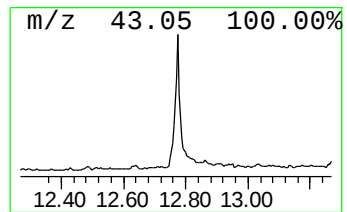
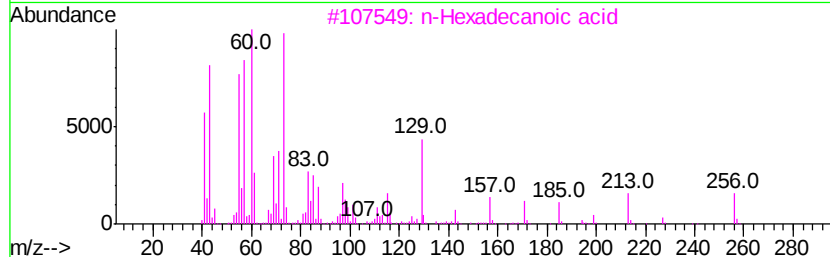
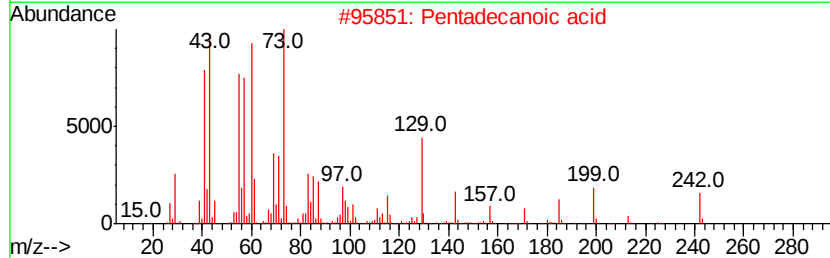
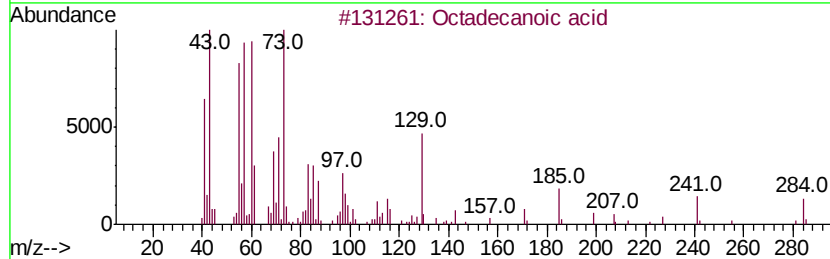
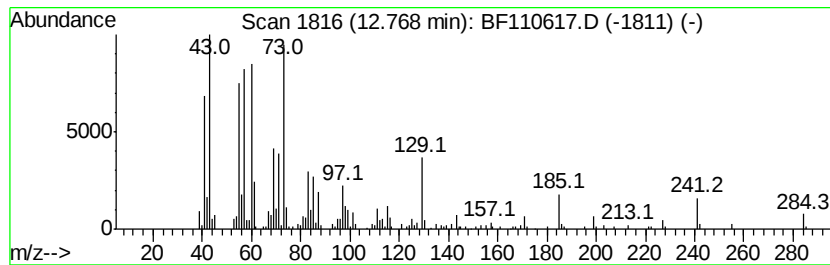
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	24.84 ng	596046	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Tridecanoic acid	214	C13H26O2	000638-53-9	83



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TS-D

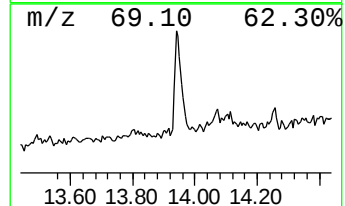
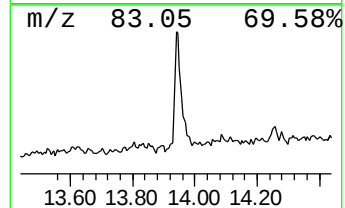
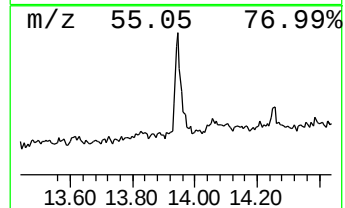
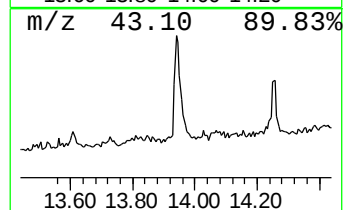
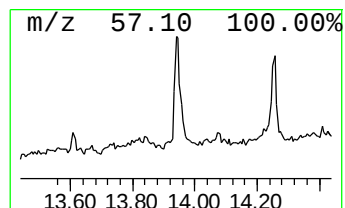
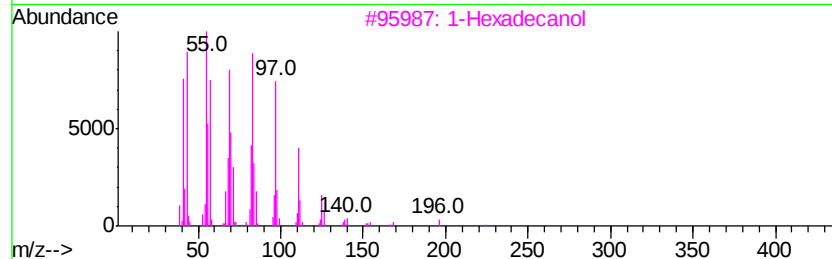
