

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
 Data File : BF117890.D
 Acq On : 20 Nov 2019 13:58
 Operator : JU
 Sample : K5908-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-8-3-(6-12)

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-BF111319.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	2.187	11	17	30	rVB	656927	871766	21.99%	2.363%
2	5.128	512	517	526	rVB	557675	651824	16.44%	1.767%
3	5.528	580	585	588	rBV	3039030	2858855	72.12%	7.749%
4	6.539	751	757	768	rBV	3346745	3370676	85.03%	9.136%
5	6.686	777	782	785	rBV	3521341	3371272	85.05%	9.138%
6	6.916	817	821	824	rBV	1267125	988377	24.93%	2.679%
7	7.075	844	848	851	rBV	3079422	2671436	67.39%	7.241%
8	7.475	907	916	919	rBV	2082210	1856301	46.83%	5.031%
9	8.204	1036	1040	1043	rBV	1321112	1094475	27.61%	2.967%
10	9.280	1219	1223	1226	rBV	4675250	3963996	100.00%	10.744%
11	9.392	1238	1242	1246	rVB2	44302	50731	1.28%	0.138%
12	9.675	1286	1290	1298	rVB	649442	573397	14.47%	1.554%
13	9.963	1333	1339	1343	rBV	1537456	1373148	34.64%	3.722%
14	10.757	1469	1474	1477	rBV	2445082	2287690	57.71%	6.201%
15	10.880	1490	1495	1502	rVB3	43574	65321	1.65%	0.177%
16	11.316	1563	1569	1573	rBV3	31215	44885	1.13%	0.122%
17	11.457	1589	1593	1596	rBV	1639079	1329384	33.54%	3.603%
18	11.686	1627	1632	1637	rBV7	24466	46042	1.16%	0.125%
19	11.980	1675	1682	1693	rBV	932345	965643	24.36%	2.617%
20	12.545	1775	1778	1781	rBV	45706	45565	1.15%	0.124%
21	12.674	1796	1800	1806	rBV	109721	177863	4.49%	0.482%
22	12.768	1812	1816	1824	rBV	739593	751734	18.96%	2.038%
23	12.904	1836	1839	1846	rVB2	69811	100963	2.55%	0.274%
24	13.045	1859	1863	1866	rBV	3599235	3161583	79.76%	8.569%
25	13.274	1900	1902	1904	rBV	61630	47861	1.21%	0.130%
26	13.615	1958	1960	1963	rVB	77974	57885	1.46%	0.157%
27	13.945	2013	2016	2023	rBV	356429	475313	11.99%	1.288%
28	14.104	2037	2043	2046	rVB	1147090	1053280	26.57%	2.855%
29	14.262	2067	2070	2073	rBV	188160	154490	3.90%	0.419%
30	14.568	2119	2122	2124	rBV	221485	203081	5.12%	0.550%
31	14.868	2170	2173	2174	rBV	92916	98568	2.49%	0.267%
32	14.886	2174	2176	2180	rVB	248552	242674	6.12%	0.658%
33	15.245	2233	2237	2240	rVB	200254	217327	5.48%	0.589%
34	15.615	2295	2300	2303	rBV	886594	1134535	28.62%	3.075%

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ClientSampleId :
B-8-3-(6-12)

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	15.645	2303	2305	2309	rVB	146300	145902	3.68%	0.395%
36	16.104	2379	2383	2388	rVB	129778	194128	4.90%	0.526%
37	17.345	2589	2594	2599	rBV5	102679	195671	4.94%	0.530%

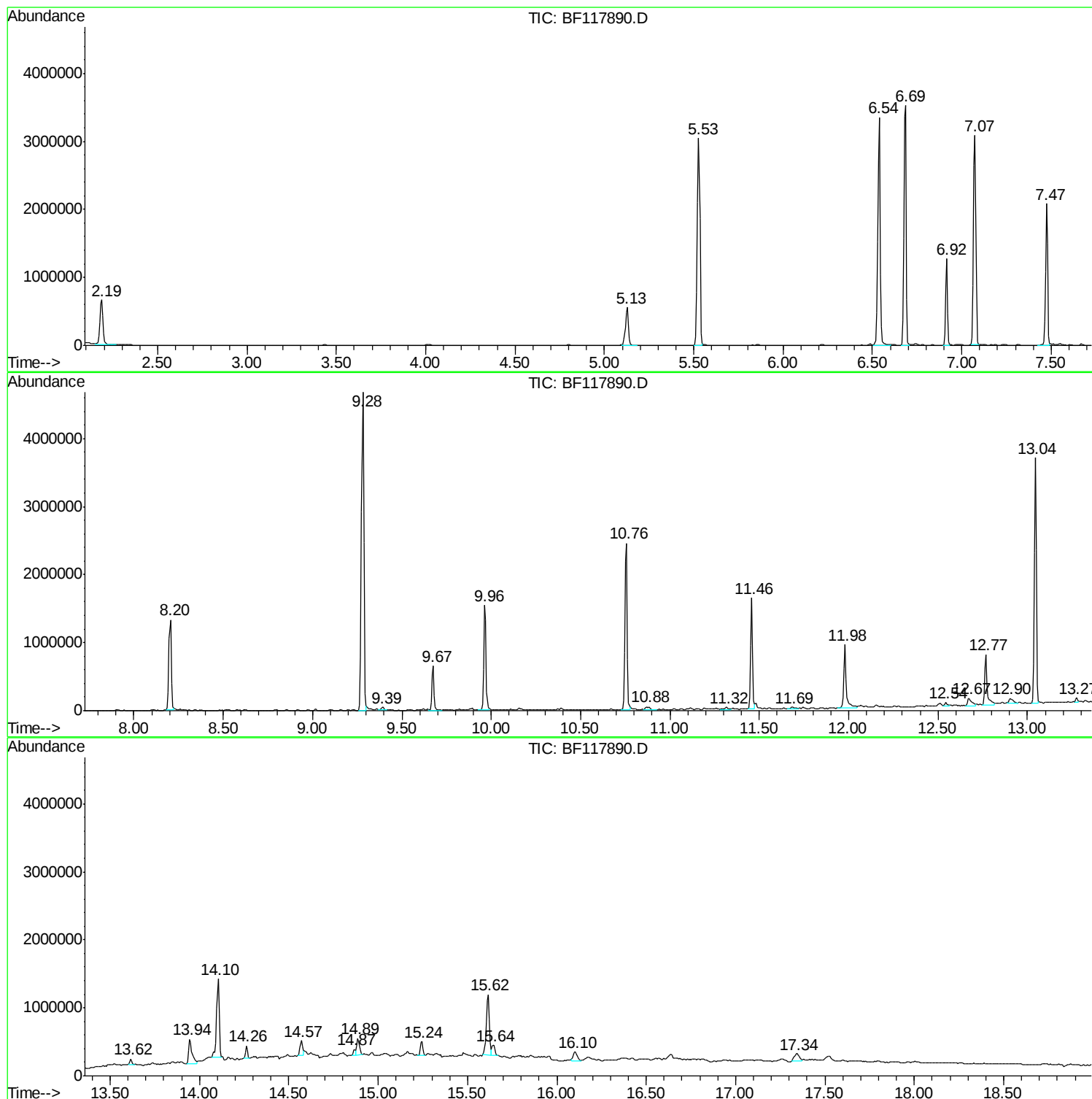
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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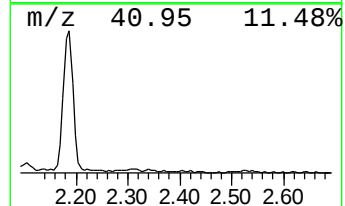
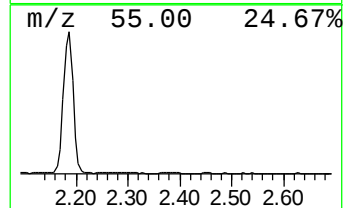
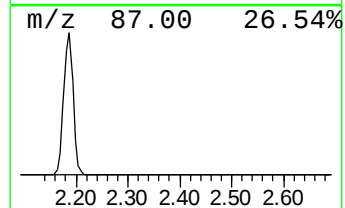
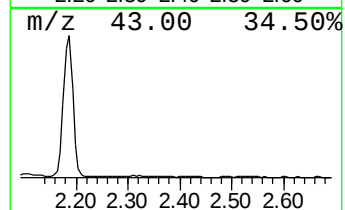
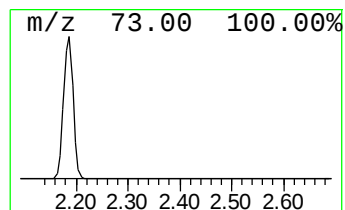
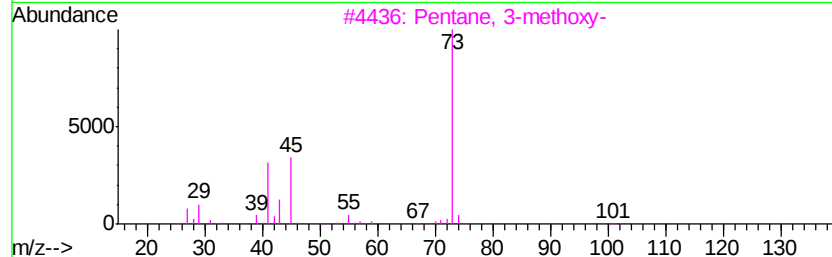
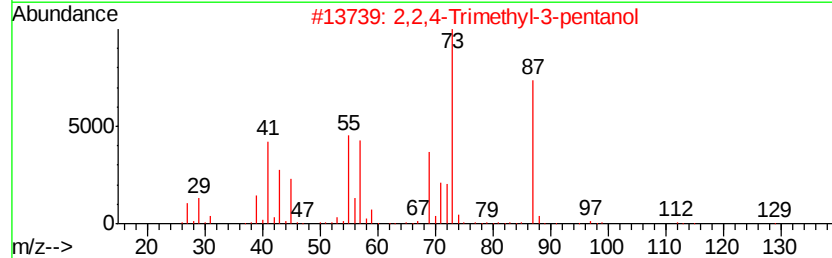
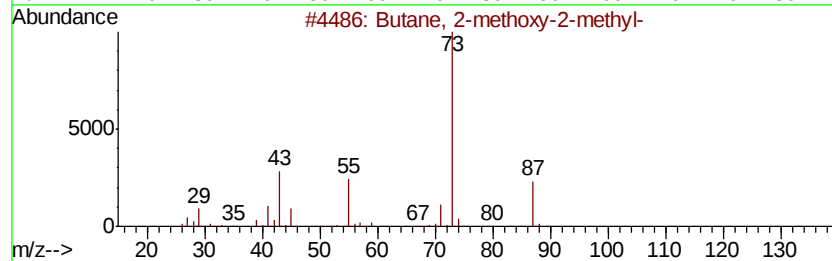
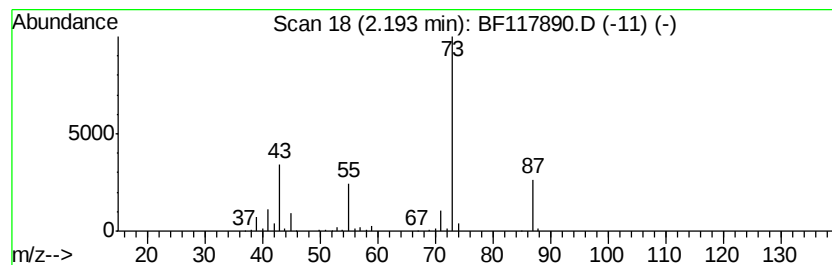
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.19	17.64 ng	871766	1,4-Dichlorobenzene-d4	6.92

