

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
 Data File : BF112649.D
 Acq On : 21 Feb 2019 13:41
 Operator : JU/SJ
 Sample : K1538-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 M-11-A-S

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-BF012519.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	5.039	499	502	517	rBV	48337	74814	3.39%	0.364%
2	5.457	570	573	603	rBV	1425090	1662498	75.22%	8.093%
3	6.475	742	746	763	rBV	1607023	1757008	79.50%	8.553%
4	6.598	763	767	782	rVB	2085420	1928957	87.28%	9.390%
5	6.822	801	805	815	rBV	536561	512388	23.18%	2.494%
6	6.975	827	831	846	rBV	1608291	1470323	66.53%	7.158%
7	7.386	897	901	921	rBV	1126995	1146546	51.88%	5.581%
8	8.104	1019	1023	1041	rBV	646747	676062	30.59%	3.291%
9	9.174	1201	1205	1216	rBV	2460384	2210093	100.00%	10.759%
10	9.574	1269	1273	1279	rBV	99972	99122	4.48%	0.483%
11	9.857	1317	1321	1335	rVB2	880400	819146	37.06%	3.988%
12	10.651	1452	1456	1471	rBV	1438212	1531632	69.30%	7.456%
13	11.345	1571	1574	1584	rBV	806322	847192	38.33%	4.124%
14	11.863	1659	1662	1676	rBV2	226992	302902	13.71%	1.475%
15	12.404	1748	1754	1762	rVB8	15146	33930	1.54%	0.165%
16	12.568	1777	1782	1786	rBV	45375	56496	2.56%	0.275%
17	12.645	1792	1795	1806	rBV	94680	136133	6.16%	0.663%
18	12.798	1815	1821	1828	rVB2	35474	59144	2.68%	0.288%
19	12.927	1838	1843	1846	rBV	2387052	2049478	92.73%	9.977%
20	13.139	1876	1879	1882	rVB5	22861	26905	1.22%	0.131%
21	13.480	1933	1937	1943	rBV2	37006	53812	2.43%	0.262%
22	13.815	1990	1994	2001	rBV	147517	228249	10.33%	1.111%
23	13.998	2021	2025	2035	rVB	593060	646154	29.24%	3.146%
24	14.127	2043	2047	2050	rBV	125657	118194	5.35%	0.575%
25	14.433	2095	2099	2102	rBV	192147	203701	9.22%	0.992%
