

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
 Data File : BF118230.D
 Acq On : 17 Dec 2019 17:02
 Operator : JU
 Sample : K6299-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SHORE-RD-BH-02

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-BF120619.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	2.128	3	7	21	rVB	299301	409219	14.15%	1.458%
2	5.069	502	507	519	rVB	332500	390922	13.52%	1.393%
3	5.475	572	576	596	rBV	2293153	2175741	75.25%	7.752%
4	6.492	744	749	768	rBV	2366427	2355576	81.47%	8.393%
5	6.628	768	772	775	rBV	2911816	2485354	85.96%	8.855%
6	6.857	807	811	820	rBV	922121	723698	25.03%	2.578%
7	7.016	834	838	841	rBV	2341484	1936623	66.98%	6.900%
8	7.422	902	907	910	rBV	1571410	1393177	48.19%	4.964%
9	8.145	1026	1030	1042	rBV	1032165	979762	33.89%	3.491%
10	9.222	1209	1213	1225	rBV	3235500	2891209	100.00%	10.301%
11	9.616	1277	1280	1290	rVB	204888	187051	6.47%	0.666%
12	9.904	1325	1329	1333	rBV	1349352	1157665	40.04%	4.125%
13	10.698	1460	1464	1478	rBV	2334967	2038163	70.50%	7.262%
14	11.398	1579	1583	1586	rBV	1319306	1198270	41.45%	4.269%
15	11.421	1586	1587	1591	rVV	215275	148948	5.15%	0.531%
16	11.474	1591	1596	1600	rVB3	40376	59460	2.06%	0.212%
17	11.921	1666	1672	1680	rBV2	167201	208902	7.23%	0.744%