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	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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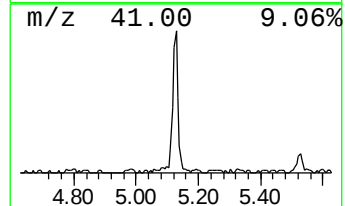
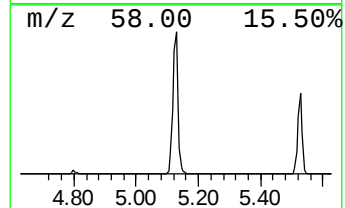
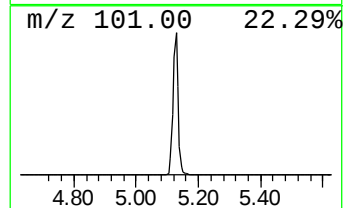
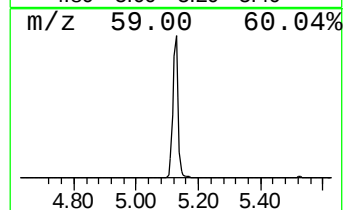
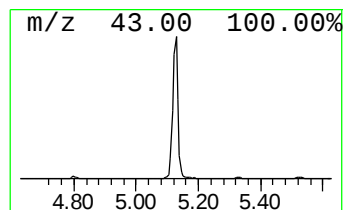
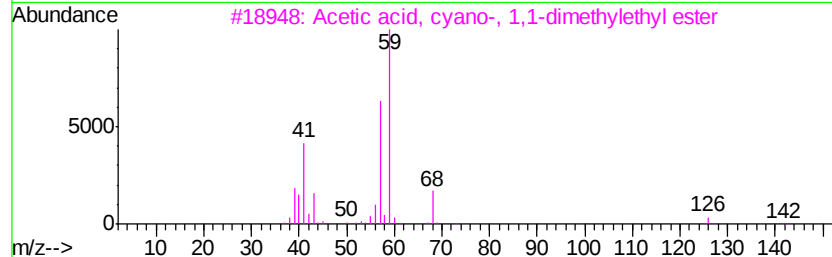
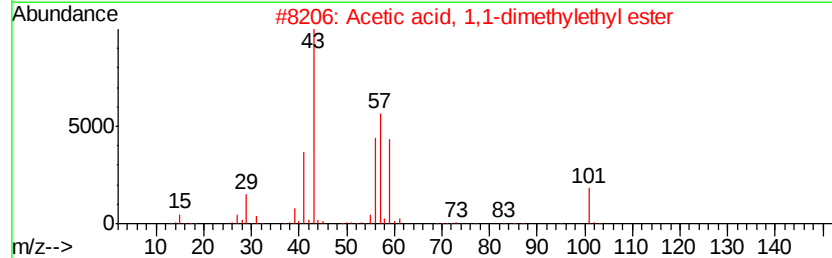
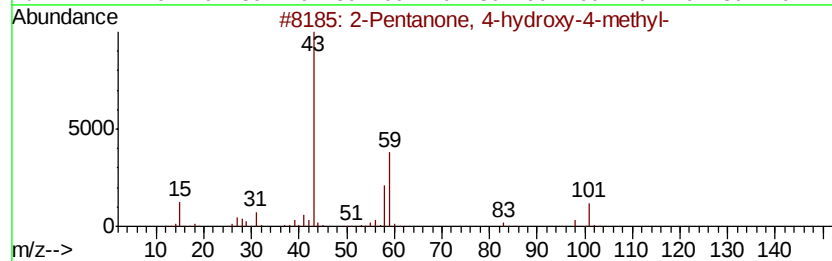
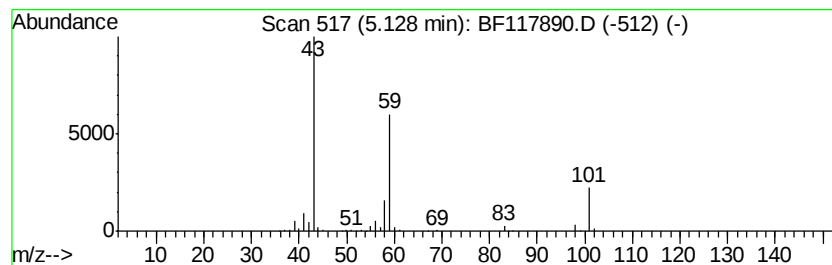
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	13.19 ng	651824	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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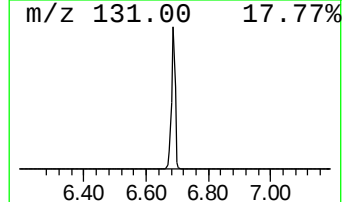
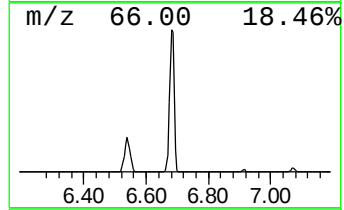
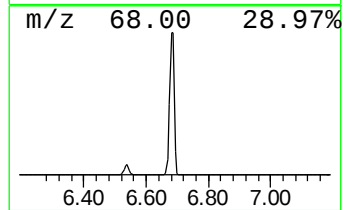
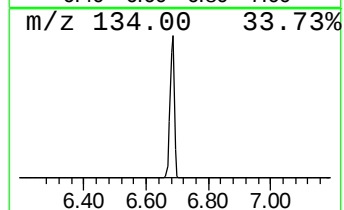
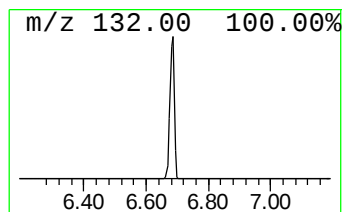
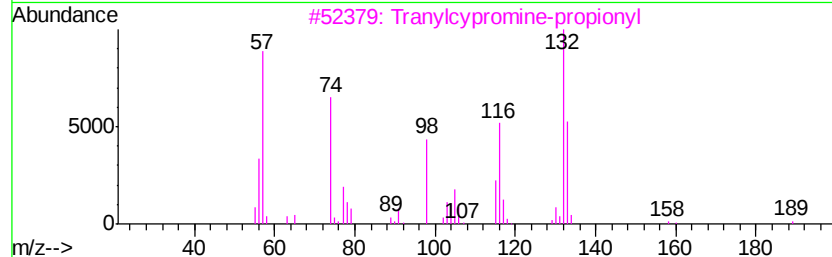
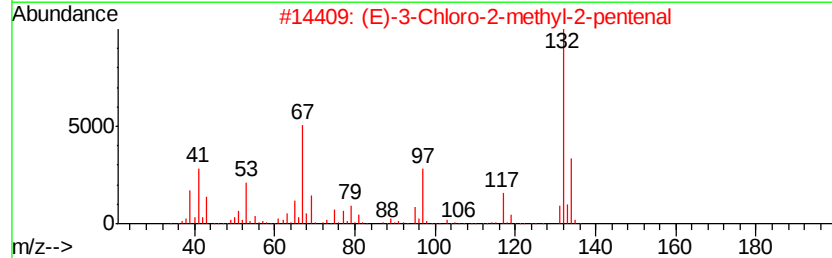
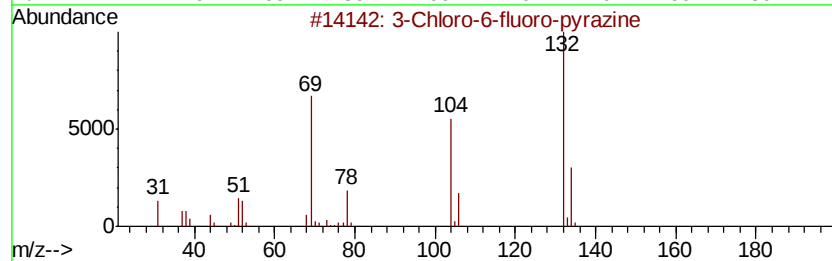
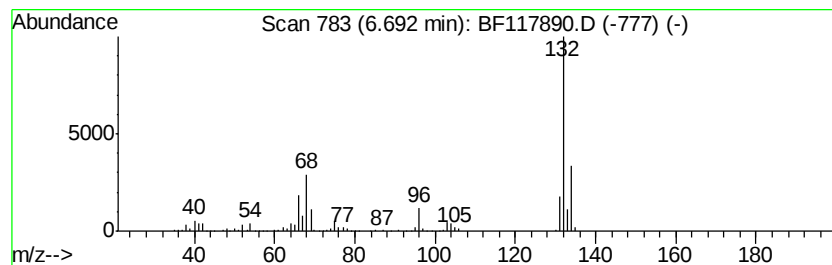
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	68.22 ng	3371270	1,4-Dichlorobenzene-d4	6.92

