

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
 Data File : BF111149.D
 Acq On : 6 Dec 2018 20:22
 Operator : JU/SJ
 Sample : J6204-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HLSP-SB-1A-(0-2)

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-BF120518.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	3.234	193	195	214	rBV	121288	294457	2.94%	0.311%
2	5.016	489	498	504	rBV	405112	585743	5.85%	0.619%
3	5.422	562	567	570	rBV	9600802	9013031	90.08%	9.522%
4	6.434	733	739	743	rBV	9635280	9922915	99.17%	10.483%
5	6.575	758	763	766	rBV	10163754	9336814	93.31%	9.864%
6	6.798	797	801	806	rBV2	3922227	4806522	48.04%	5.078%
7	6.963	825	829	832	rBV	8538746	7132668	71.28%	7.535%
8	7.363	892	897	900	rBV	6828019	6124060	61.20%	6.470%
9	7.969	996	1000	1002	rBV	336582	293661	2.93%	0.310%
10	8.087	1015	1020	1023	rBV	4382146	3670457	36.68%	3.878%
11	8.904	1155	1159	1167	rBV	259124	315198	3.15%	0.333%
12	9.163	1198	1203	1206	rBV	11719345	10006117	100.00%	10.571%
13	9.551	1266	1269	1273	rBV	1369997	1168841	11.68%	1.235%
14	9.839	1310	1318	1322	rBV2	4792141	4015344	40.13%	4.242%
15	10.504	1427	1431	1434	rBV	492502	433194	4.33%	0.458%
16	10.569	1437	1442	1447	rBV	240459	219370	2.19%	0.232%
17	10.622	1447	1451	1455	rBV	6125018	5514431	55.11%	5.826%
18	11.322	1566	1570	1573	rBV	4436910	3642886	36.41%	3.849%
19	11.851	1656	1660	1670	rBV	712314	829277	8.29%	0.876%