18	12.615	1787	1790	1800	rBV	164797	167883	5.81%	0.598%
19	12.710	1803	1806	1812	rBV2	49922	67176	2.32%	0.239%
20	12.845	1824	1829	1836	rVB	145888	172083	5.95%	0.613%
21	12.992	1849	1854	1857	rBV	3254551	2868489	99.21%	10.220%
22	13.468	1930	1935	1945	rBV	582217	549734	19.01%	1.959%
23	13.886	2002	2006	2017	rBV	270871	377182	13.05%	1.344%
24	14.051	2026	2034	2037	rBV	988839	970917	33.58%	3.459%
25	14.074	2037	2038	2046	rVB	78821	70193	2.43%	0.250%
26	14.204	2057	2060	2066	rBV	59681	65767	2.27%	0.234%
27	14.509	2109	2112	2120	rBV	99090	114705	3.97%	0.409%
28	14.821	2160	2165	2169	rBV	128356	139520	4.83%	0.497%
29	14.898	2175	2178	2183	rVB	37105	39372	1.36%	0.140%
30	15.104	2209	2213	2220	rBV2	46643	91881	3.18%	0.327%
31	15.162	2220	2223	2229	rVB	130495	155012	5.36%	0.552%
32	15.409	2261	2265	2272	rVB	34671	53950	1.87%	0.192%
33	15.474	2272	2276	2281	rBV2	40718	53870	1.86%	0.192%
34	15.545	2282	2288	2300	rVB	667266	1011098	34.97%	3.602%

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SHORE-RD-BH-02

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-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.998	2360	2365	2370	rBV	97415	138687	4.80%	0.494%
36	16.062	2372	2376	2384	rVV6	20044	41347	1.43%	0.147%
37	16.515	2446	2453	2460	rBV	49429	92775	3.21%	0.331%