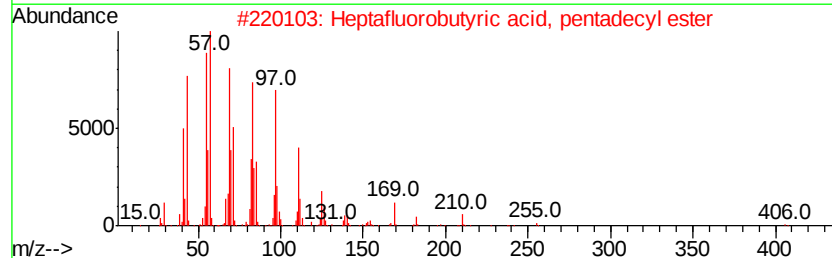
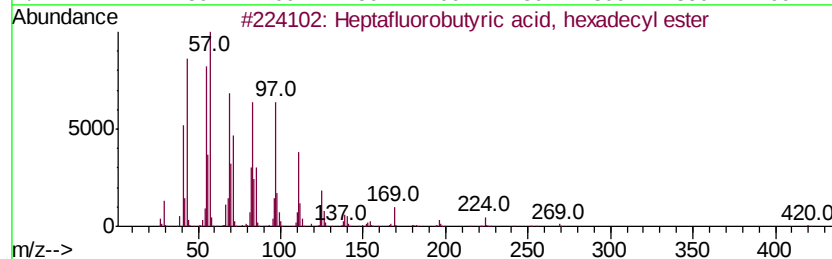
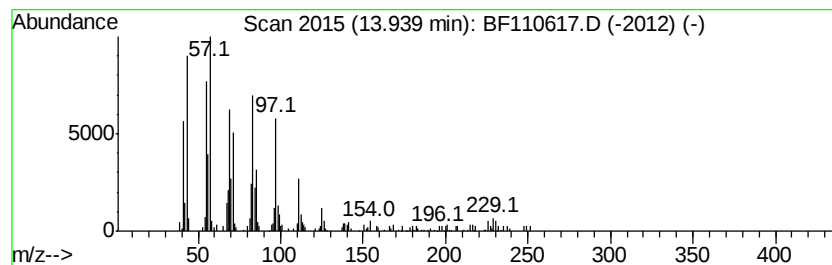
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.69 ng	191579	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		1-Hexadecanol	242	C16H34O	036653-82-4	93
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110617.D
Acq On : 9 Nov 2018 10:31
Operator : JU/SJ
Sample : J5813-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-D

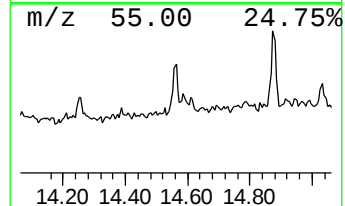
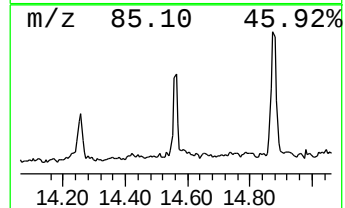
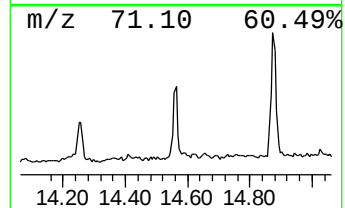
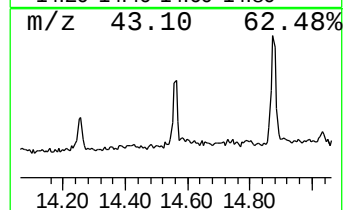
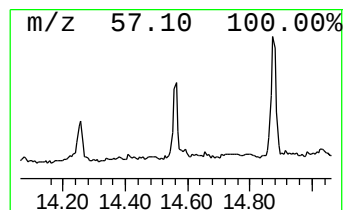
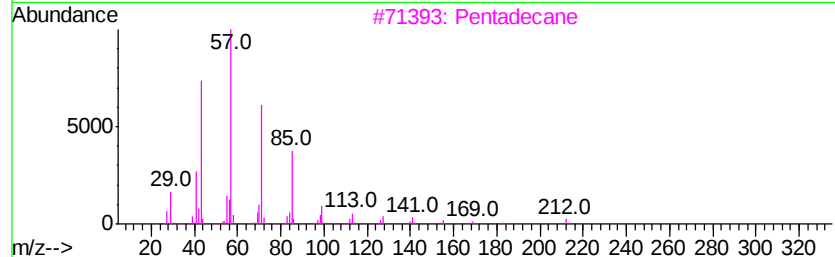