20	12.527	1767	1775	1779	rBV4	67052	125859	1.26%	0.133%
21	12.639	1790	1794	1804	rBV	309817	363294	3.63%	0.384%
22	12.816	1818	1824	1825	rBV4	125340	163497	1.63%	0.173%
23	12.869	1826	1833	1836	rVV5	296651	750178	7.50%	0.793%
24	12.910	1836	1840	1843	rVV	8020483	7506730	75.02%	7.931%
25	12.945	1843	1846	1849	rVB4	243402	335450	3.35%	0.354%
26	13.404	1920	1924	1926	rBV2	374382	340944	3.41%	0.360%
27	13.733	1977	1980	1989	rVB7	72189	128121	1.28%	0.135%
28	13.810	1989	1993	2002	rBV	515267	651747	6.51%	0.689%
29	13.951	2013	2017	2021	rBV	2462456	2347209	23.46%	2.480%
30	14.063	2034	2036	2040	rVB4	128133	145175	1.45%	0.153%
31	14.451	2098	2102	2119	rBV2	261464	624984	6.25%	0.660%
32	14.821	2161	2165	2169	rVB	332708	334779	3.35%	0.354%
33	15.080	2205	2209	2211	rBV	209782	245556	2.45%	0.259%
34	15.392	2257	2262	2267	rVB	2137638	2455664	24.54%	2.594%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.451	2269	2272	2276	rVB2	128736	151040	1.51%	0.160%
36	15.874	2340	2344	2348	rBV	207462	293742	2.94%	0.310%
37	15.921	2349	2352	2356	rBV5	82610	133996	1.34%	0.142%
38	17.404	2600	2604	2610	rVB8	118236	233112	2.33%	0.246%

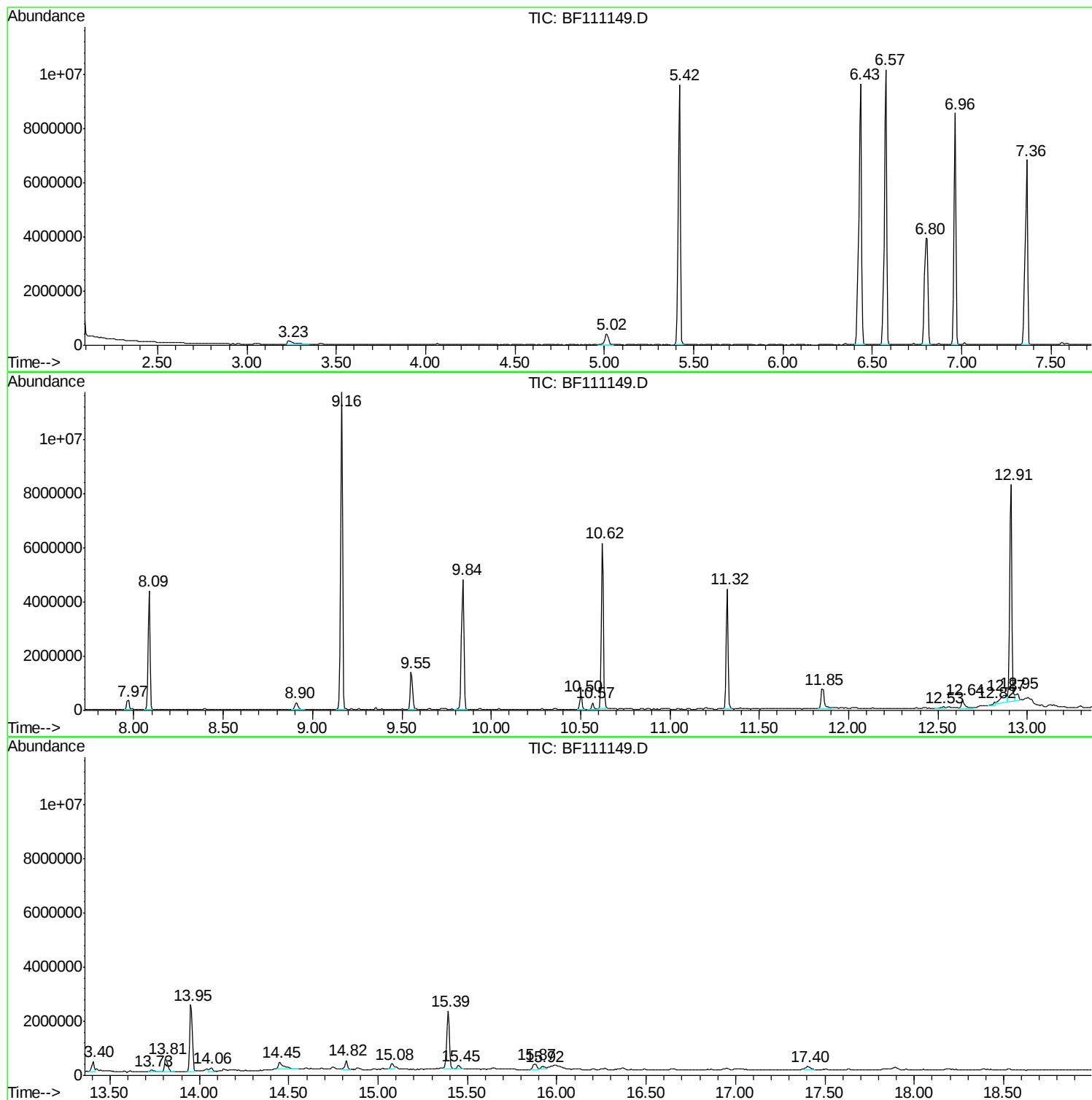
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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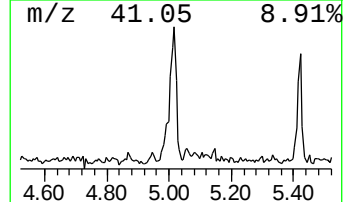
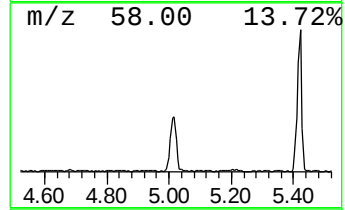