38	17.050	2538	2544	2549	rBV4	17548	37981	1.31%	0.135%
39	17.121	2551	2556	2562	rVB6	22171	48205	1.67%	0.172%

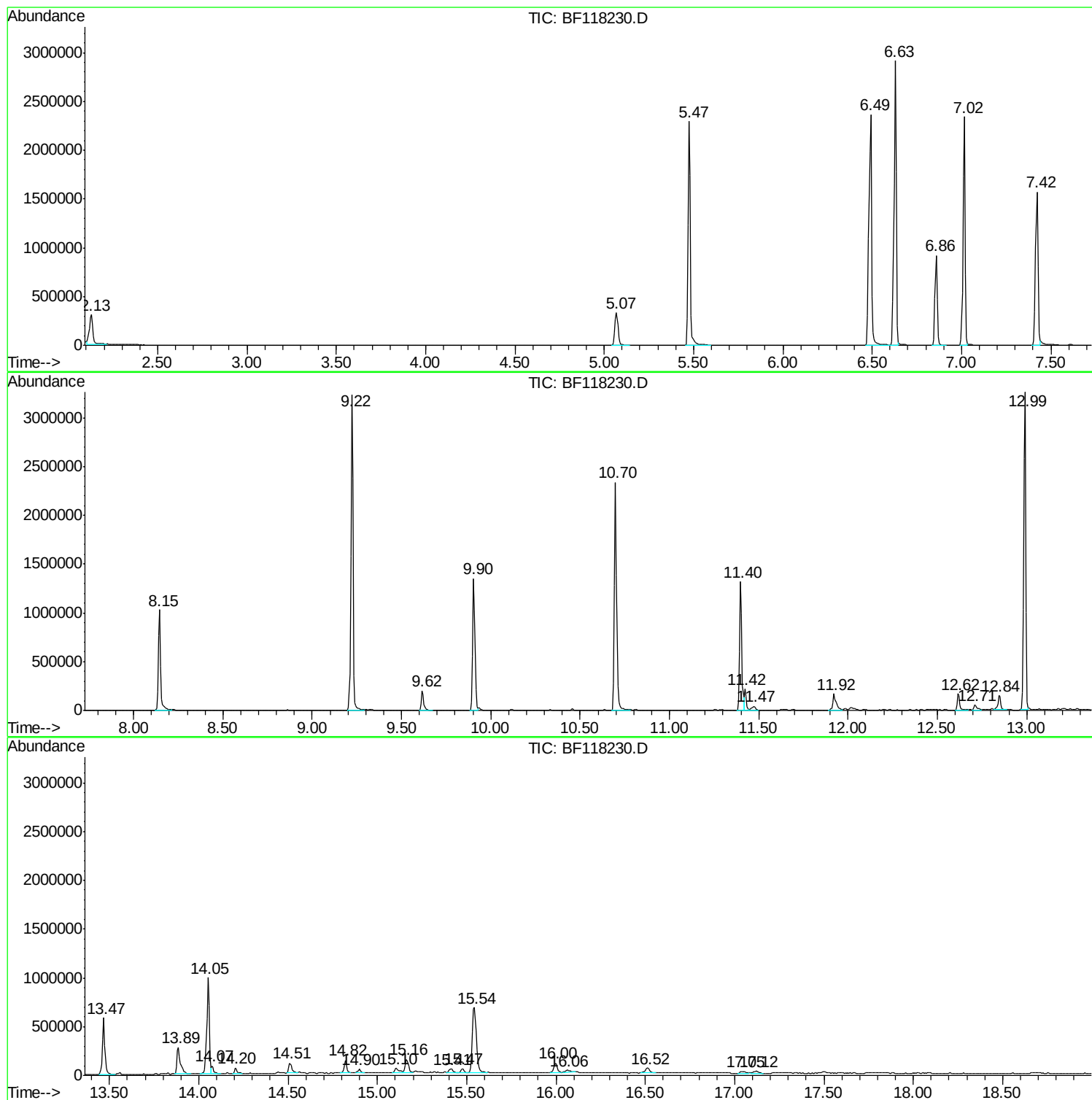
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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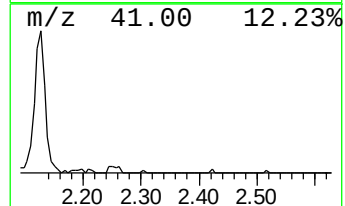
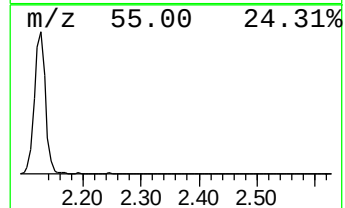
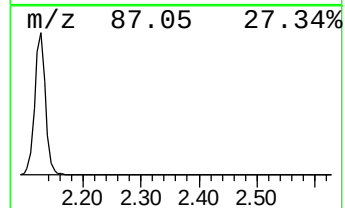
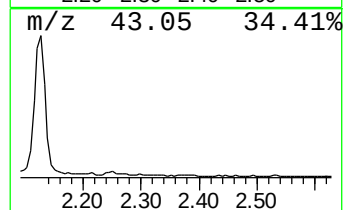
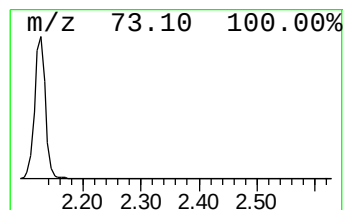
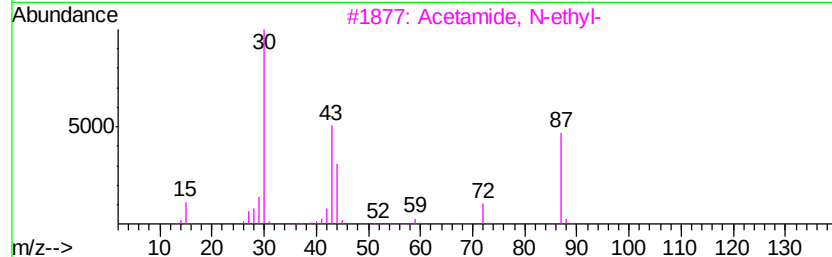
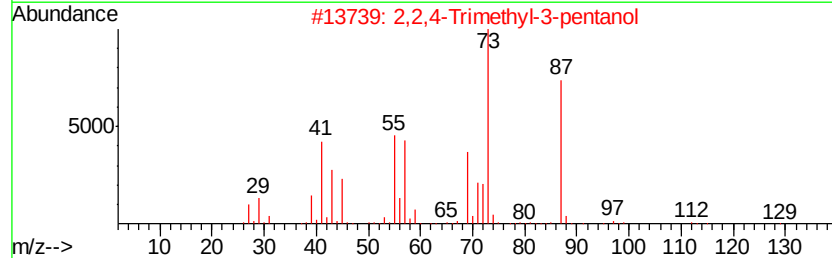
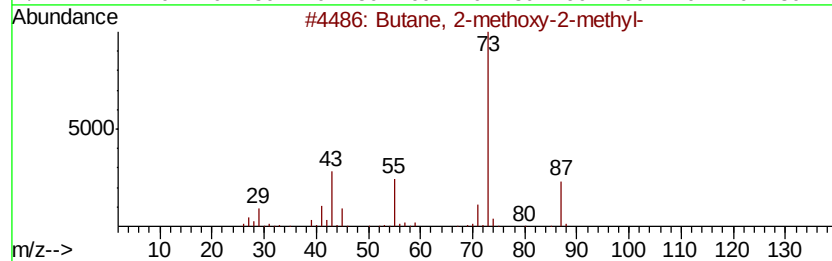
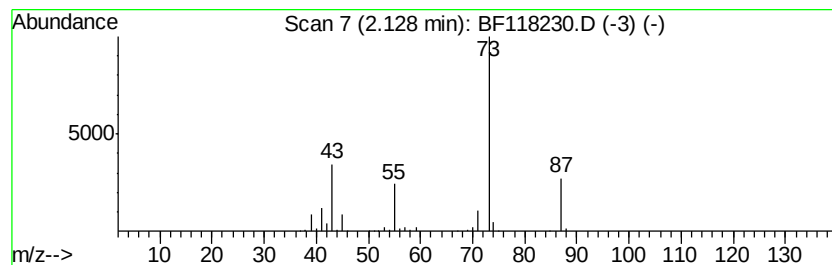
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	11.31 ng	409219	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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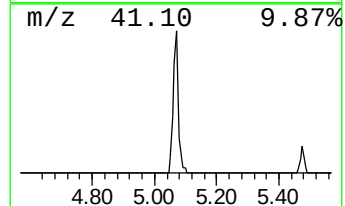
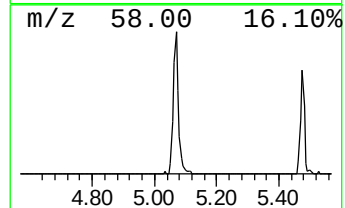
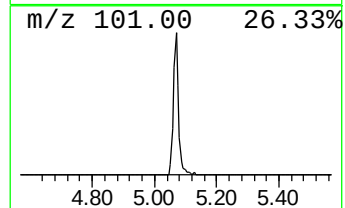
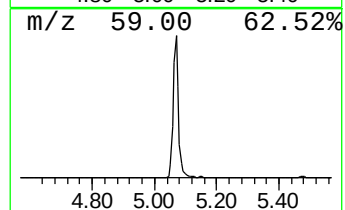
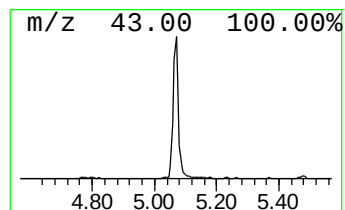
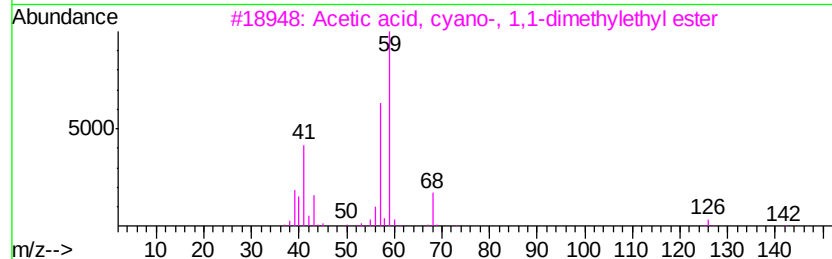
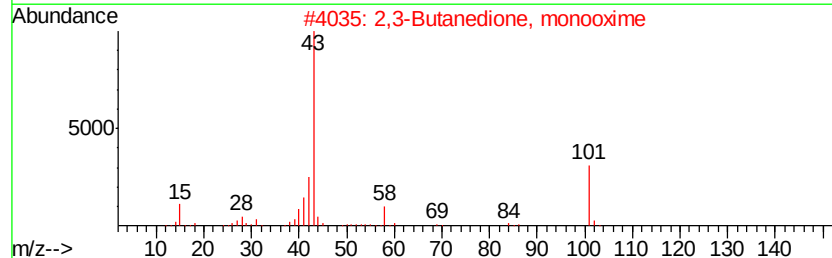
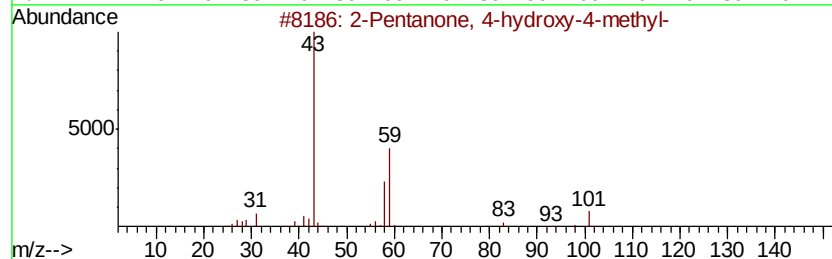
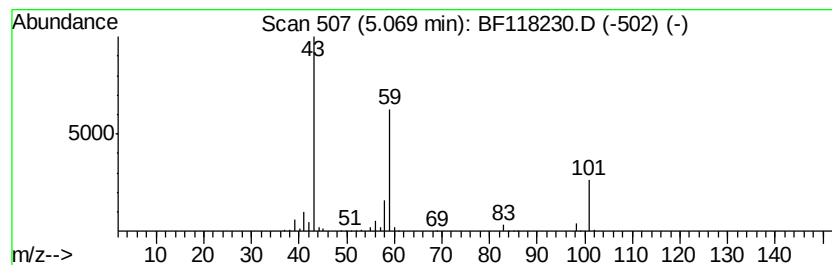
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	10.80 ng	390922	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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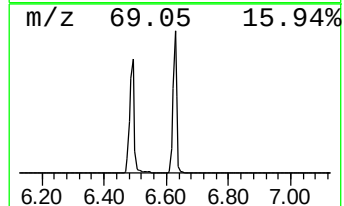