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		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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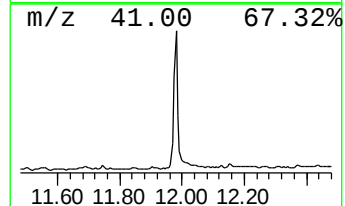
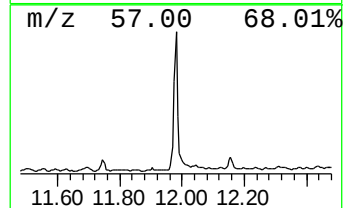
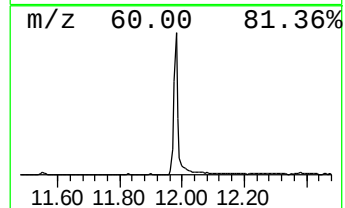
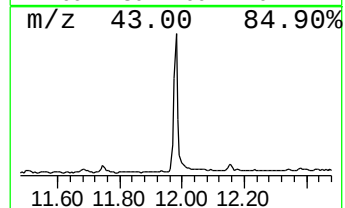
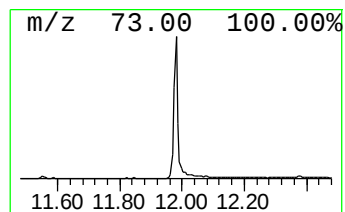
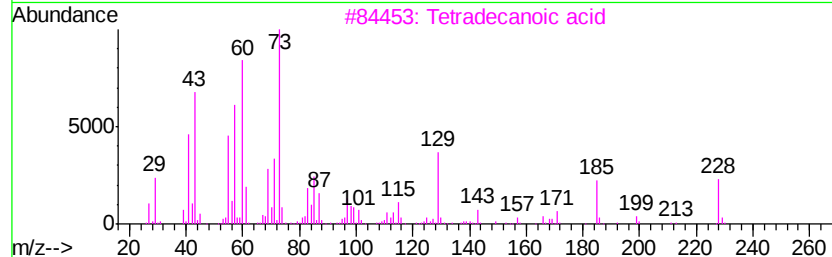
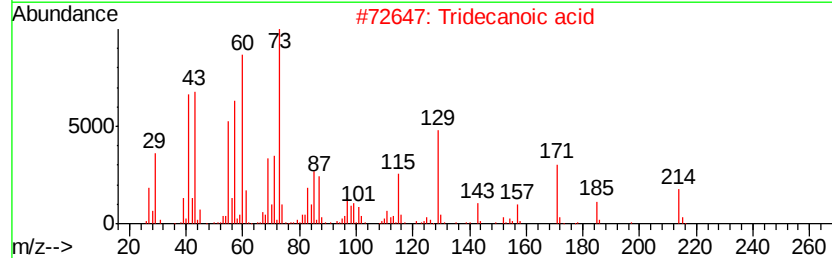
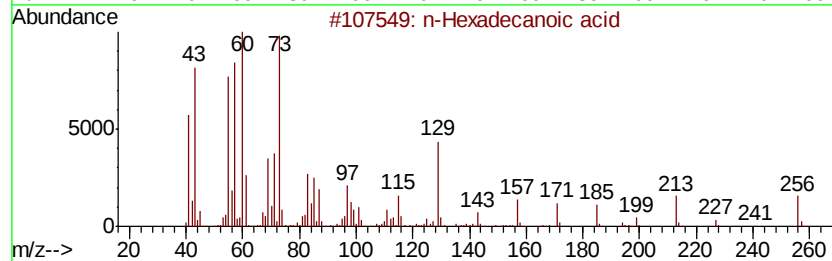
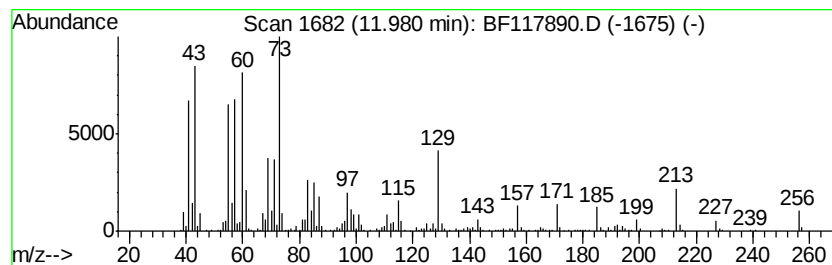
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 TIC Integration Parameters: LSCINT.P