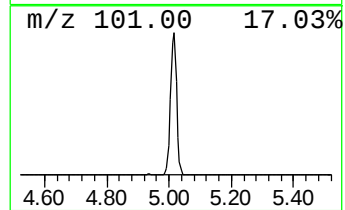
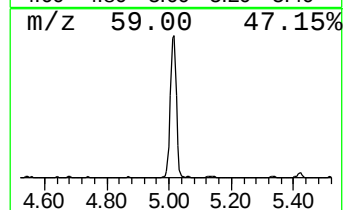
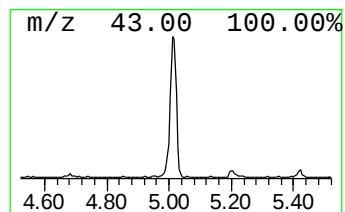
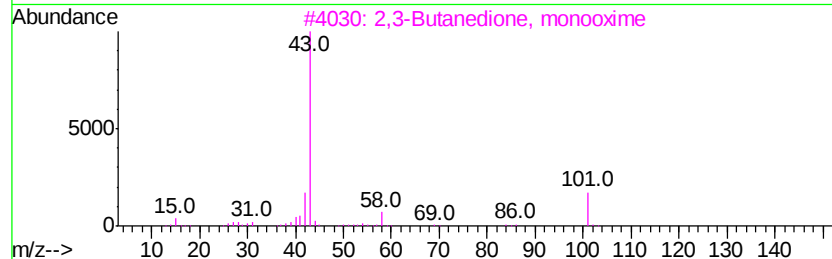
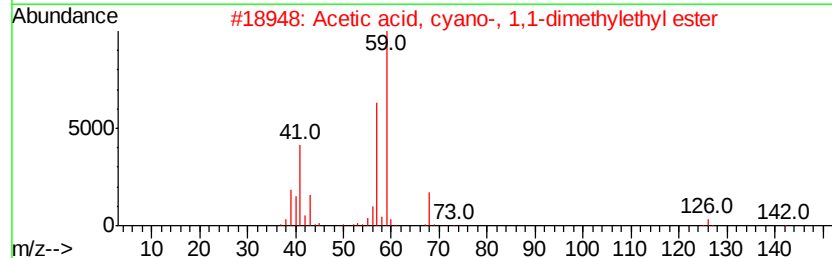
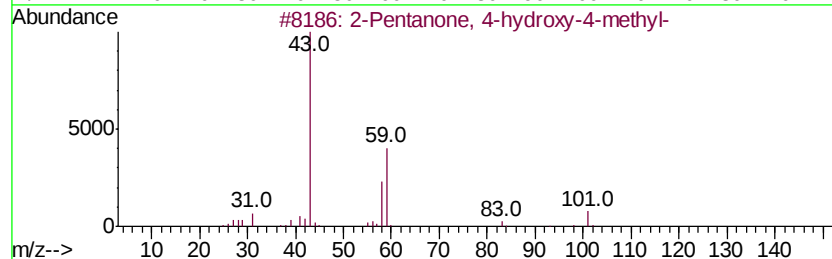
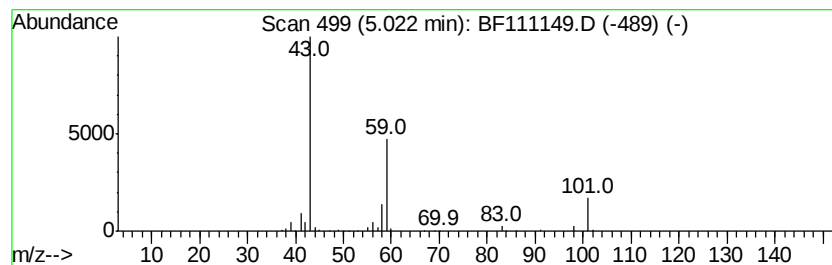
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.44 ng	585743	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		2-Pentanone	86	C5H10O	000107-87-9	10
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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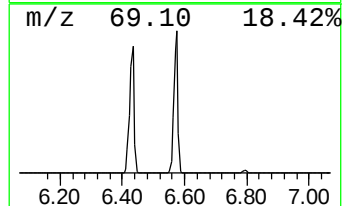
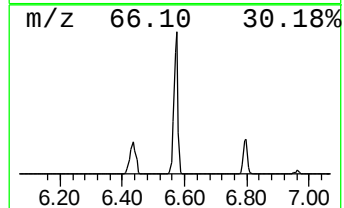
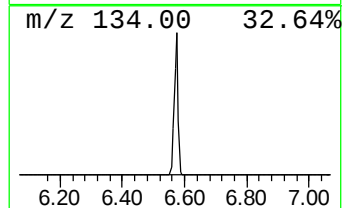
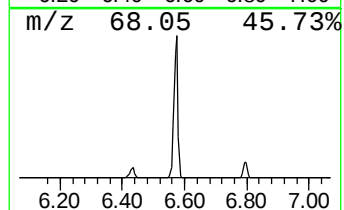
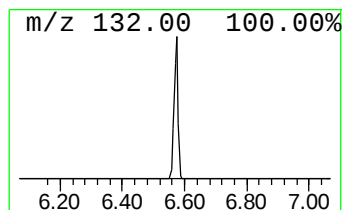
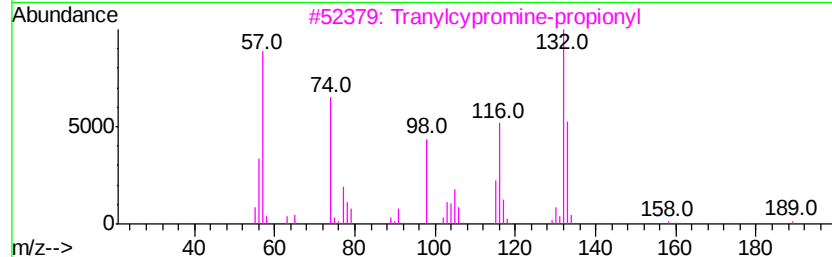
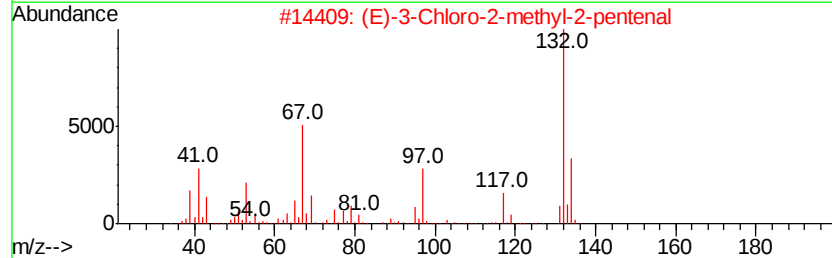
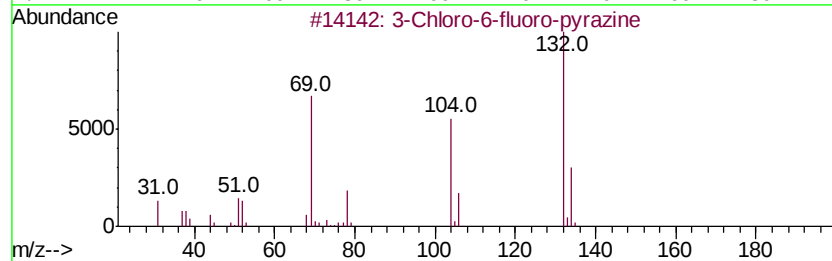
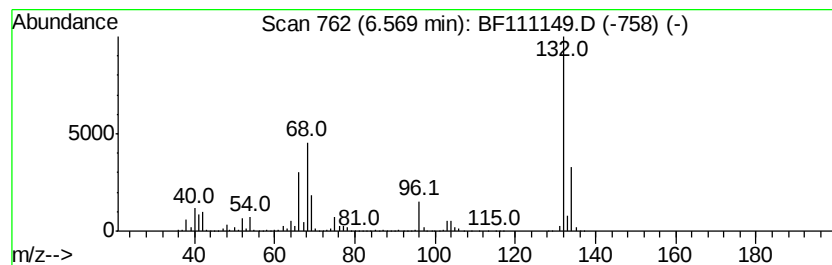
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	38.85 ng	9336810	1,4-Dichlorobenzene-d4	6.80

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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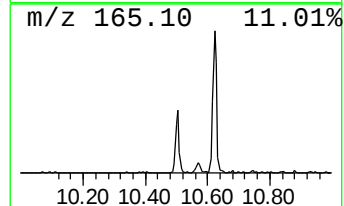
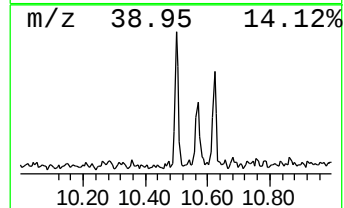
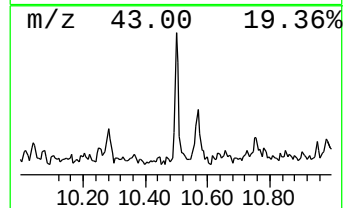
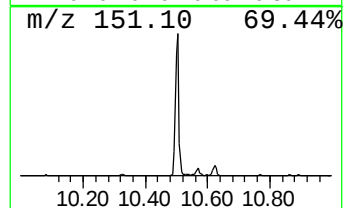
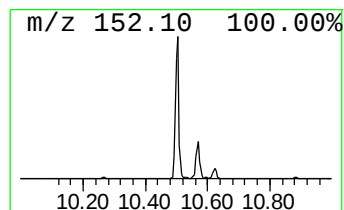
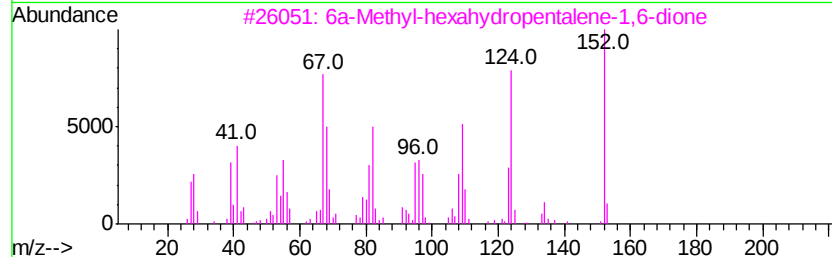