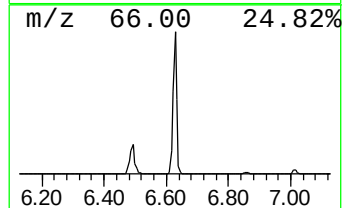
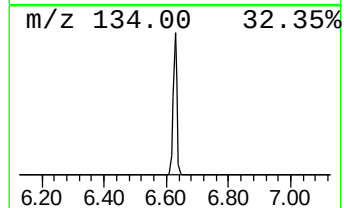
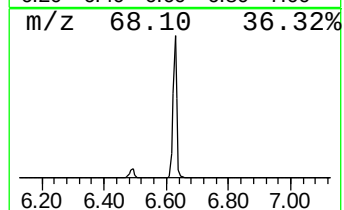
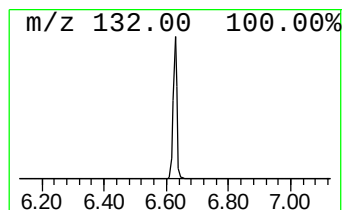
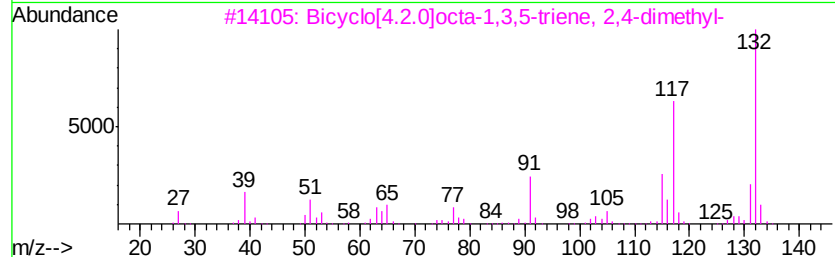
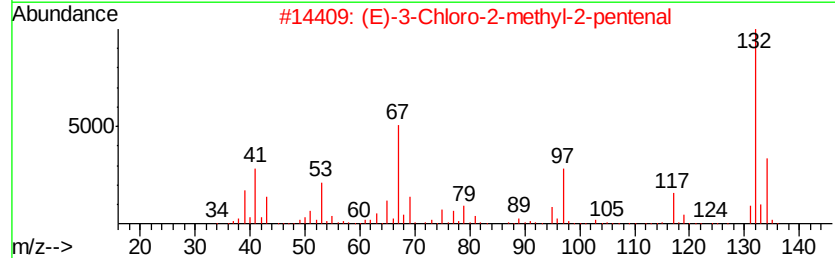
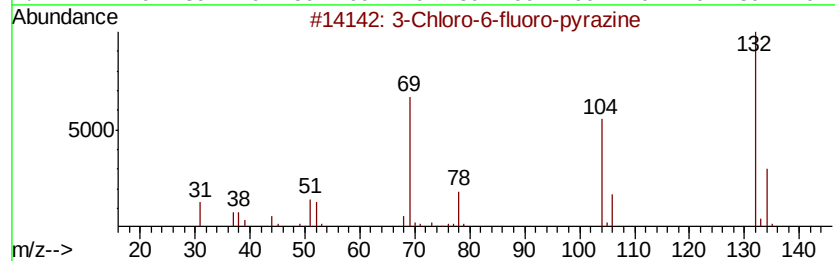
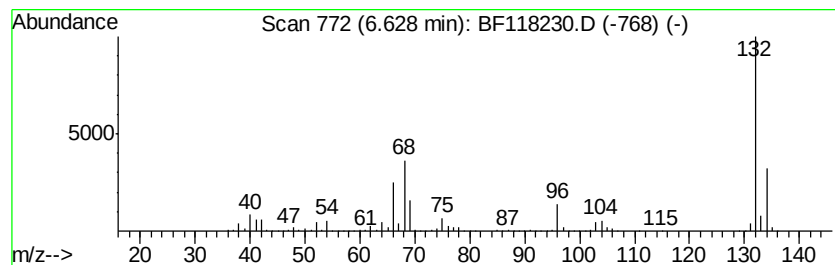
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	68.68 ng	2485350	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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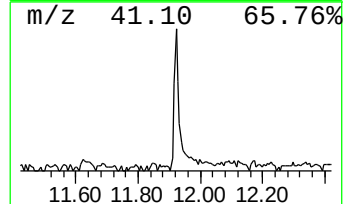
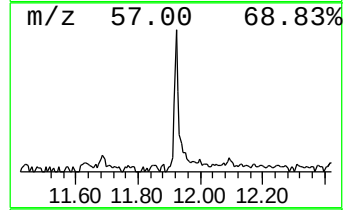
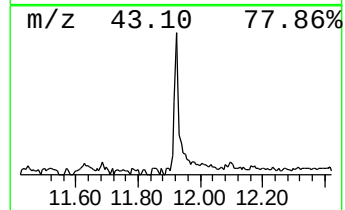
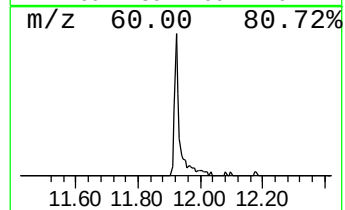
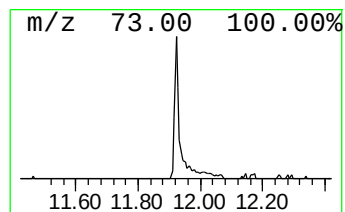
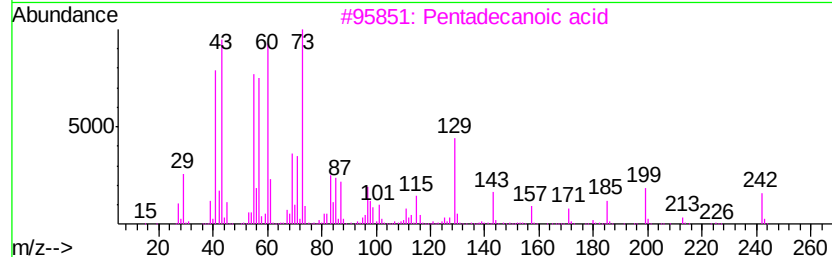
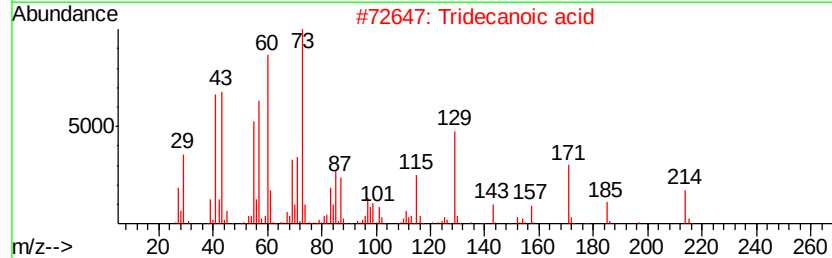
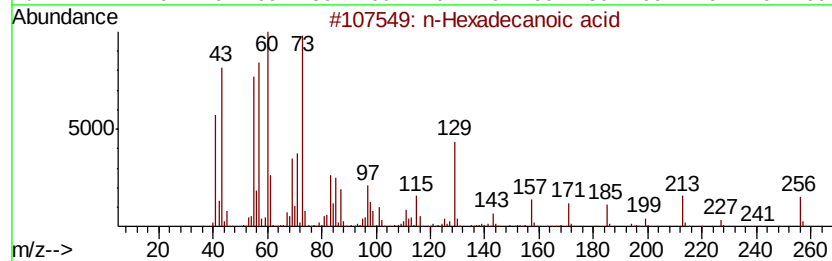
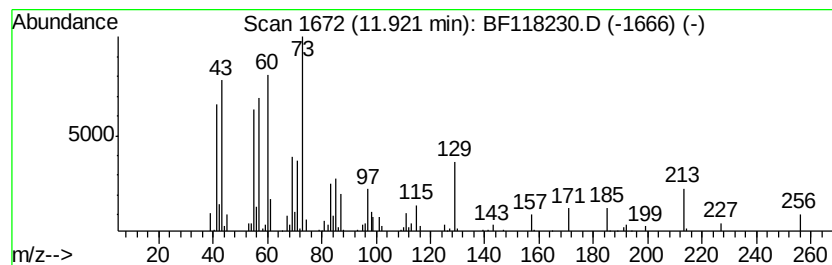
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.49 ng	208902	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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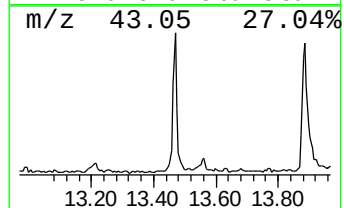
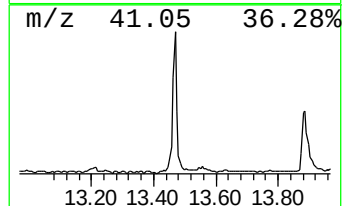
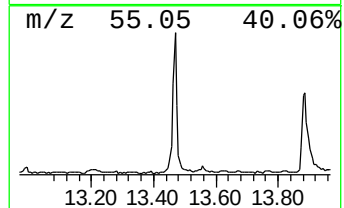