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.98	14.53 ng	965643	Phenanthrene-d10		11.46	
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	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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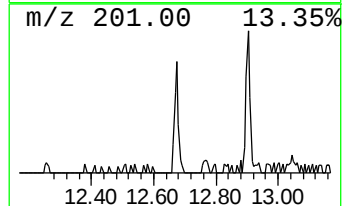
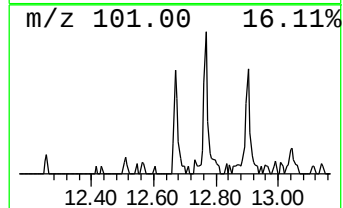
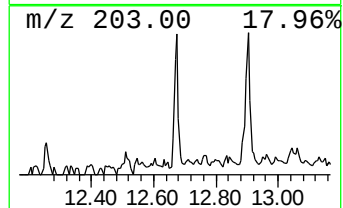
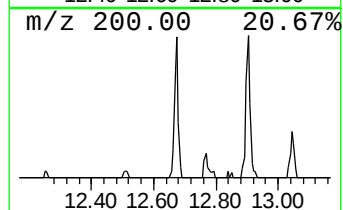
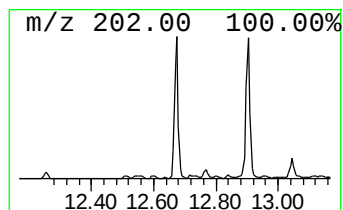
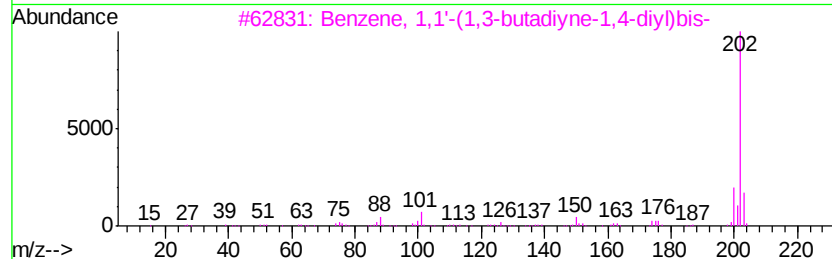
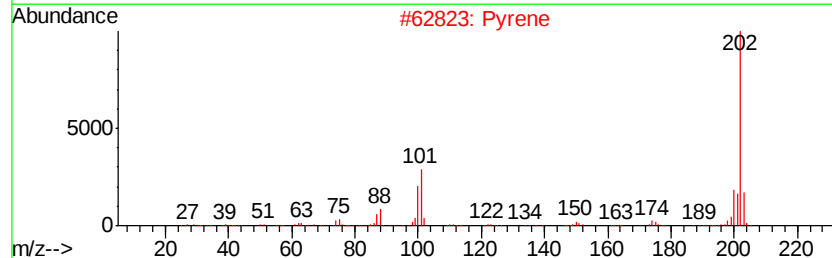
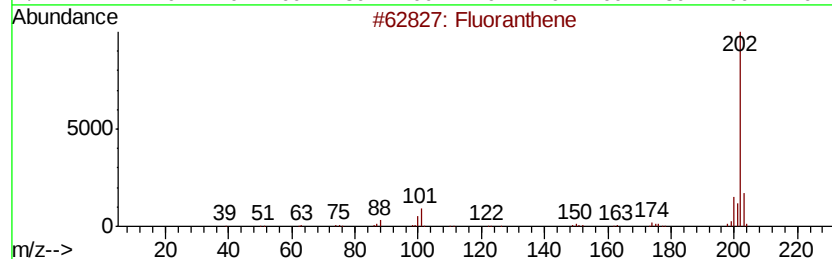
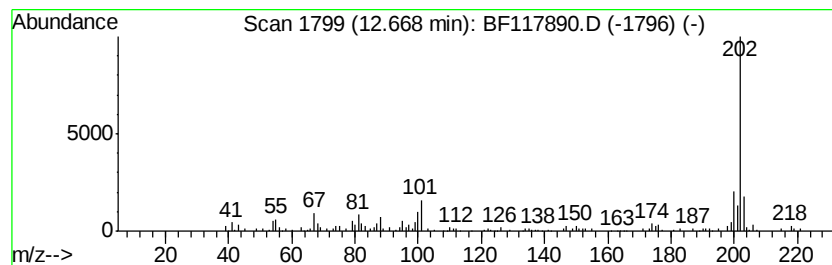
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.67	2.68 ng	177863	Phenanthrene-d10	11.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	95
2	Pyrene	202	C16H10	000129-00-0	81
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	72
5	1H-Indole-3-propanoic acid, 1-(t...	275	C15H21NO2Si	056196-72-6	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117890.D
Acq On : 20 Nov 2019 13:58
Operator : JU
Sample : K5908-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-8-3-(6-12)

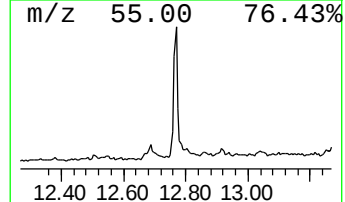
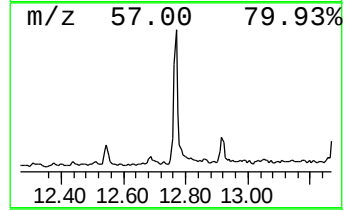
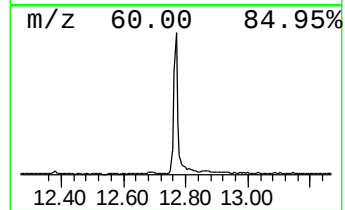
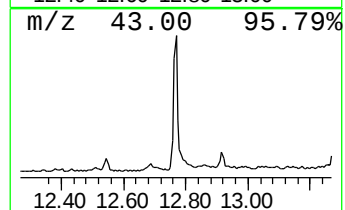
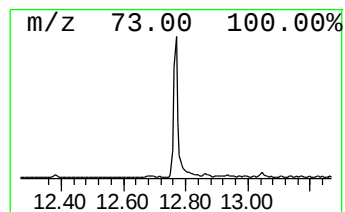
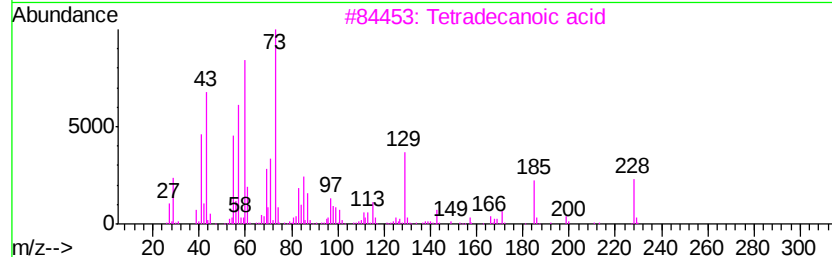
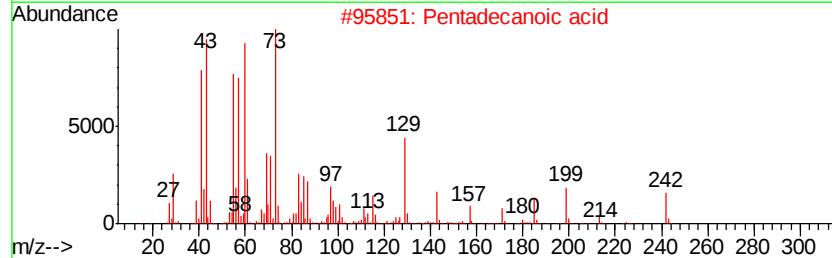
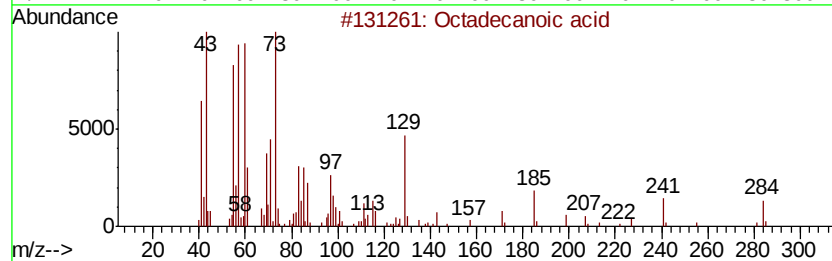
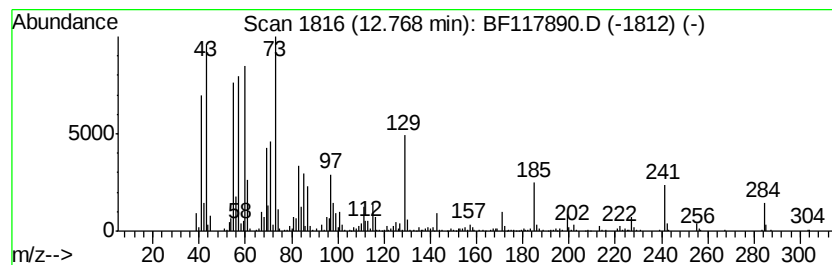
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	11.31 ng	751734	Phenanthrene-d10	11.46