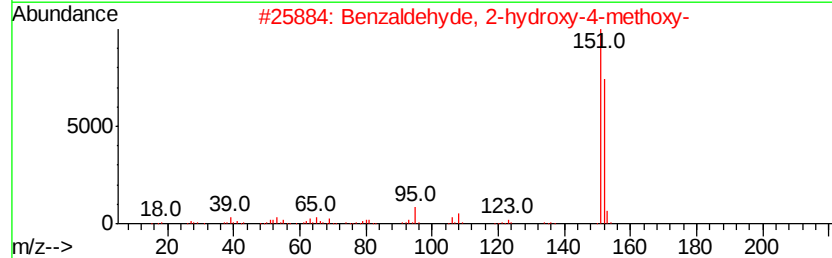
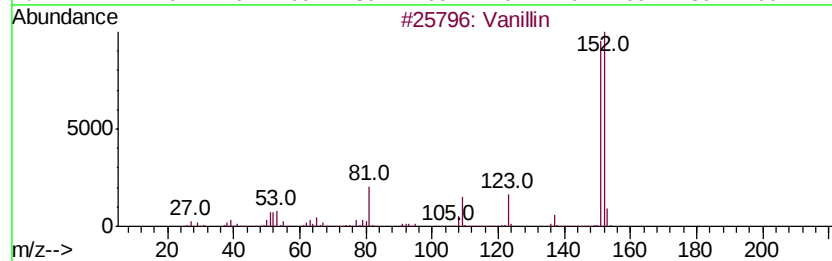
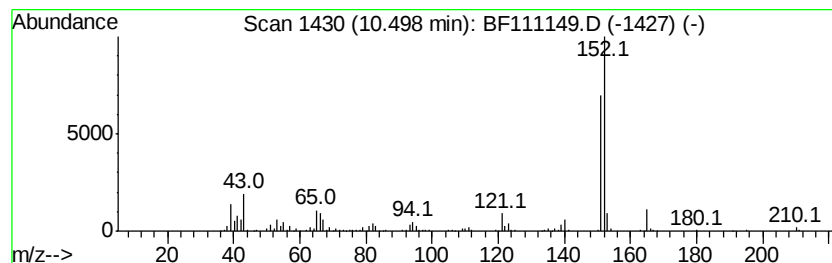
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Vanillin Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	2.16 ng	433194	Acenaphthene-d10	9.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin		152	C8H8O3	000121-33-5	59
2	Benzaldehyde, 2-hydroxy-4-methoxy-		152	C8H8O3	000673-22-3	43
3	6a-Methyl-hexahydopentalene-1,6...		152	C9H12O2	092485-86-4	38
4	d-Proline, n-propargyloxycarbonyl...		253	C13H19NO4	1000328-06-7	37
5	Benzaldehyde, 3-(chloroacetoxy)-...		228	C10H9ClO4	066267-38-7	37



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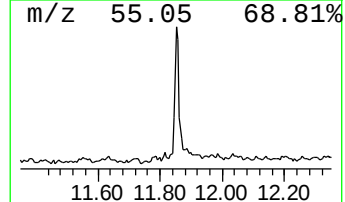
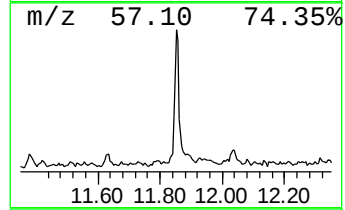
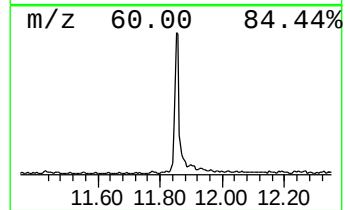
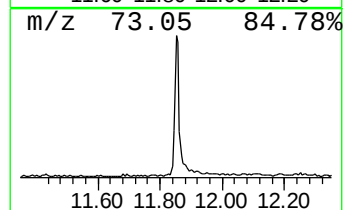
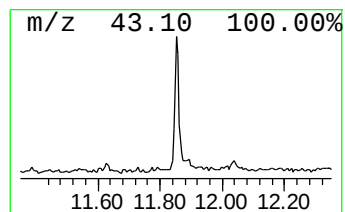
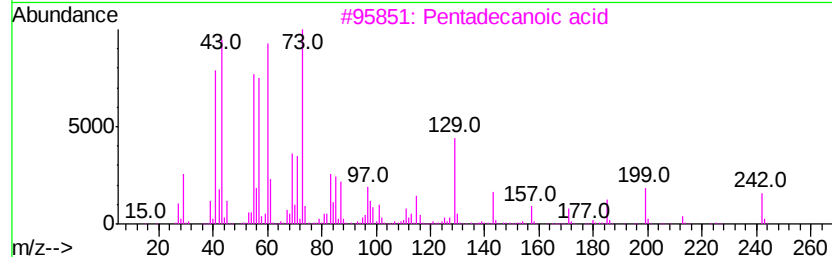
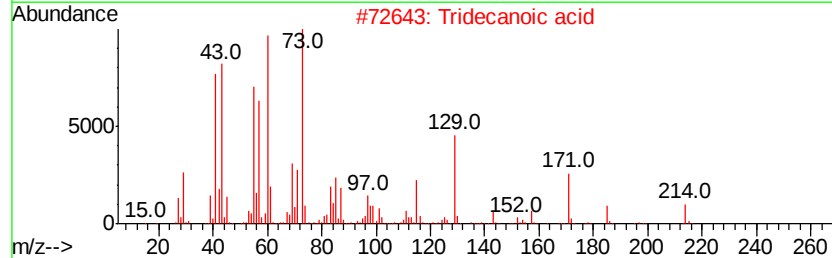
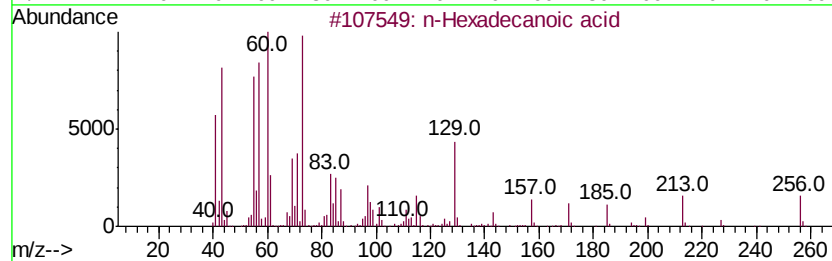
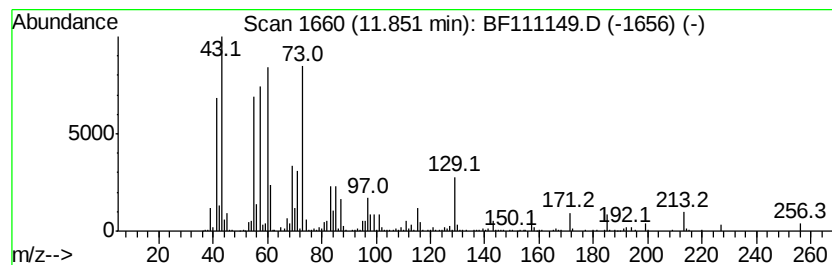
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.85	4.55 ng	829277	Phenanthrene-d10		11.32	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Undecanoic acid		186	C11H22O2	000112-37-8	87
5	Dodecanoic acid		200	C12H24O2	000143-07-7	72



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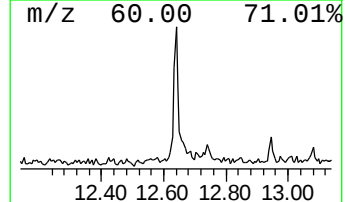