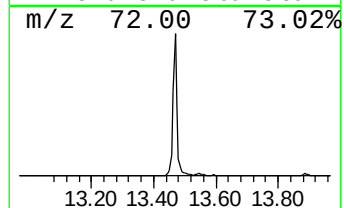
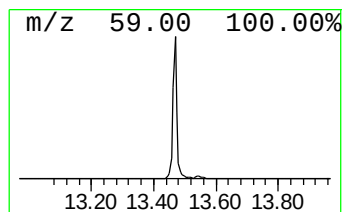
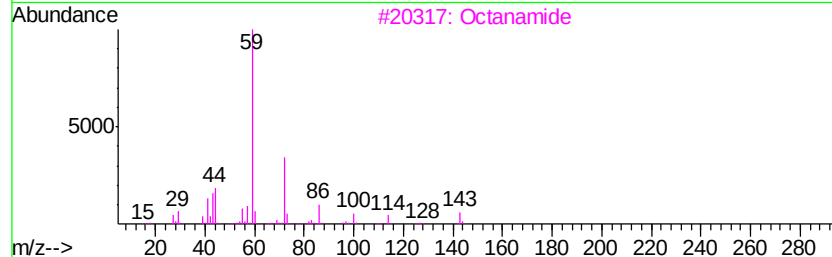
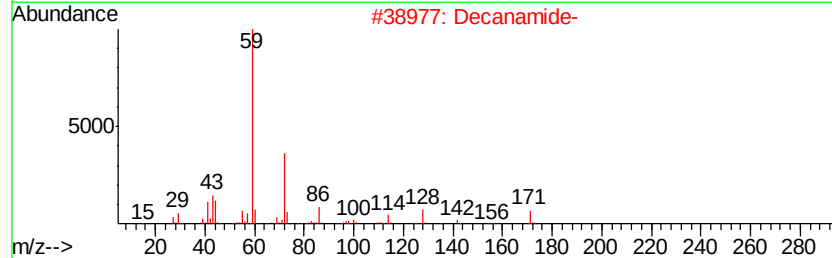
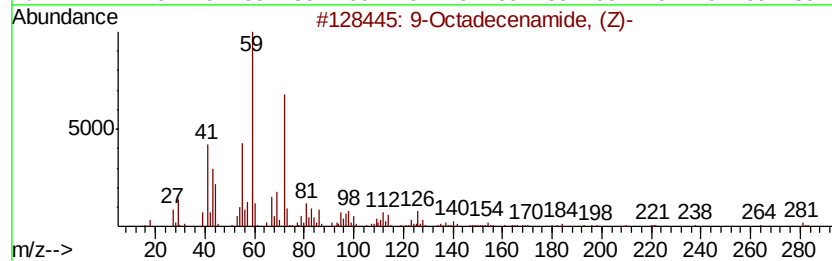
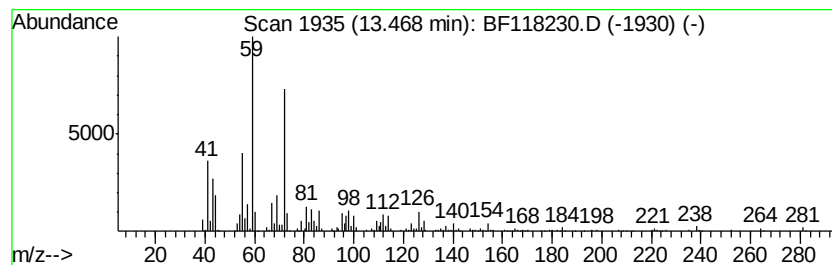
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	11.32 ng	549734	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Decanamide-	171	C10H21NO	002319-29-1	53
3		Octanamide	143	C8H17NO	000629-01-6	53
4		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	43
5		2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118230.D
Acq On : 17 Dec 2019 17:02
Operator : JU
Sample : K6299-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

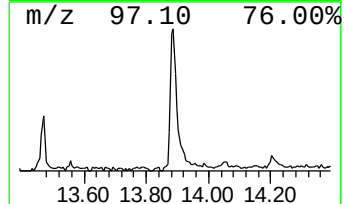
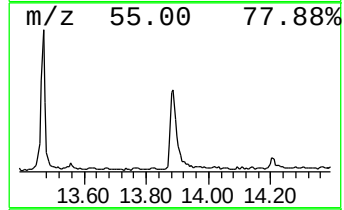
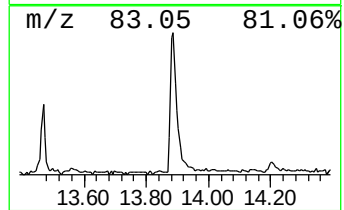
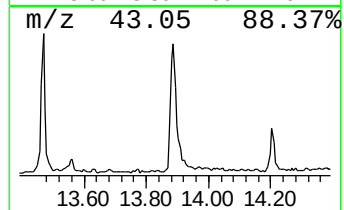
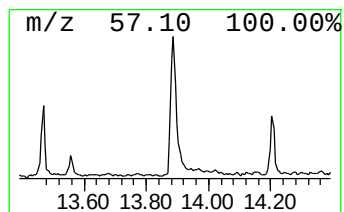
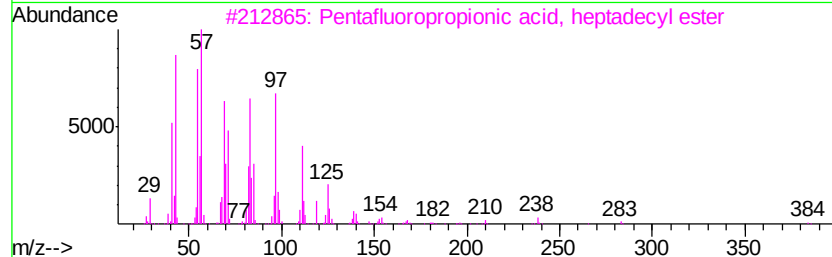
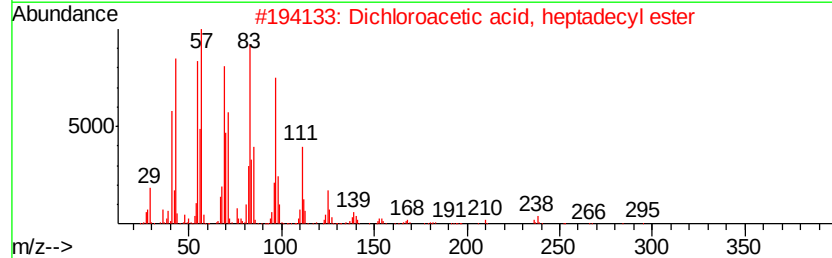
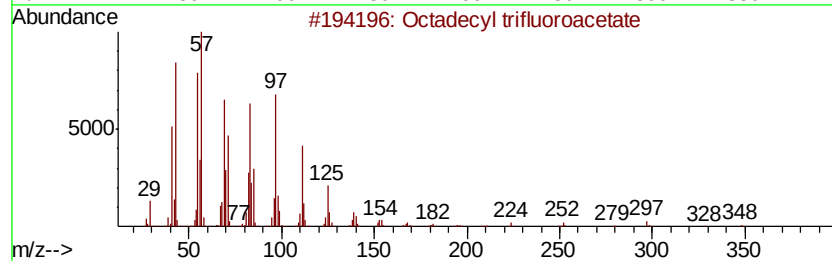
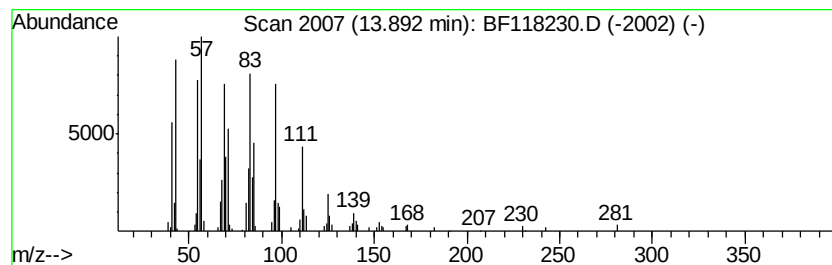
Instrument :
BNA_F
ClientSampleId :
SHORE-RD-BH-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.89	7.77 ng	377182	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118230.D
Acq On : 17 Dec 2019 17:02
Operator : JU