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		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117890.D
Acq On : 20 Nov 2019 13:58
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Misc :
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ClientSampleId :
B-8-3-(6-12)

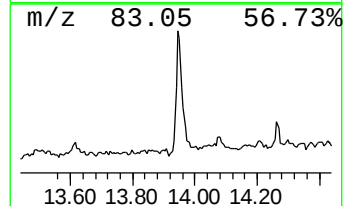
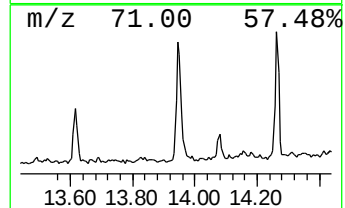
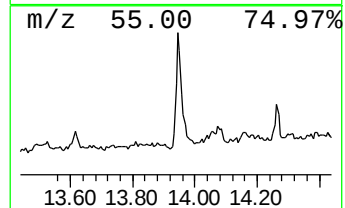
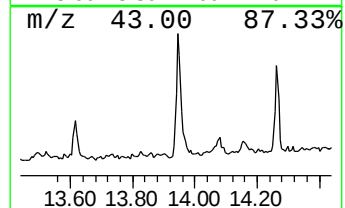
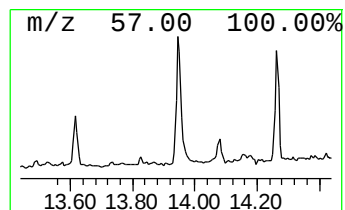
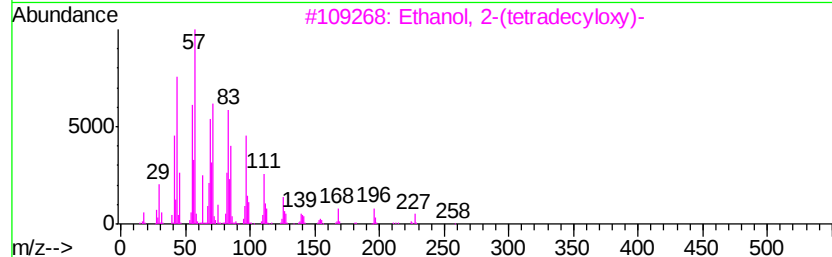
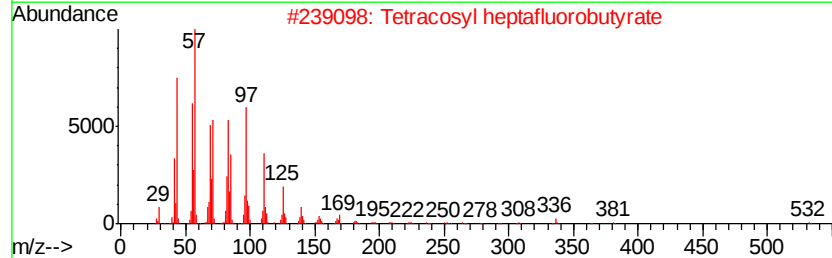
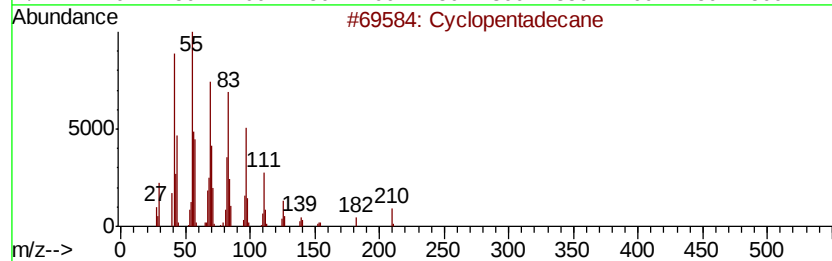
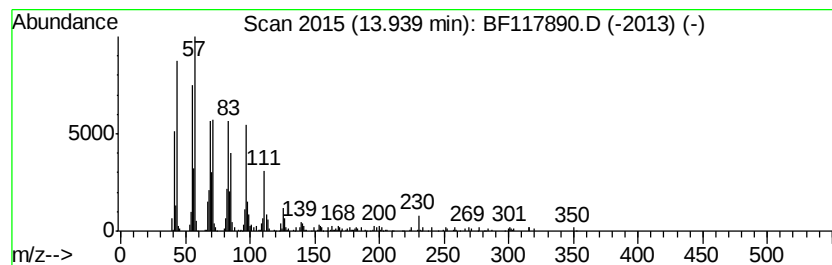
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	9.03 ng	475313	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	90
2		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
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 Acq On : 20 Nov 2019 13:58
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 Sample : K5908-04
 Misc :
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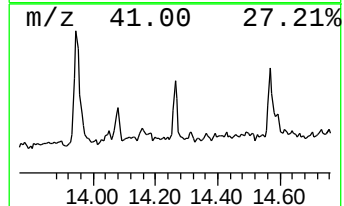
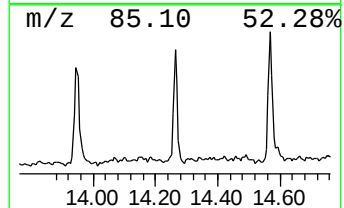
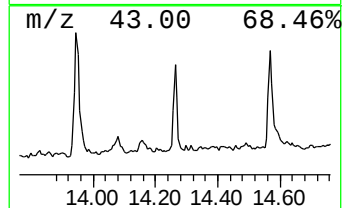
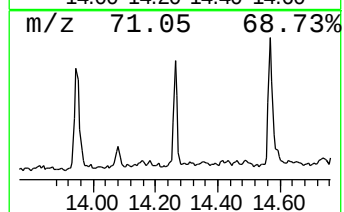
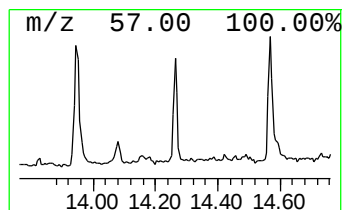
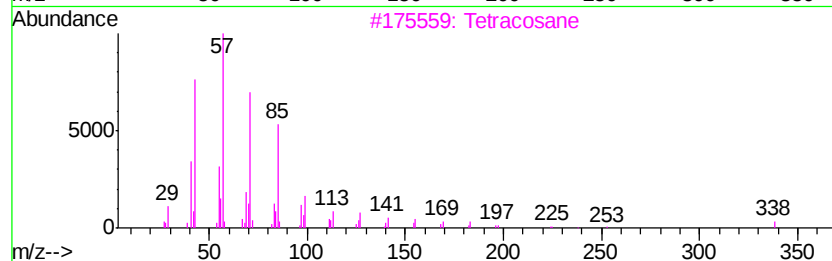
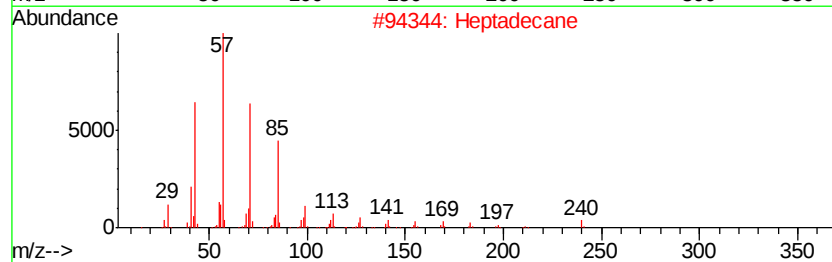
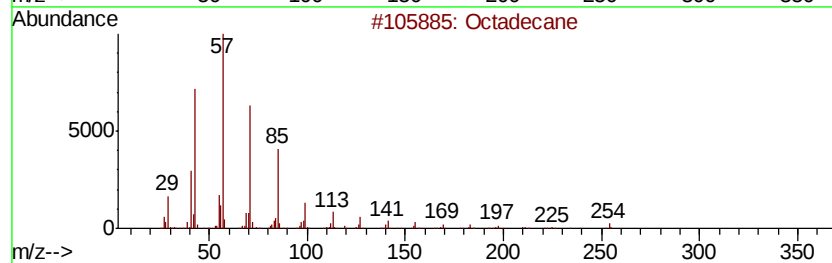
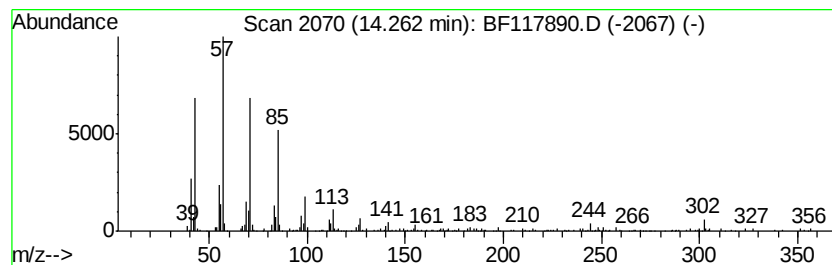
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.26	2.93 ng	154490	Chrysene-d12		14.10
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Heptadecane	240	C17H36	000629-78-7	94
3	Tetracosane	338	C24H50	000646-31-1	94
4	Heneicosane	296	C21H44	000629-94-7	87