26	14.733	2146	2150	2153	rBV	231966	236357	10.69%	1.151%
27	14.804	2160	2162	2167	rVB	74743	73316	3.32%	0.357%
28	15.062	2202	2206	2210	rVB2	224045	269363	12.19%	1.311%
29	15.433	2265	2269	2272	rBV	202214	259751	11.75%	1.264%
30	15.468	2272	2275	2286	rVB	432314	598846	27.10%	2.915%
31	15.856	2337	2341	2346	rVB	177087	241167	10.91%	1.174%
32	16.350	2421	2425	2437	rVB3	99481	212315	9.61%	1.034%

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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

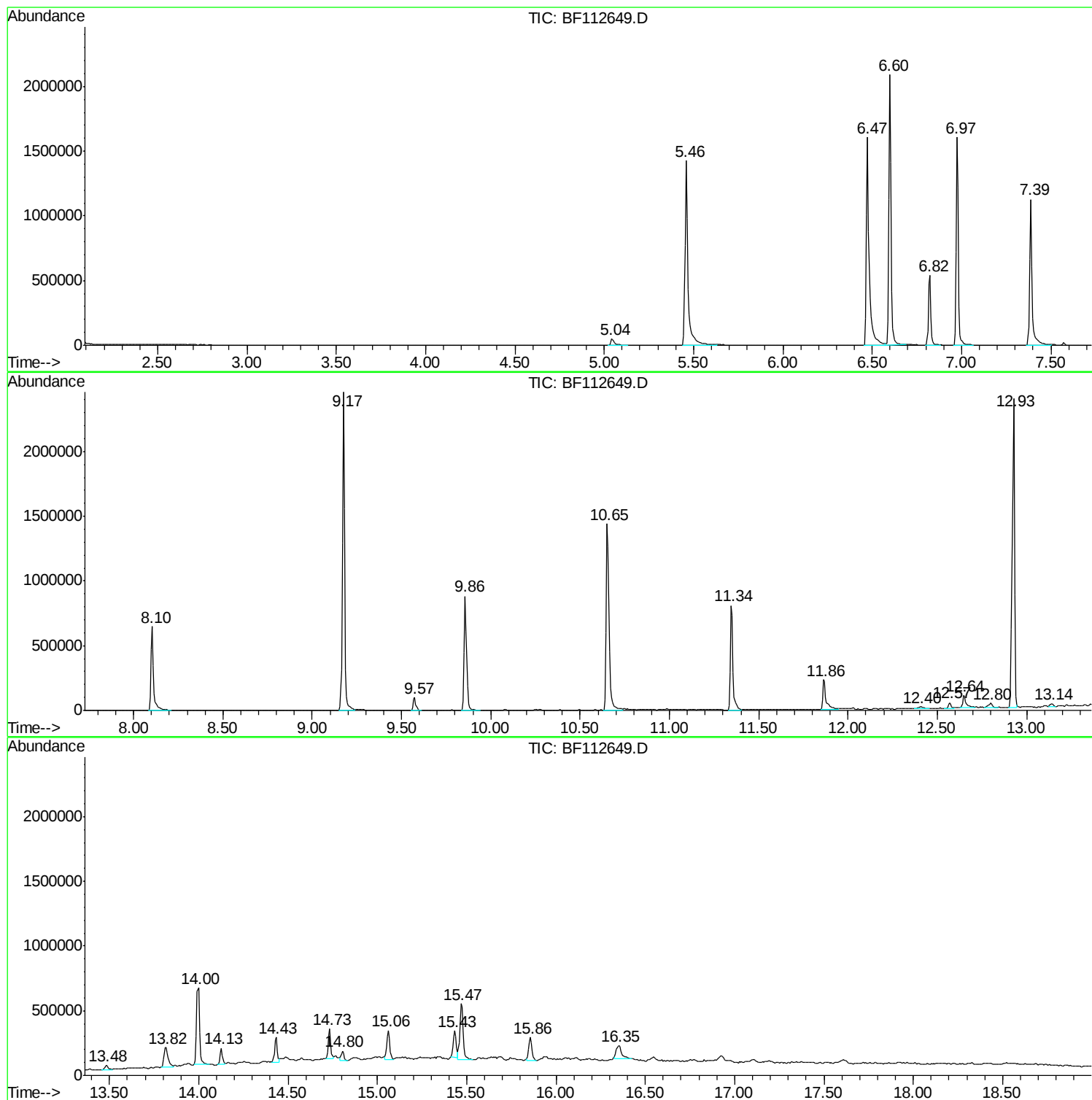
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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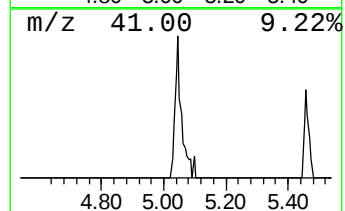
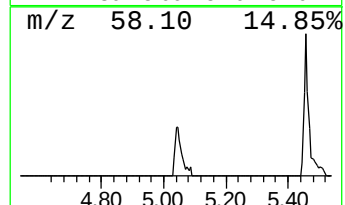
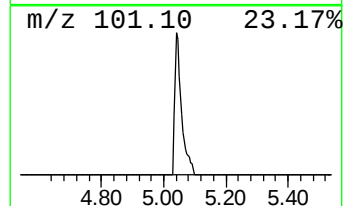
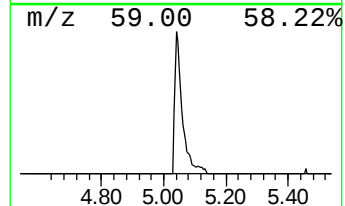
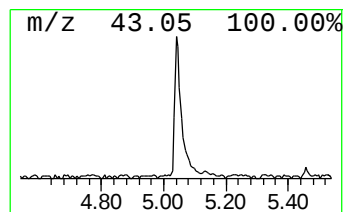
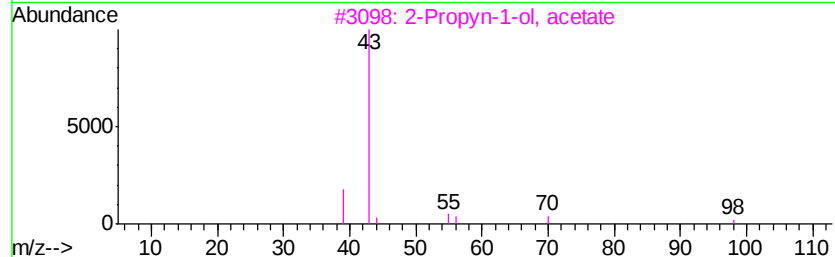