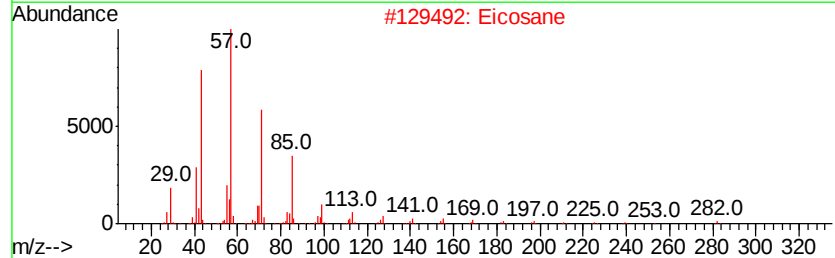
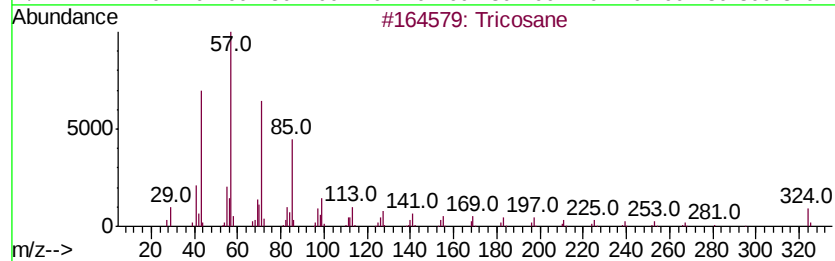
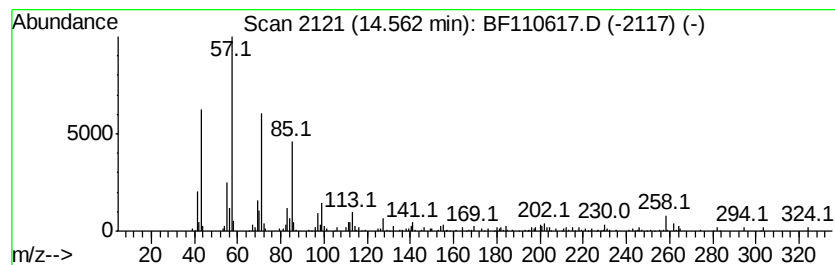
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tricosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	4.72 ng	117426	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	93
2	Eicosane		282	C20H42	000112-95-8	91
3	Pentadecane		212	C15H32	000629-62-9	90
4	Hexacosane		366	C26H54	000630-01-3	87
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110617.D
Acq On : 9 Nov 2018 10:31
Operator : JU/SJ
Sample : J5813-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-D

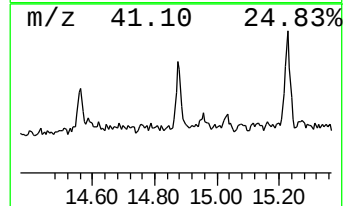
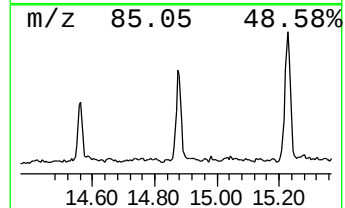