5	Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117890.D
Acq On : 20 Nov 2019 13:58
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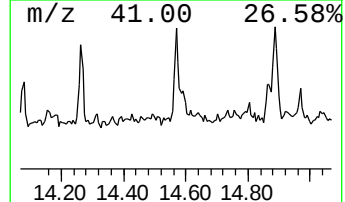
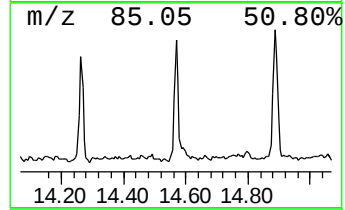
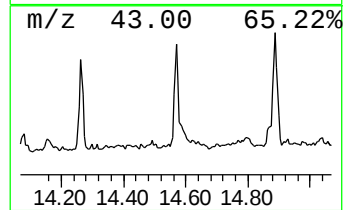
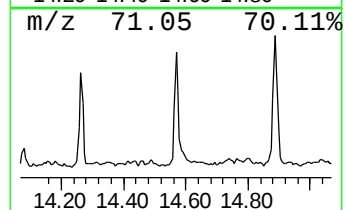
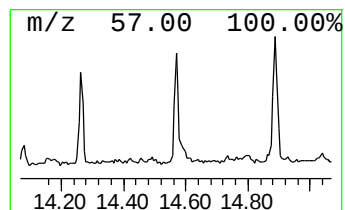
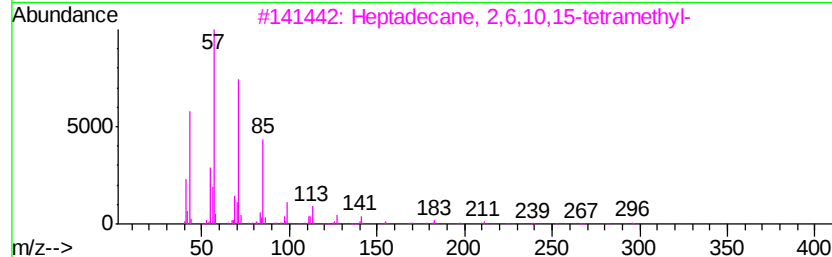
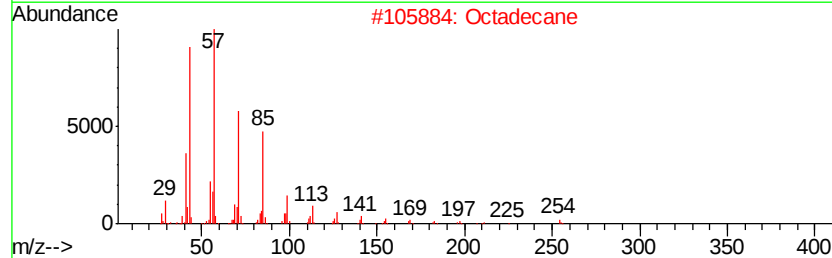
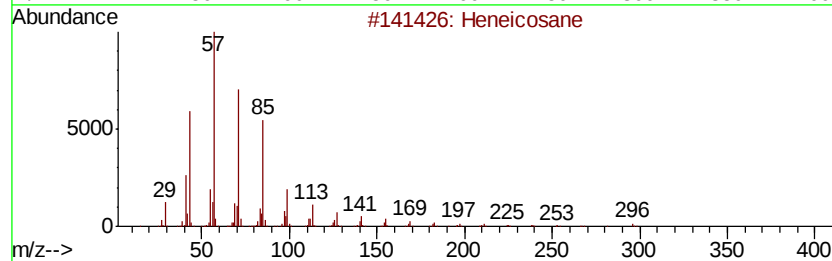
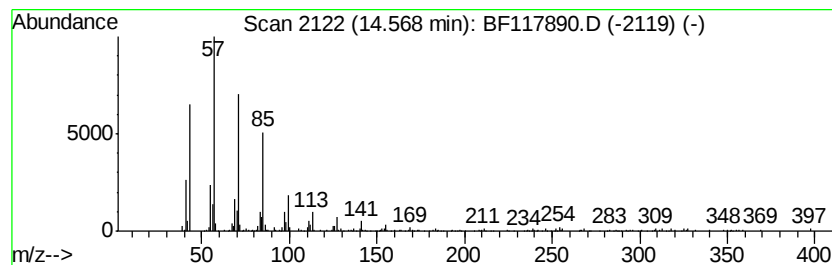
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.86 ng	203081	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	97
2		Octadecane	254	C18H38	000593-45-3	95
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4		Nonadecane	268	C19H40	000629-92-5	93
5		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
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 Misc :
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Instrument :
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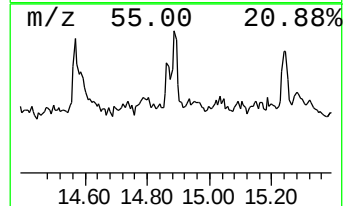
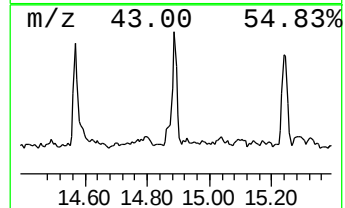
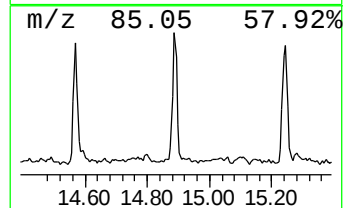
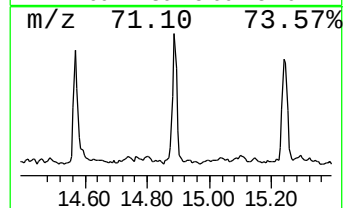
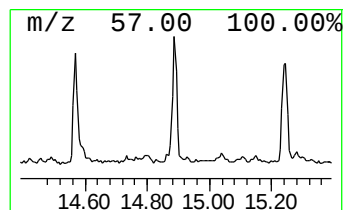
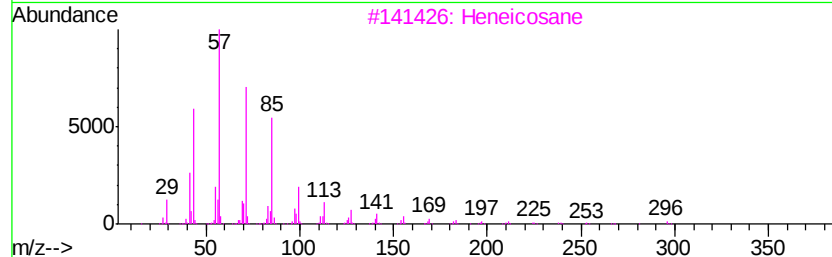
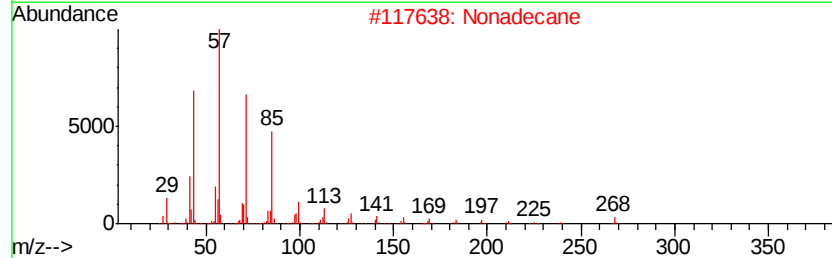
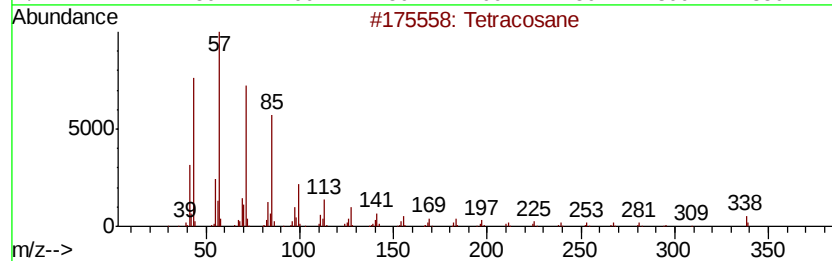
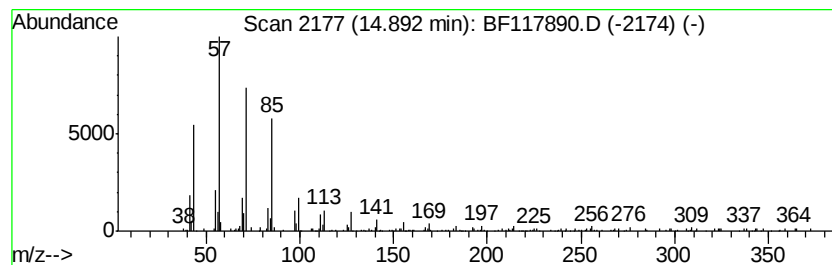
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 11 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	4.28 ng	242674	Perylene-d12	15.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	97
2			Nonadecane	268	C19H40	000629-92-5	93
3			Heneicosane	296	C21H44	000629-94-7	90
4			Octacosane	394	C28H58	000630-02-4	87
5			Hexacosane	366	C26H54	000630-01-3	87