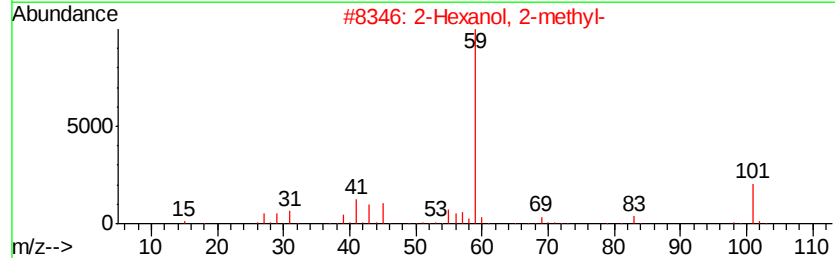
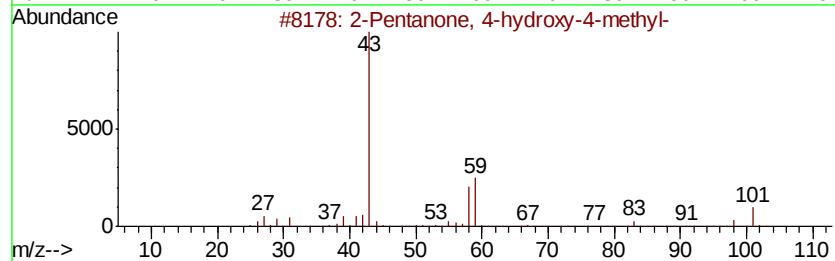
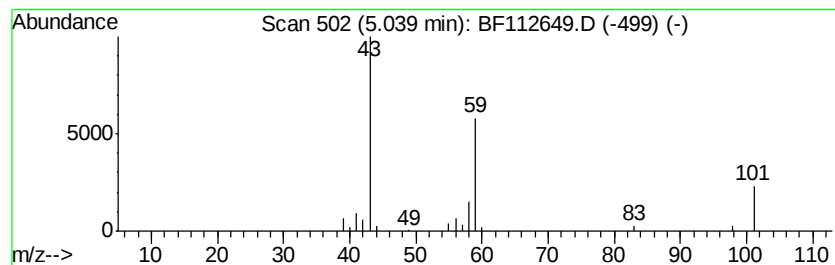
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	2.92 ng	74814	1,4-Dichlorobenzene-d4	6.82

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2-Nonanone	142	C9H18O	000821-55-6	9



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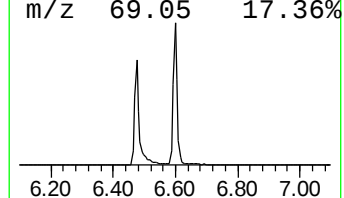
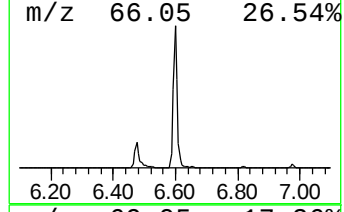
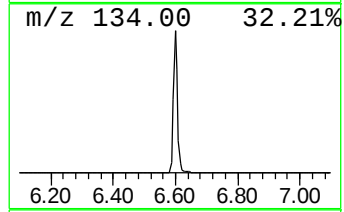
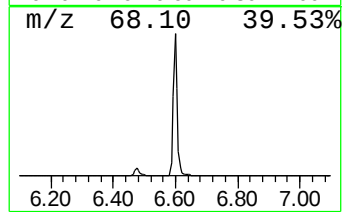
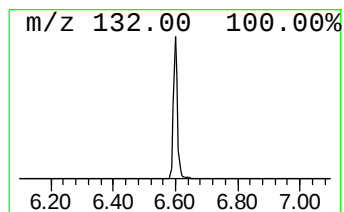
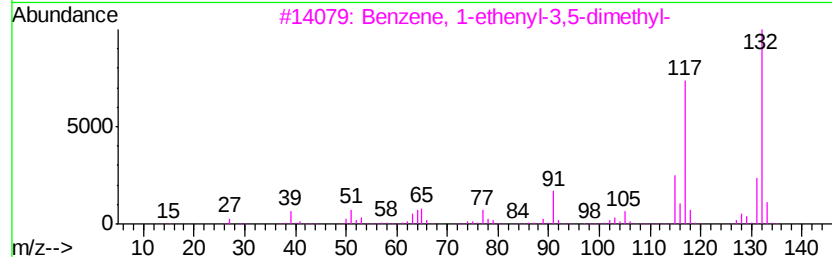
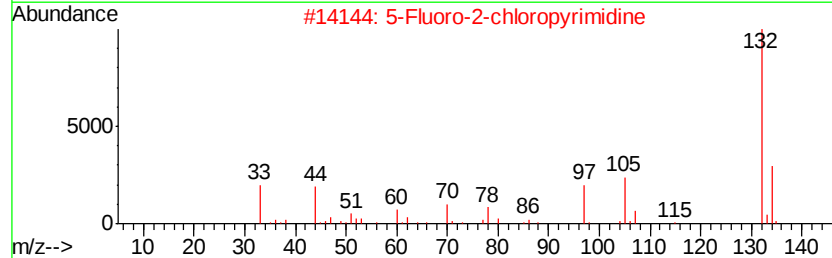
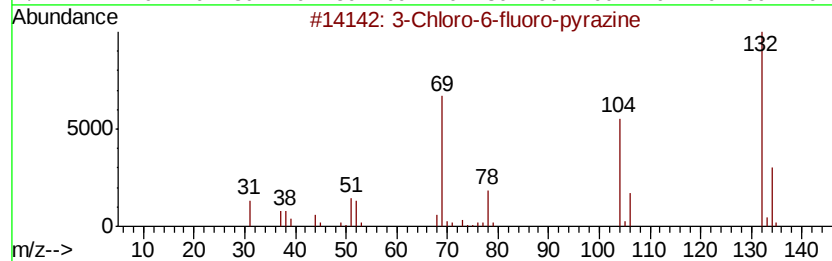
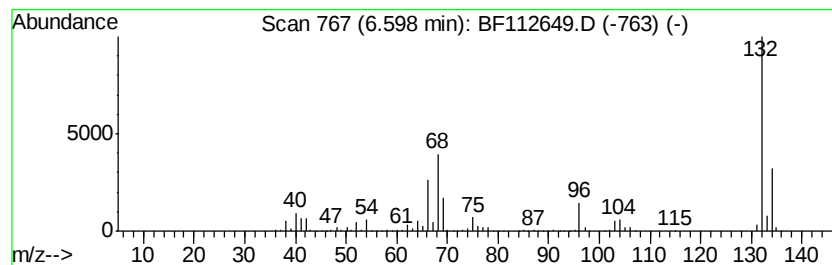
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	75.29 ng	1928960	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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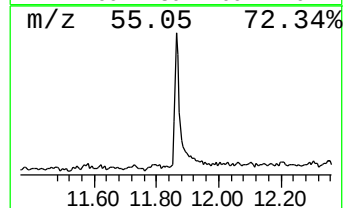