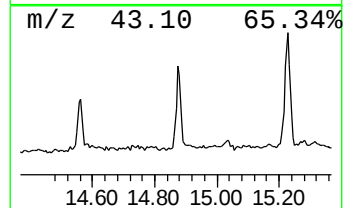
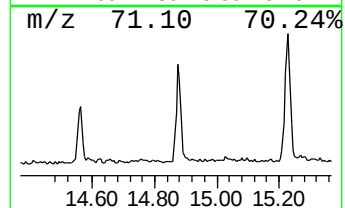
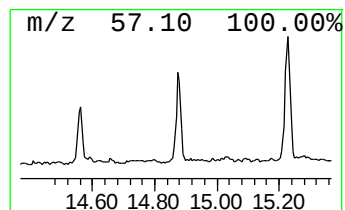
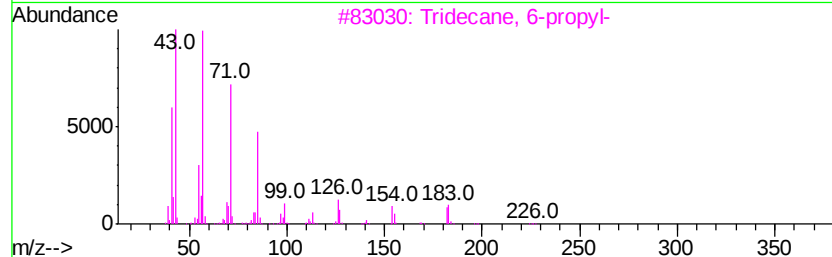
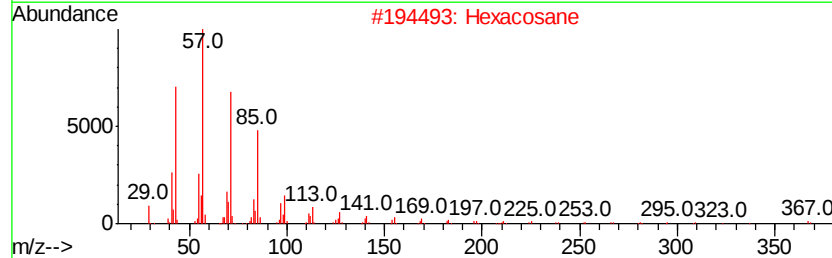
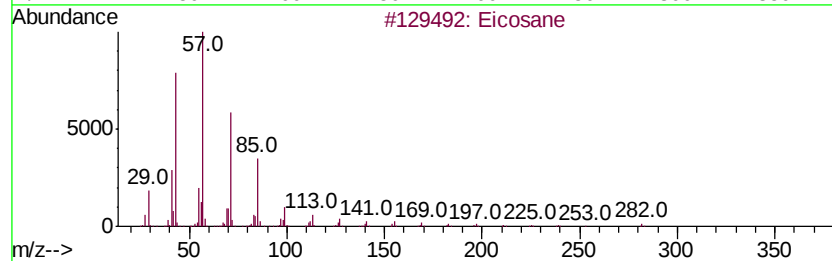
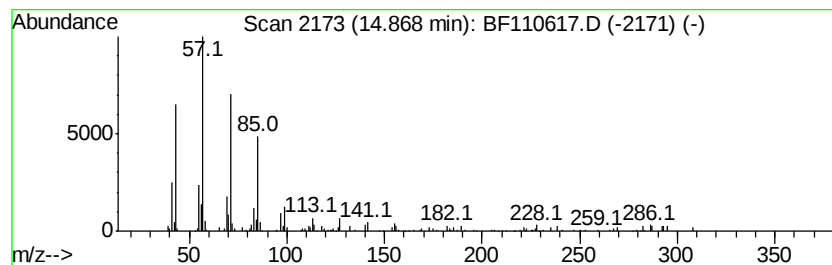
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	6.21 ng	154661	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Tridecane, 6-propyl-		226	C16H34	055045-10-8	90
4	Heneicosane		296	C21H44	000629-94-7	87
5	5-Ethyl-5-methylnonadecane		310	C22H46	1000360-42-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110617.D
Acq On : 9 Nov 2018 10:31
Operator : JU/SJ
Sample : J5813-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-D