Sample : K6299-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

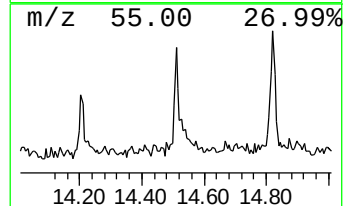
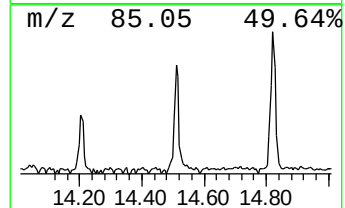
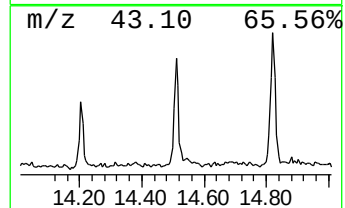
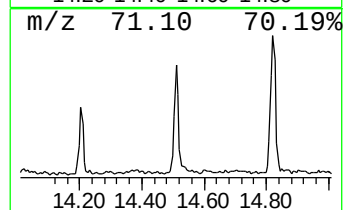
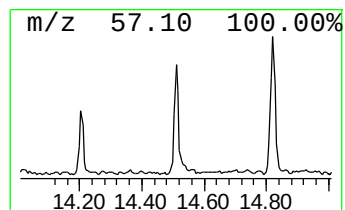
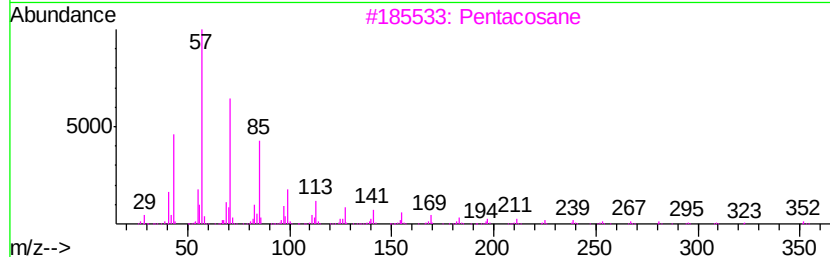
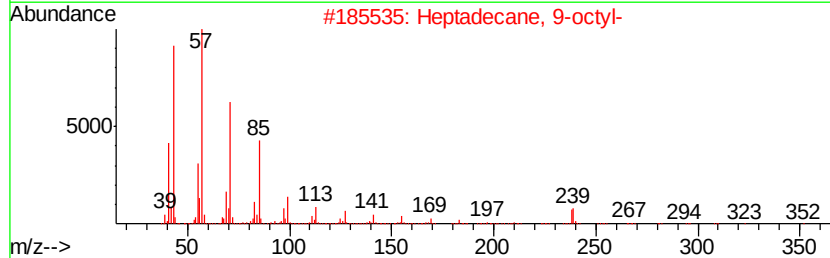
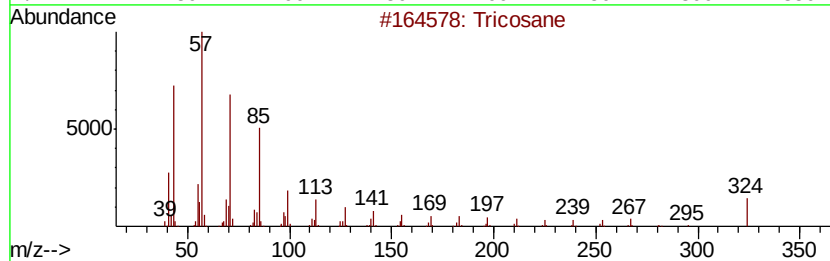
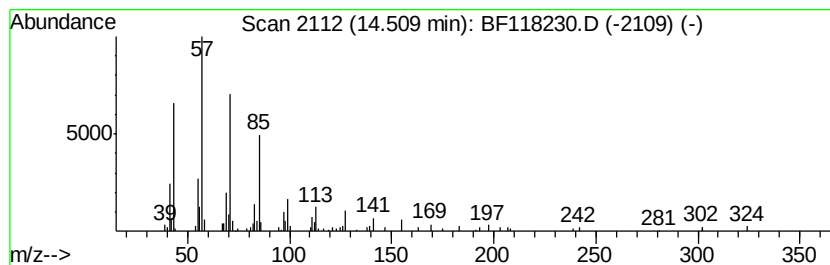
Instrument :
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ClientSampleId :
SHORE-RD-BH-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
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 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.36 ng	114705	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tricosane	324 C23H48	000638-67-5	94
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	90
3	Pentacosane	352 C25H52	000629-99-2	90
4	Octacosane	394 C28H58	000630-02-4	87
5	Docosane, 11-butyl-	366 C26H54	013475-76-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118230.D
Acq On : 17 Dec 2019 17:02
Operator : JU
Sample : K6299-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHORE-RD-BH-02

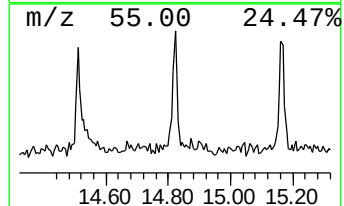
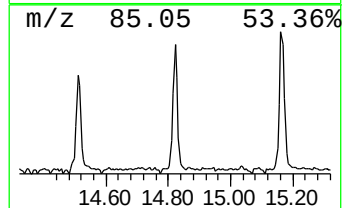
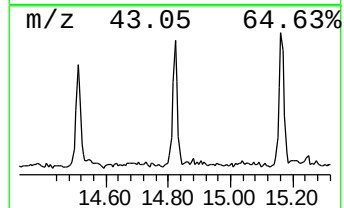