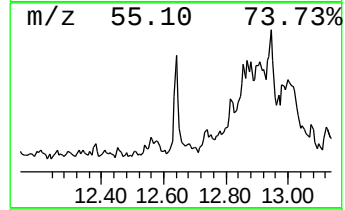
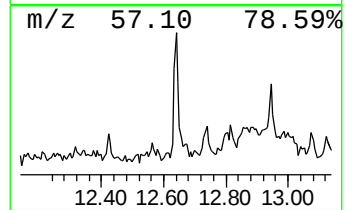
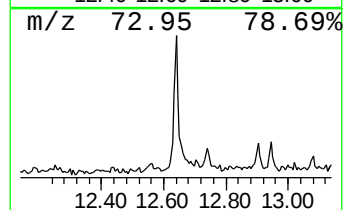
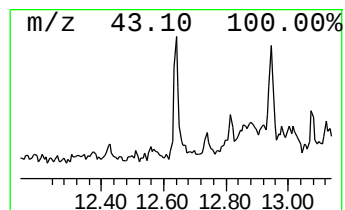
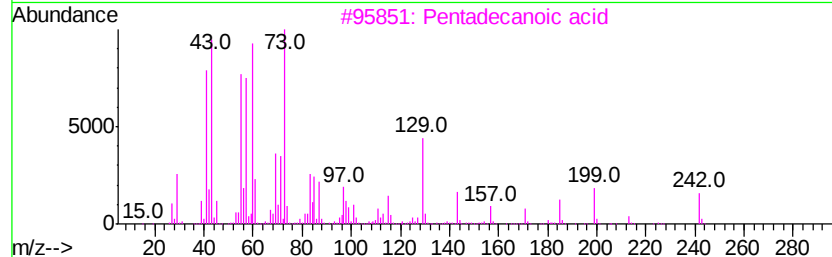
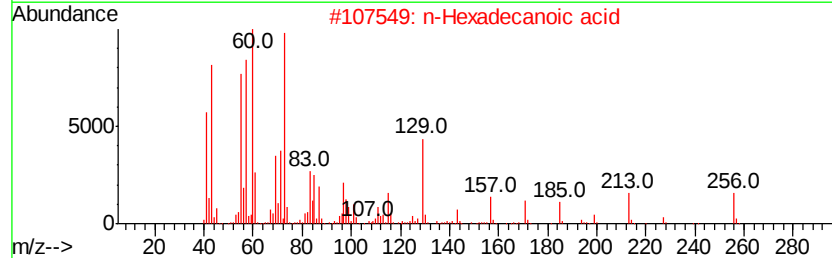
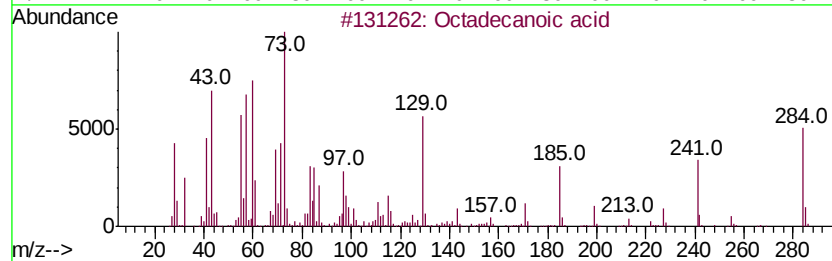
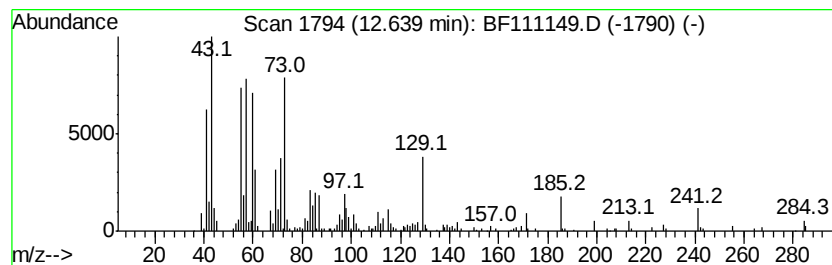
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.64	3.10 ng	363294	Chrysene-d12	13.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111149.D
Acq On : 6 Dec 2018 20:22
Operator : JU/SJ
Sample : J6204-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HLSP-SB-1A-(0-2)

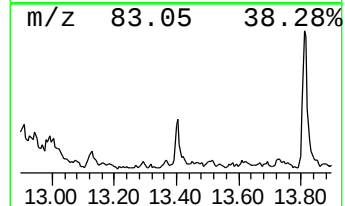
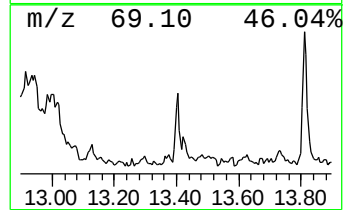
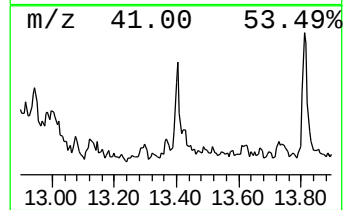
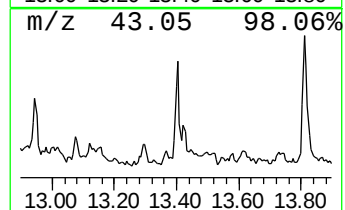
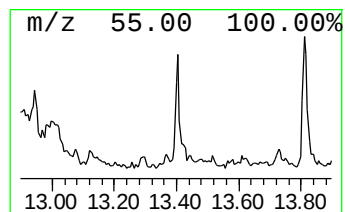
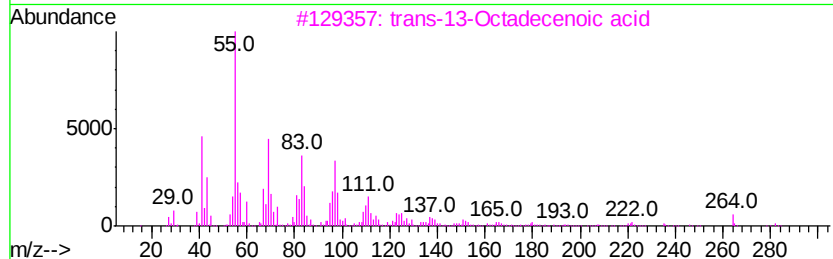
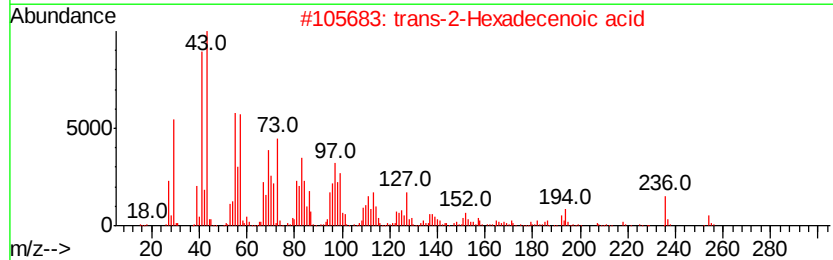
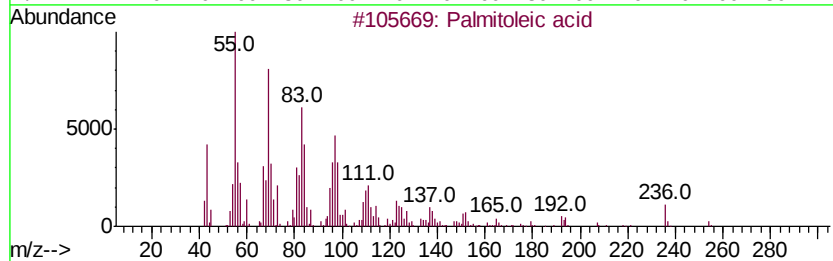
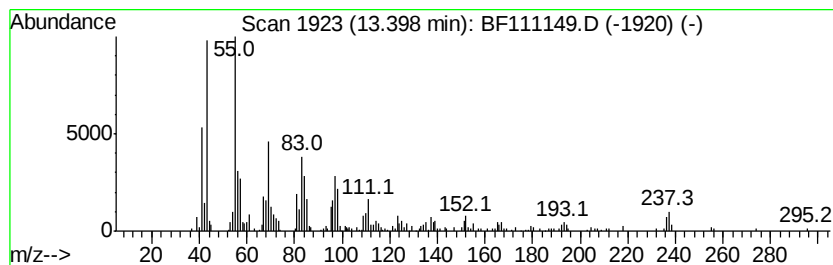
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Palmitoleic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.91 ng	340944	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Palmitoleic acid	254	C16H30O2	000373-49-9	93
2		trans-2-Hexadecenoic acid	254	C16H30O2	000929-79-3	72
3		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	50
4		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	47