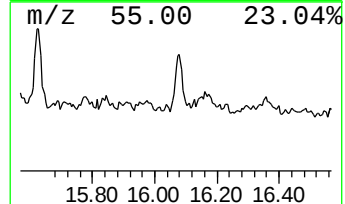
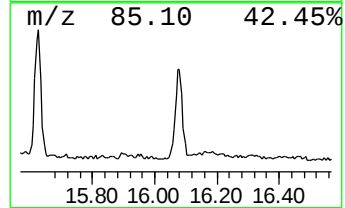
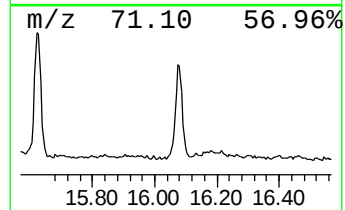
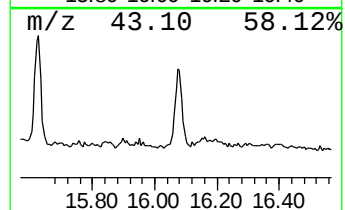
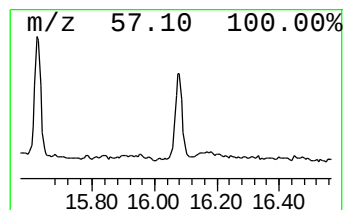
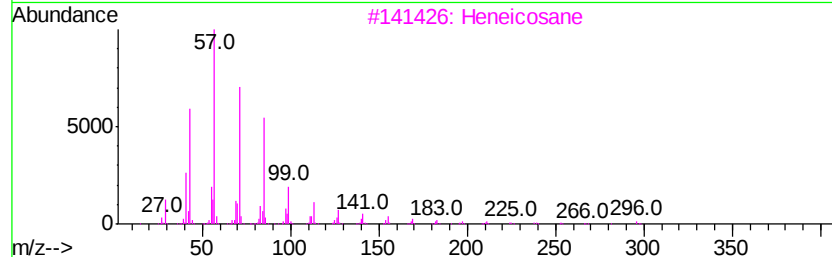
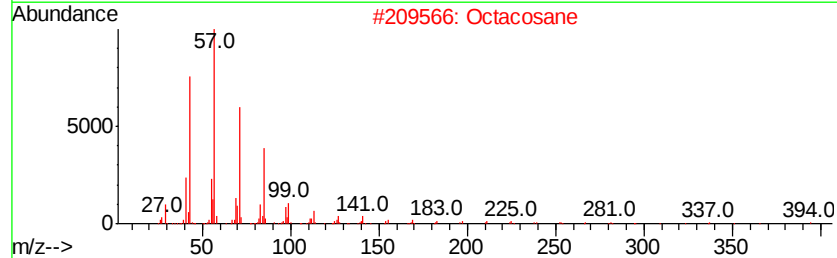
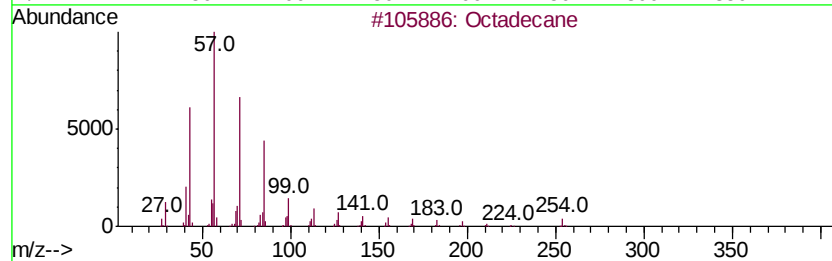
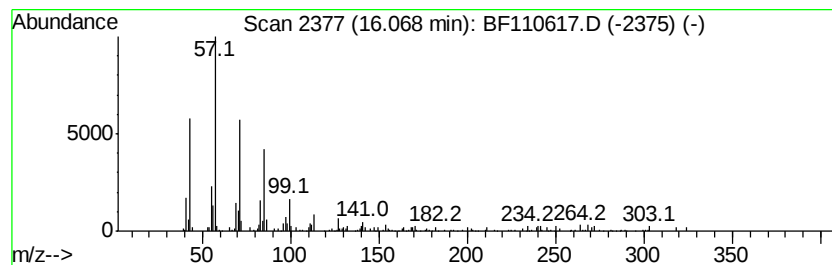
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	12.94 ng	192248	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	93
2		Octacosane	394	C28H58	000630-02-4	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110617.D
Acq On : 9 Nov 2018 10:31
Operator : JU/SJ