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ALS Vial : 9 Sample Multiplier: 1

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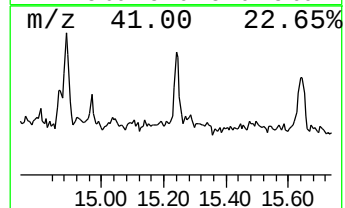
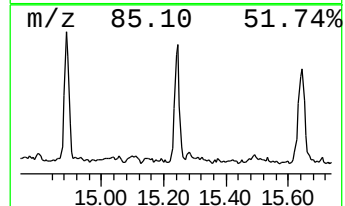
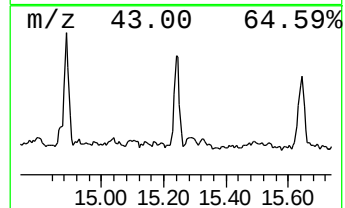
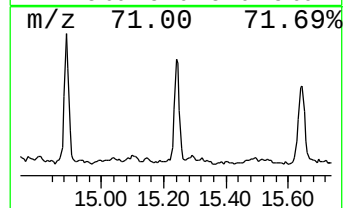
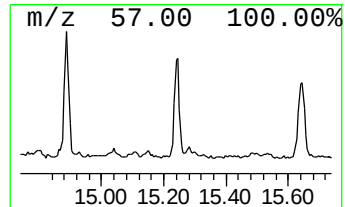
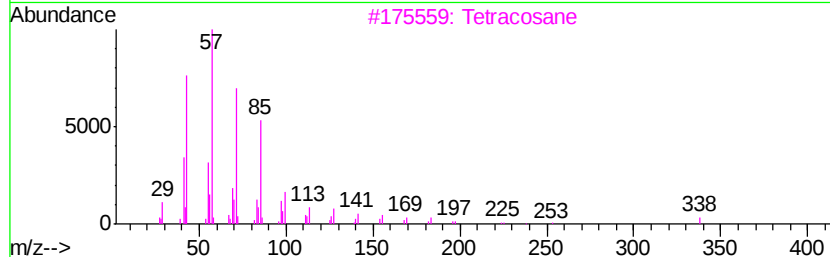
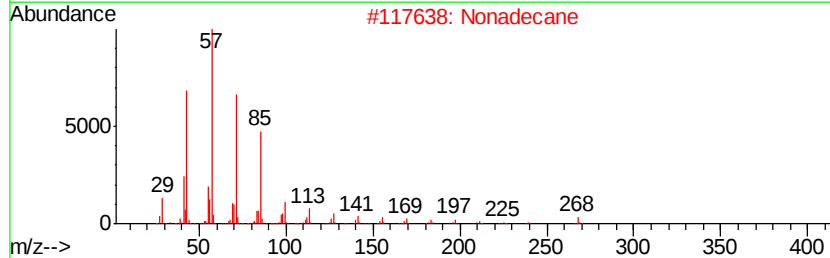
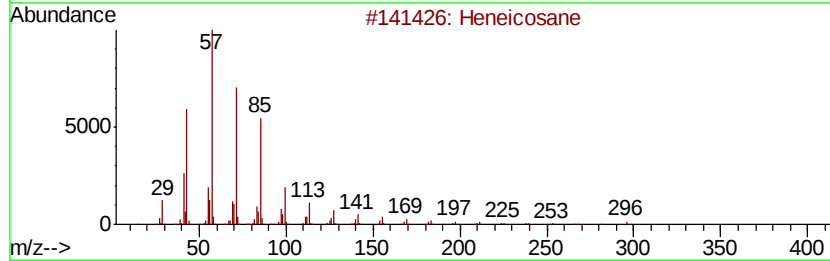
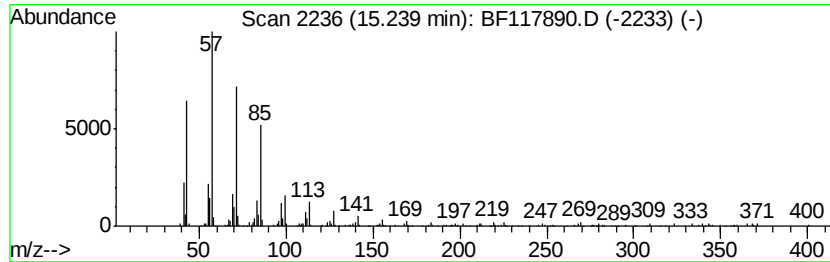
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	3.83 ng	217327	Perylene-d12	15.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Nonadecane	268	C19H40	000629-92-5	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			Docosane	310	C22H46	000629-97-0	86
5			Eicosane	282	C20H42	000112-95-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
 Data File : BF117890.D
 Acq On : 20 Nov 2019 13:58
 Operator : JU
 Sample : K5908-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 B-8-3-(6-12)