5		Oxacyclohexadecan-2-one, 16-methyl-	254	C16H30O2	004459-57-8	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111149.D
Acq On : 6 Dec 2018 20:22
Operator : JU/SJ
Sample : J6204-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

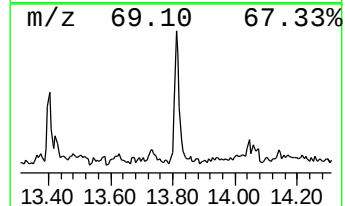
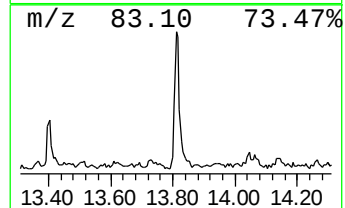
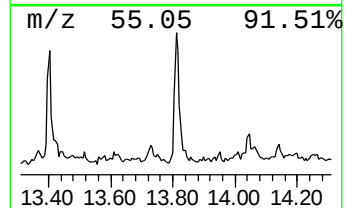
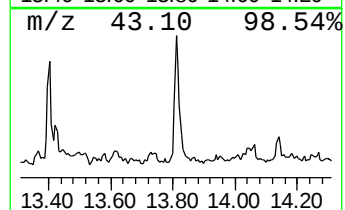
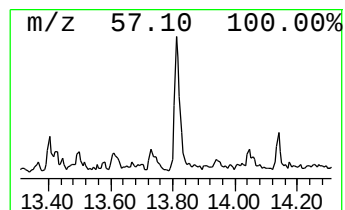
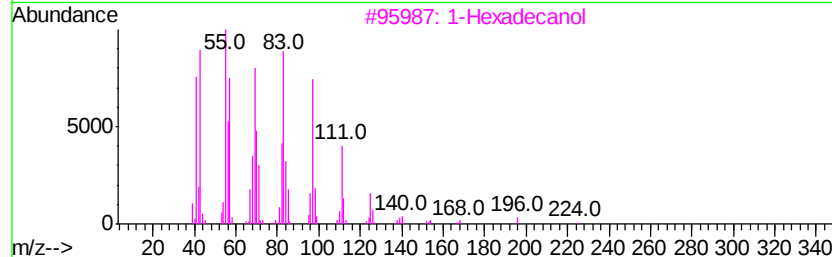
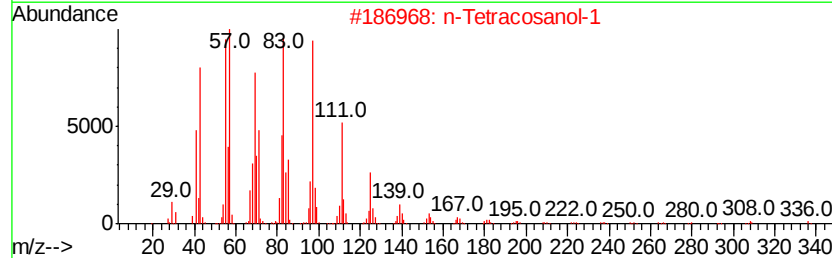
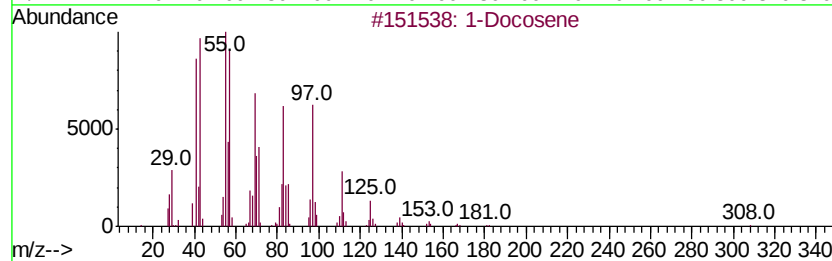
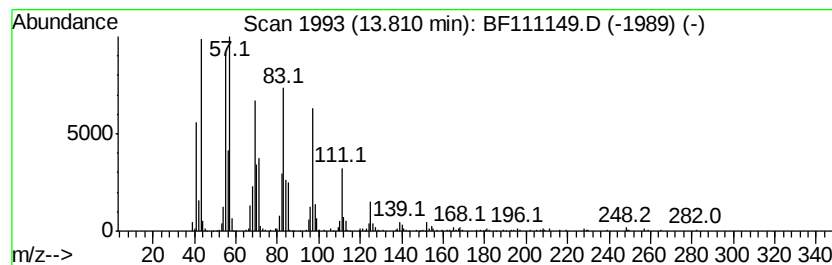
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ClientSampleId :
HLSP-SB-1A-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.81	5.55 ng	651747	Chrysene-d12		13.95
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111149.D
Acq On : 6 Dec 2018 20:22
Operator : JU/SJ
Sample : J6204-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

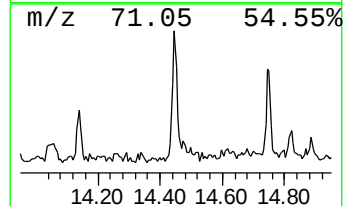
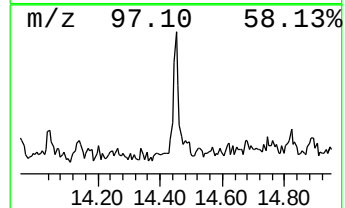
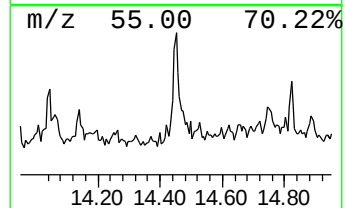
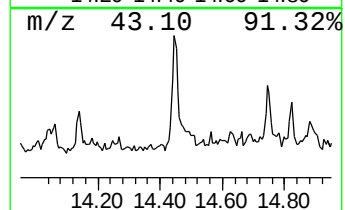
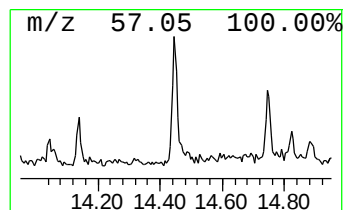
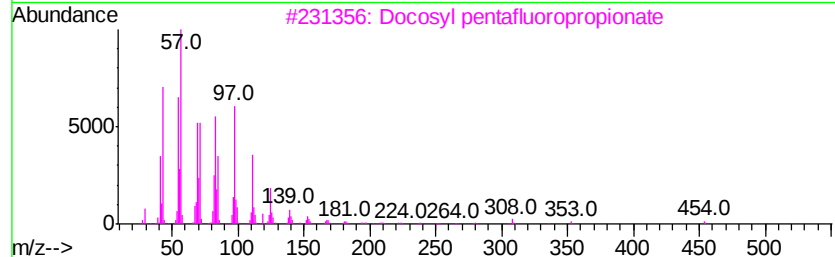
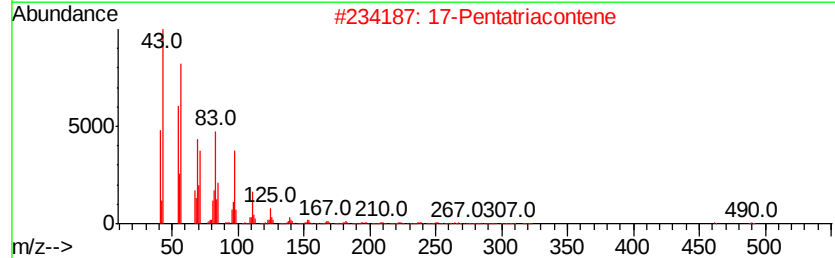
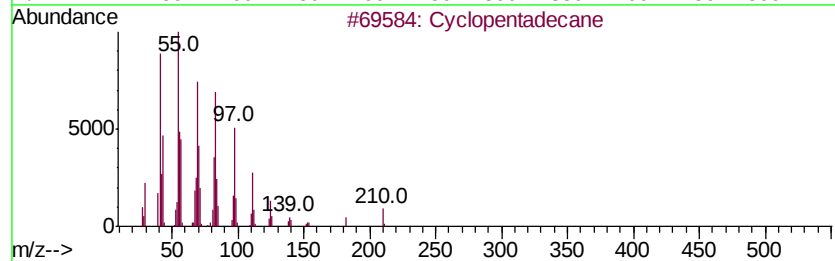
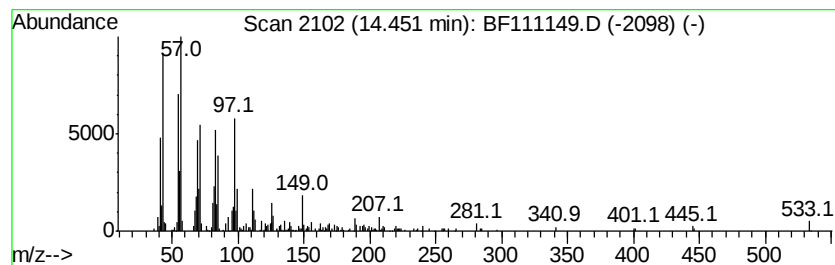
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	5.33 ng	624984	Chrysene-d12	13.95