Sample : J5813-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

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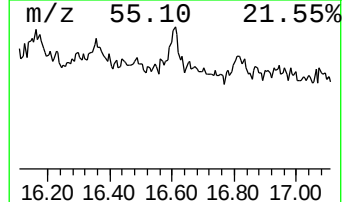
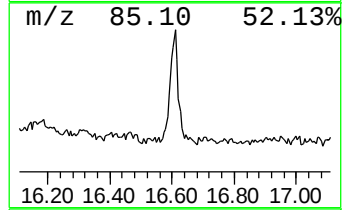
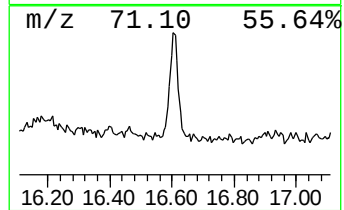
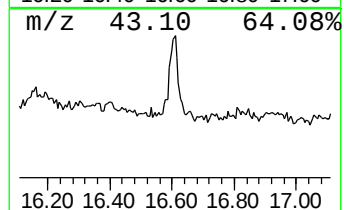
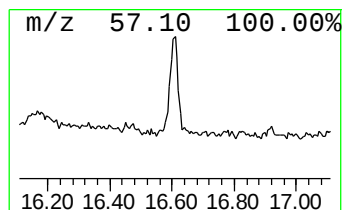
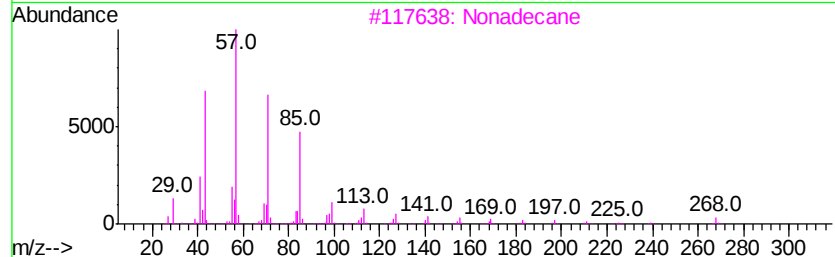
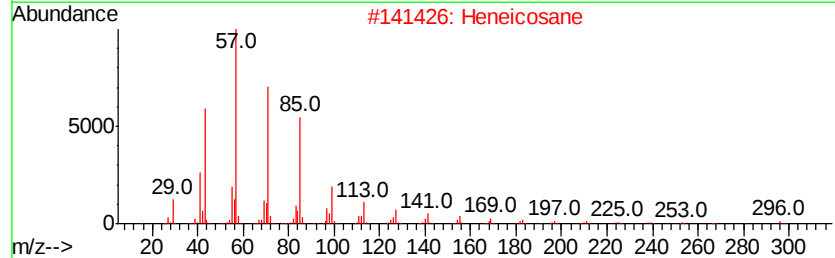
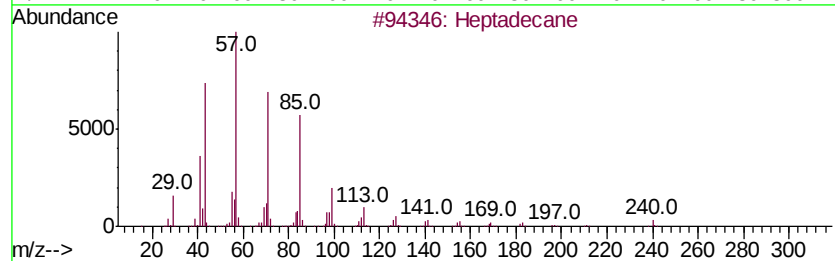
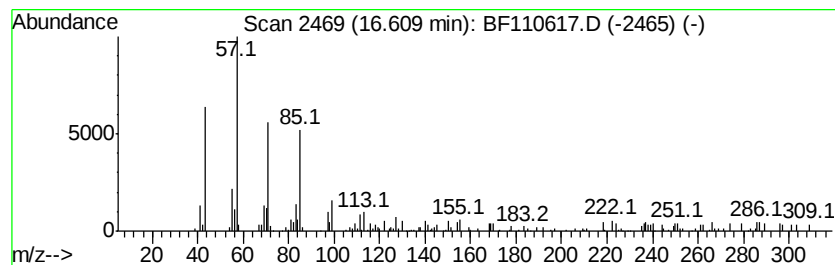
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	6.10 ng	90582	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Nonadecane	268	C19H40	000629-92-5	58
4		Tetracosane	338	C24H50	000646-31-1	58
5		Octadecane	254	C18H38	000593-45-3	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110617.D
Acq On : 9 Nov 2018 10:31
Operator : JU/SJ
Sample : J5813-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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	2.0	ng	48679	1	6.95	477659	20.0
unknown6.72	6.72	82.3	ng	1965350	1	6.95	477659	20.0
Tridecanoic acid	11.99	27.7	ng	664190	4	11.48	479957	20.0
Octadecanoic acid	12.77	24.8	ng	596046	4	11.48	479957	20.0
Heptafluorobutyri...	13.94	7.7	ng	191579	5	14.13	498026	20.0
Tricosane	14.56	4.7	ng	117426	5	14.13	498026	20.0
Eicosane	14.87	6.2	ng	154661	5	14.13	498026	20.0
Octadecane	16.07	12.9	ng	192248	6	15.66	297189	20.0
Heptadecane	16.61	6.1	ng	90582	6	15.66	297189	20.0