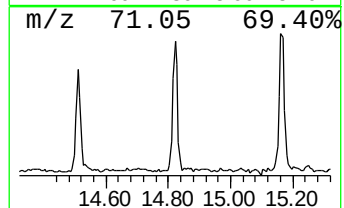
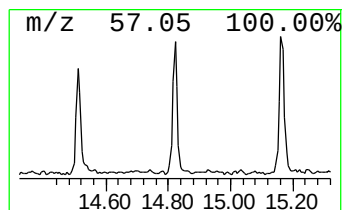
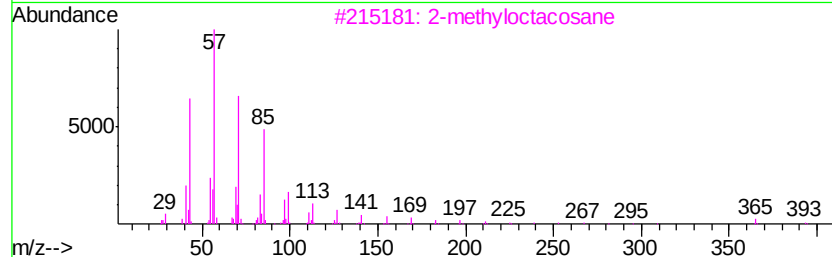
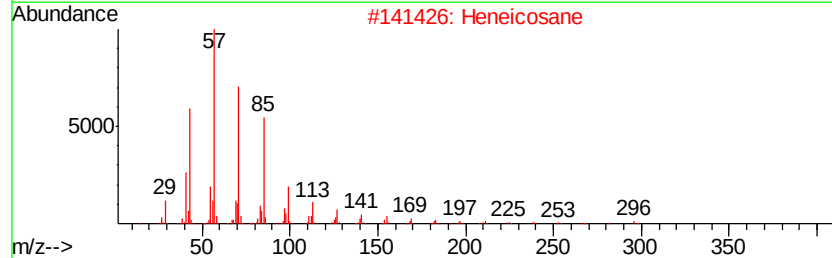
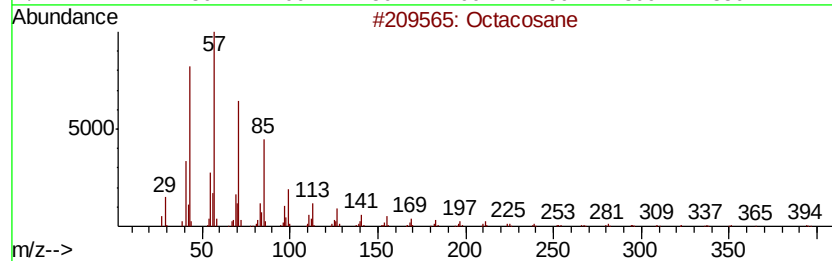
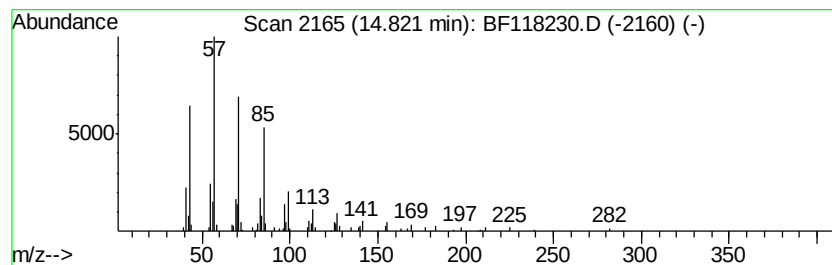
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.76 ng	139520	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118230.D
Acq On : 17 Dec 2019 17:02
Operator : JU
Sample : K6299-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHORE-RD-BH-02

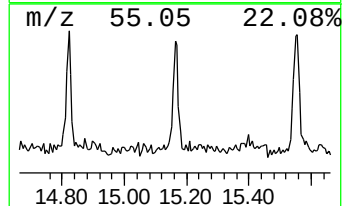
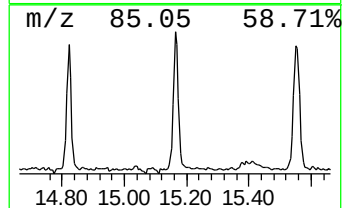
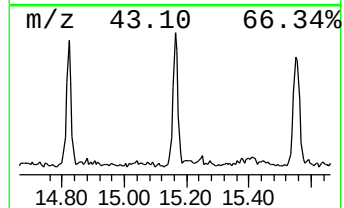
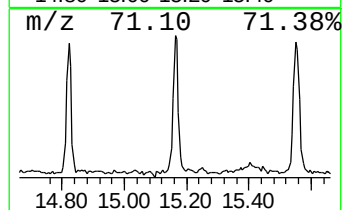
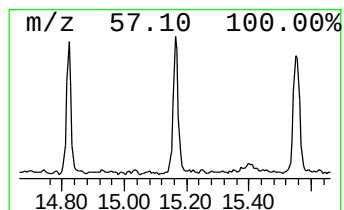
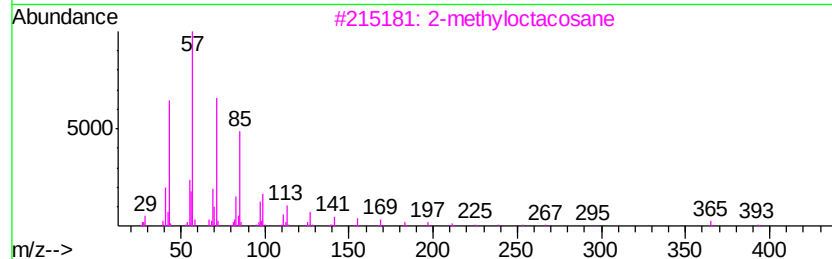
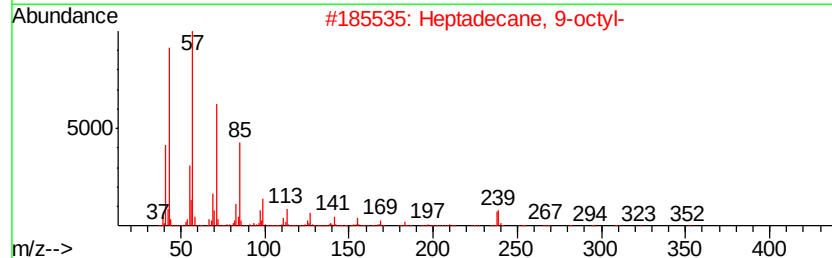
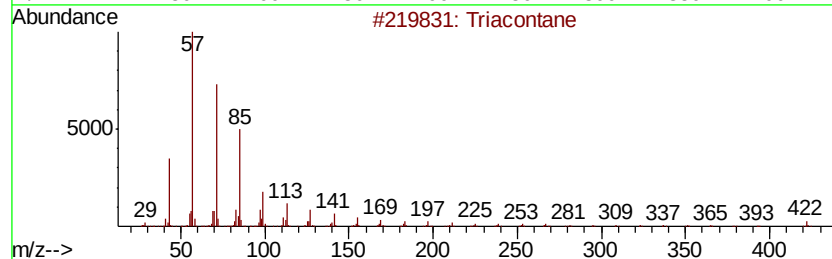
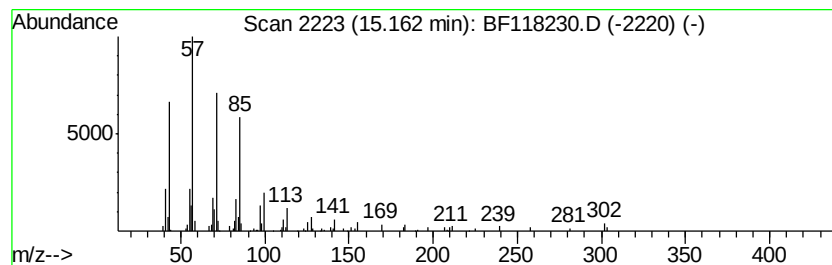
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	3.07 ng	155012	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	90
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		2-methyltetracosane	352	C25H52	1000376-72-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118230.D
Acq On : 17 Dec 2019 17:02
Operator : JU
Sample : K6299-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHORE-RD-BH-02