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentadecane	210 C15H30	000295-48-7 86
2		17-Pentatriacontene	491 C35H70	006971-40-0 76
3		Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9 76
4		Tetracosyl heptafluorobutyrte	550 C28H49F7O2	1000351-83-7 76
5		Tricosyl pentafluoropropionate	486 C26H47F5O2	1000351-81-0 76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111149.D
Acq On : 6 Dec 2018 20:22
Operator : JU/SJ
Sample : J6204-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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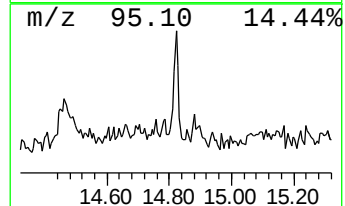
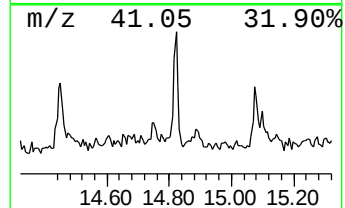
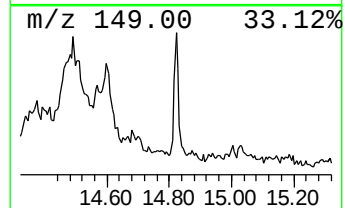
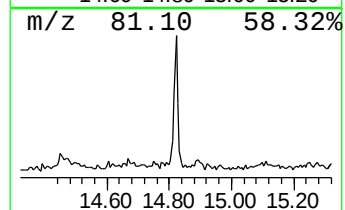
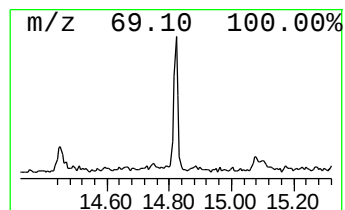
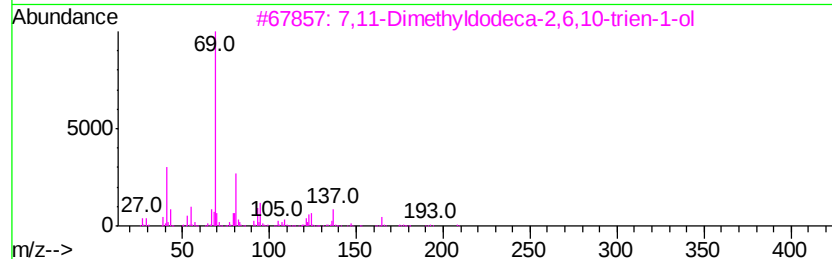
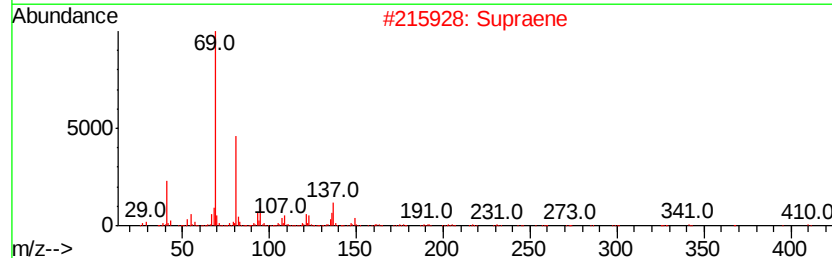
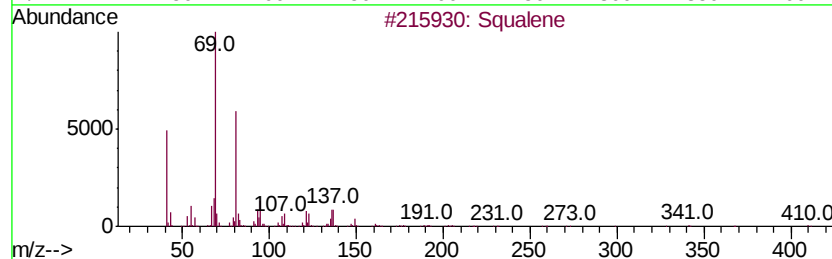
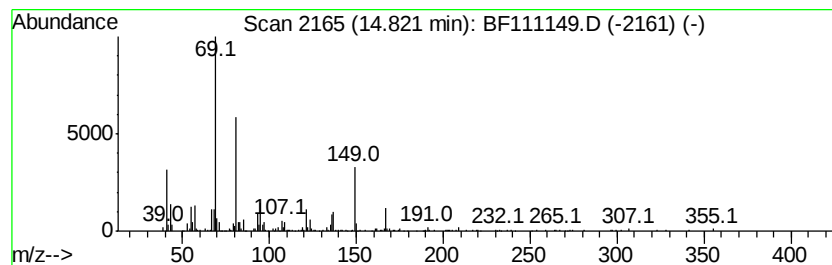
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.73 ng	334779	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	68
2		Supraene	410	C30H50	007683-64-9	58
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53
4		Farnesol isomer a	222	C15H26O	1000108-92-4	53
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111149.D
Acq On : 6 Dec 2018 20:22
Operator : JU/SJ
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HLSP-SB-1A-(0-2)