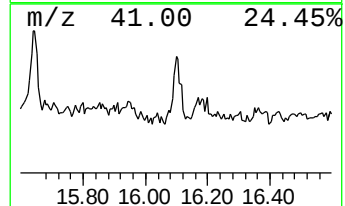
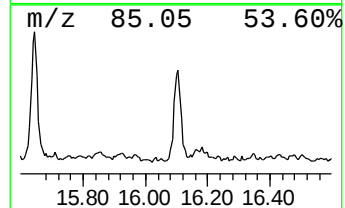
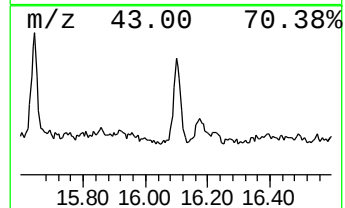
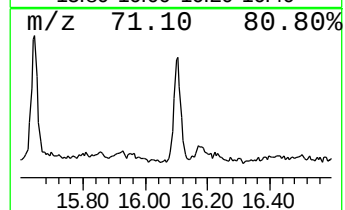
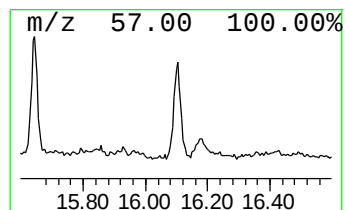
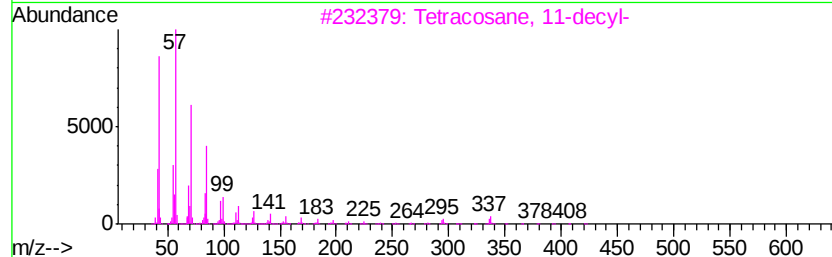
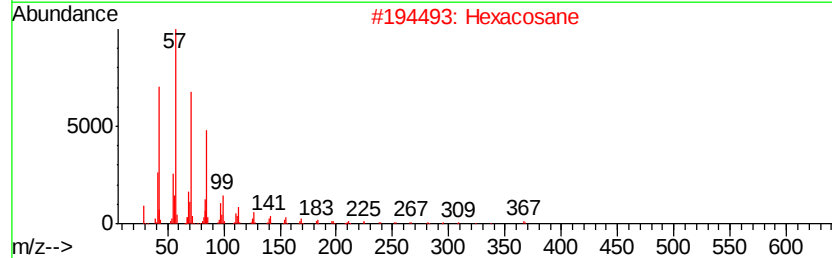
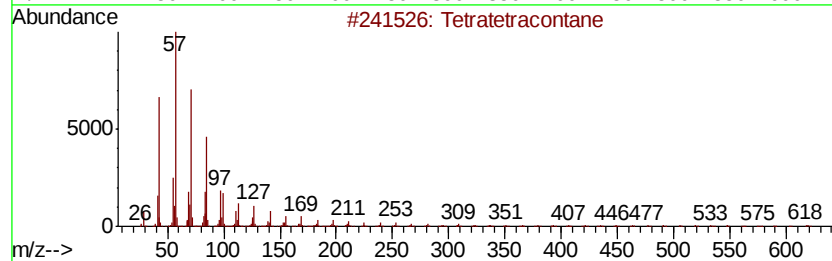
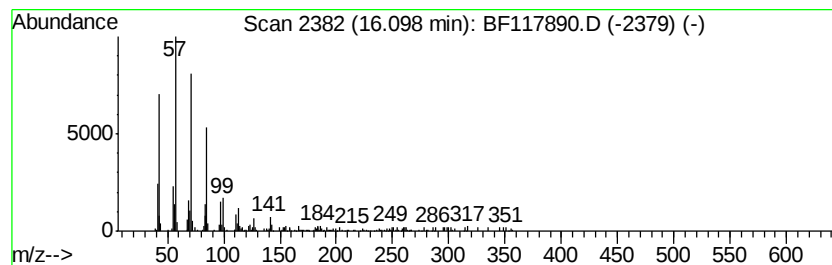
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 13 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	3.42 ng	194128	Perylene-d12	15.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117890.D
Acq On : 20 Nov 2019 13:58
Operator : JU
Sample : K5908-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-8-3-(6-12)

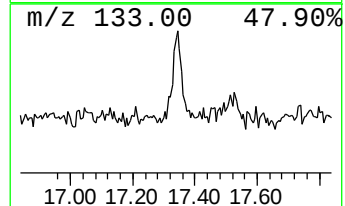
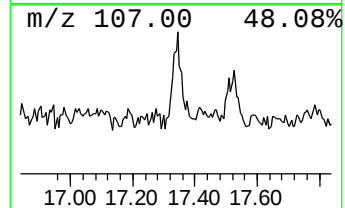
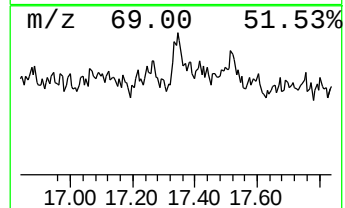
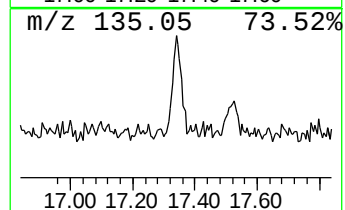
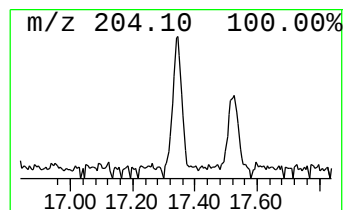
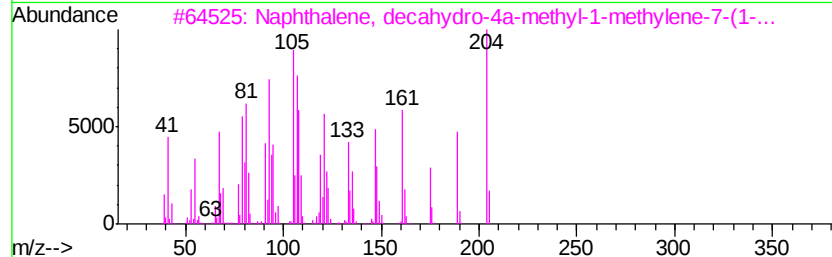
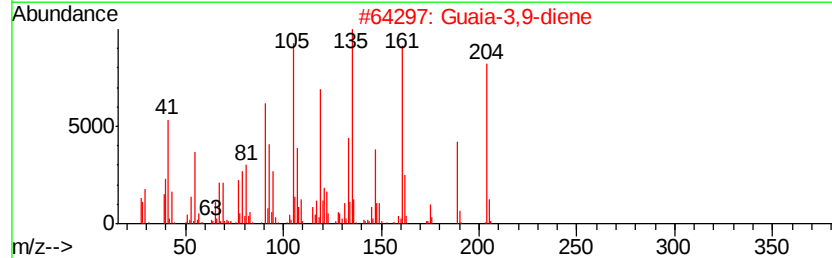
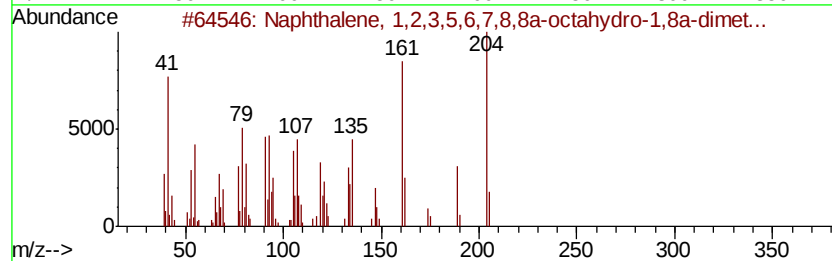
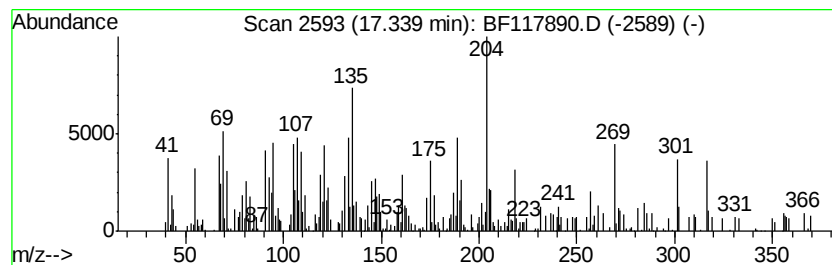
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	3.45 ng	195671	Perylene-d12	15.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	64
2		Guaia-3,9-diene	204	C15H24	000489-83-8	50
3		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49
4		Farnesyl bromide	284	C15H25Br	006874-67-5	47
5		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112019\
 Data File : BF117890.D
 Acq On : 20 Nov 2019 13:58
 Operator : JU
 Sample : K5908-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-8-3-(6-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.19	17.6	ng	871766	1	6.92	988377	20.0
2-Pentanone, 4-hy...	5.13	13.2	ng	651824	1	6.92	988377	20.0
unknown6.69	6.69	68.2	ng	3371270	1	6.92	988377	20.0
n-Hexadecanoic acid	11.98	14.5	ng	965643	4	11.46	1329380	20.0
Benzene, 1,1'-(1,...	12.67	2.7	ng	177863	4	11.46	1329380	20.0
Octadecanoic acid	12.77	11.3	ng	751734	4	11.46	1329380	20.0
Cyclopentadecane	13.94	9.0	ng	475313	5	14.10	1053280	20.0
Octadecane	14.26	2.9	ng	154490	5	14.10	1053280	20.0
Heneicosane	14.57	3.9	ng	203081	5	14.10	1053280	20.0
Tetracosane	14.89	4.3	ng	242674	6	15.62	1134540	20.0
Nonadecane	15.24	3.8	ng	217327	6	15.62	1134540	20.0
Tetratetracontane	16.10	3.4	ng	194128	6	15.62	1134540	20.0
Naphthalene, 1,2,...	17.34	3.5	ng	195671	6	15.62	1134540	20.0