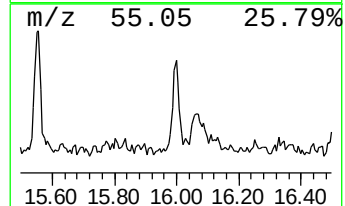
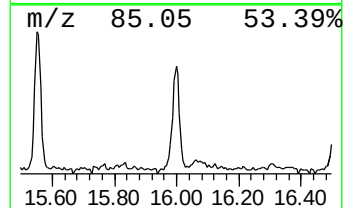
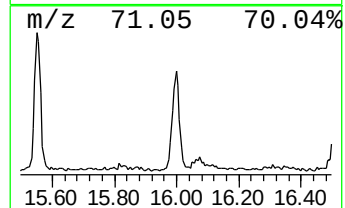
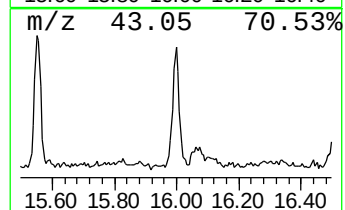
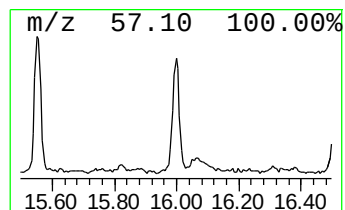
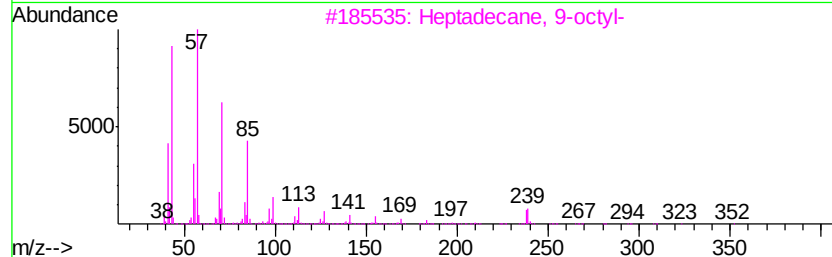
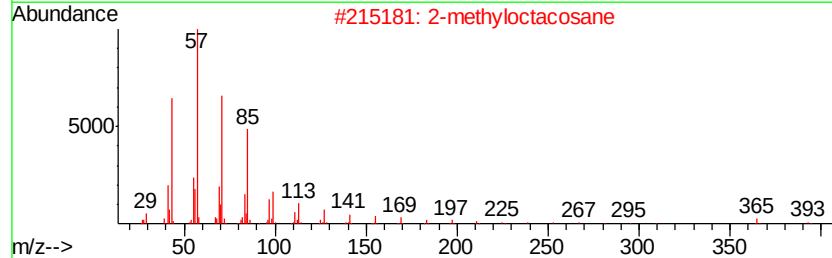
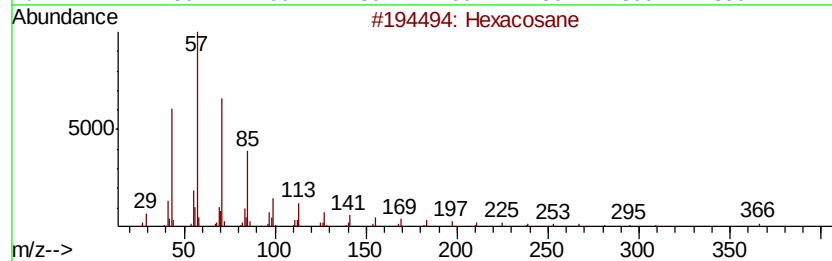
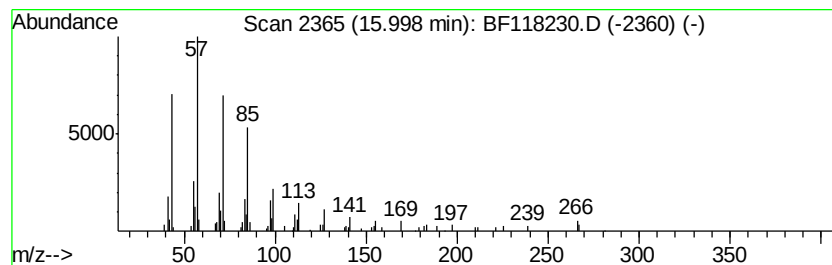
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.74 ng	138687	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
 Data File : BF118230.D
 Acq On : 17 Dec 2019 17:02
 Operator : JU
 Sample : K6299-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SHORE-RD-BH-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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...	2.13	11.3	ng	409219	1	6.86	723698	20.0
2-Pentanone, 4-hy...	5.07	10.8	ng	390922	1	6.86	723698	20.0
unknown6.63	6.63	68.7	ng	2485350	1	6.86	723698	20.0
n-Hexadecanoic acid	11.92	3.5	ng	208902	4	11.40	1198270	20.0
9-Octadecenamide,...	13.47	11.3	ng	549734	5	14.05	970917	20.0
Octadecyl trifluo...	13.89	7.8	ng	377182	5	14.05	970917	20.0
Tricosane	14.51	2.4	ng	114705	5	14.05	970917	20.0
Octacosane	14.82	2.8	ng	139520	6	15.54	1011100	20.0
Triacontane	15.16	3.1	ng	155012	6	15.54	1011100	20.0
Hexacosane	16.00	2.7	ng	138687	6	15.54	1011100	20.0