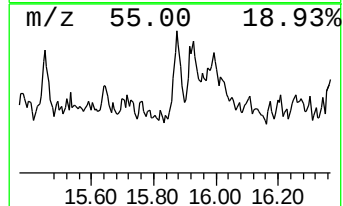
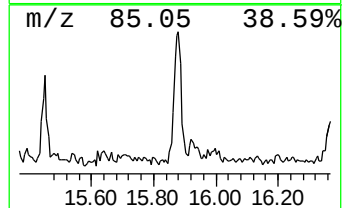
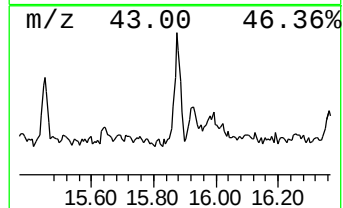
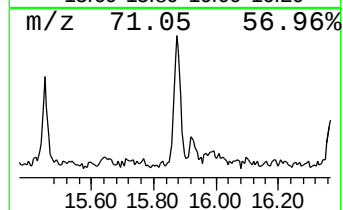
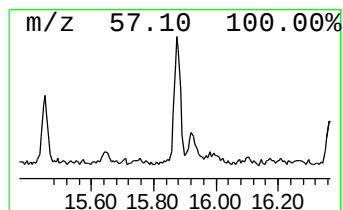
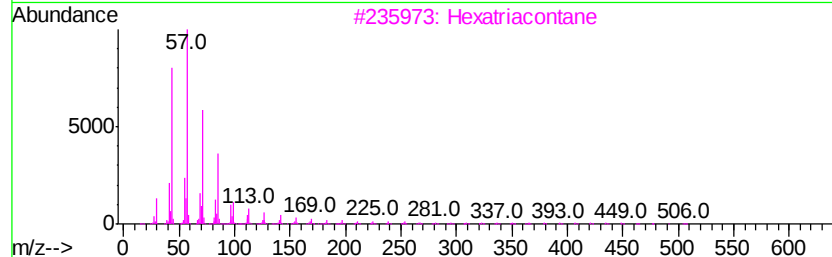
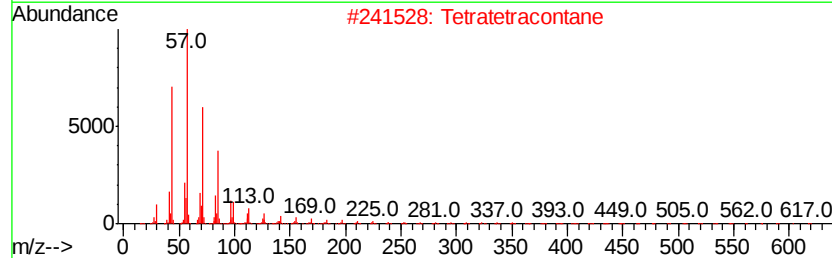
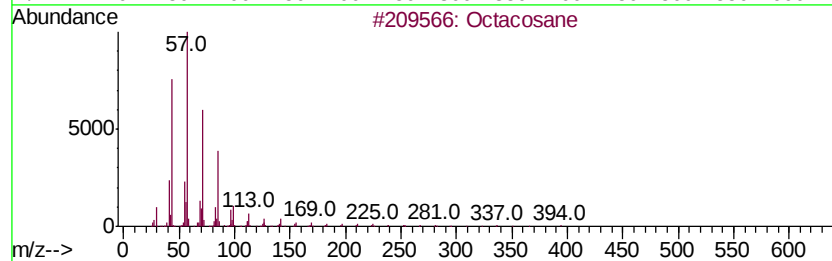
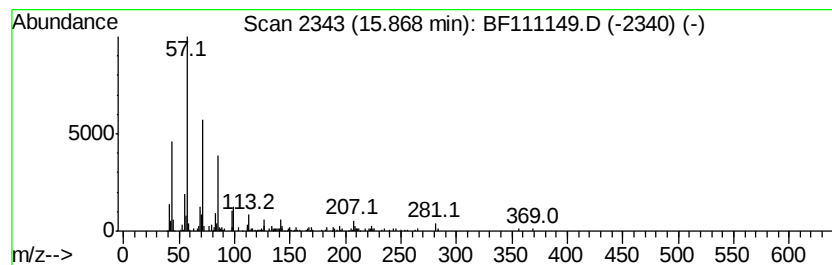
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.39 ng	293742	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Hexatriacontane	507	C36H74	000630-06-8	87
4		Octadecane	254	C18H38	000593-45-3	83
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
 Data File : BF111149.D
 Acq On : 6 Dec 2018 20:22
 Operator : JU/SJ
 Sample : J6204-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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
2-Pentanone, 4-hy...	5.02	2.4	ng	585743	1	6.80	4806520	20.0
unknown6.57	6.57	38.9	ng	9336810	1	6.80	4806520	20.0
Vanillin	10.50	2.2	ng	433194	3	9.84	4015340	20.0
n-Hexadecanoic acid	11.85	4.5	ng	829277	4	11.32	3642890	20.0
Octadecanoic acid	12.64	3.1	ng	363294	5	13.95	2347210	20.0
Palmitoleic acid	13.40	2.9	ng	340944	5	13.95	2347210	20.0
1-Docosene	13.81	5.5	ng	651747	5	13.95	2347210	20.0
Cyclopentadecane	14.45	5.3	ng	624984	5	13.95	2347210	20.0
Squalene	14.82	2.7	ng	334779	6	15.39	2455660	20.0
Octacosane	15.87	2.4	ng	293742	6	15.39	2455660	20.0