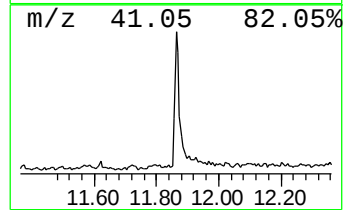
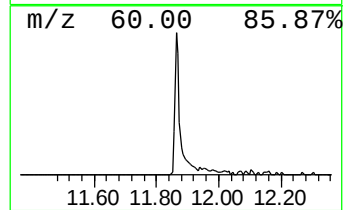
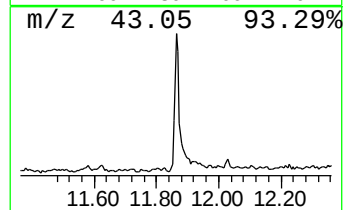
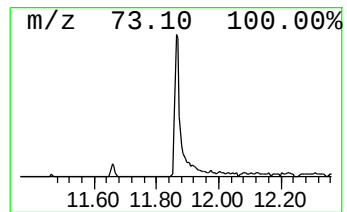
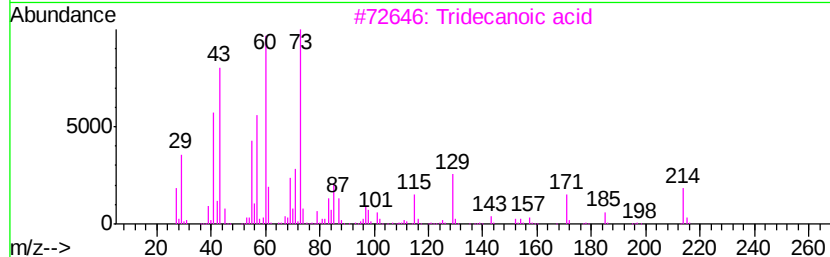
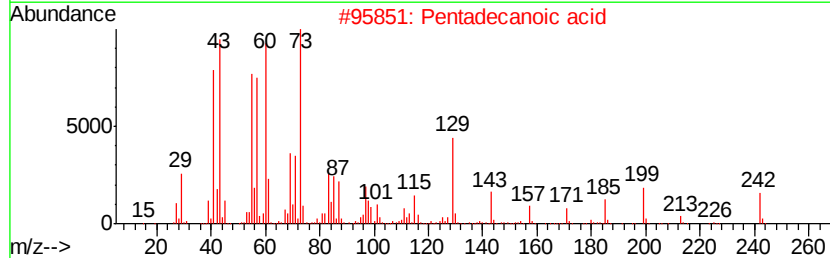
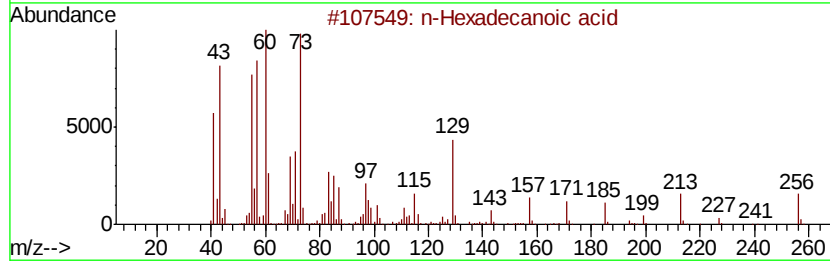
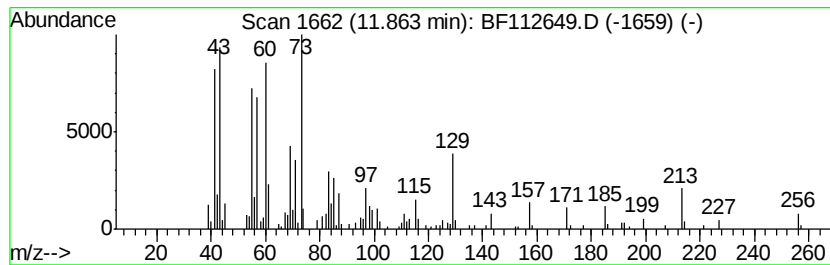
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	7.15 ng	302902	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	70



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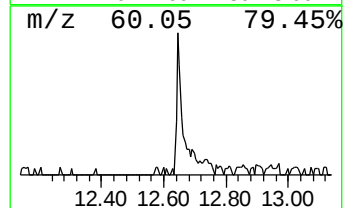
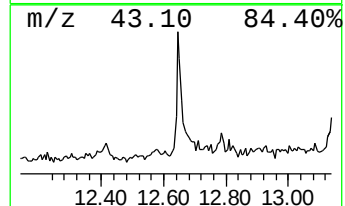
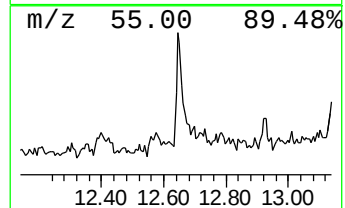
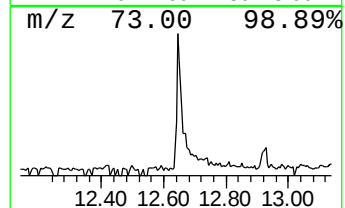
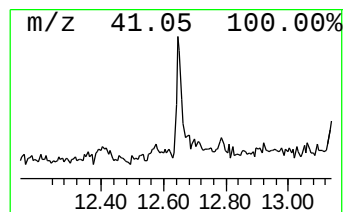
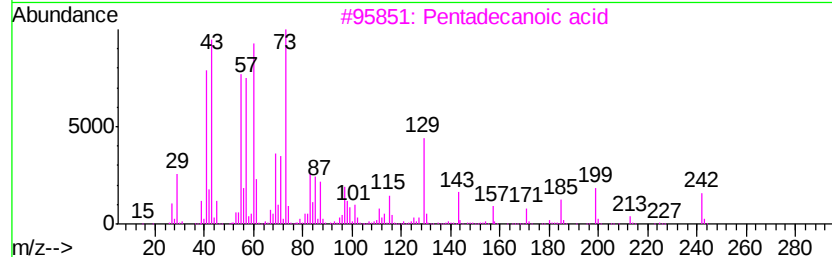
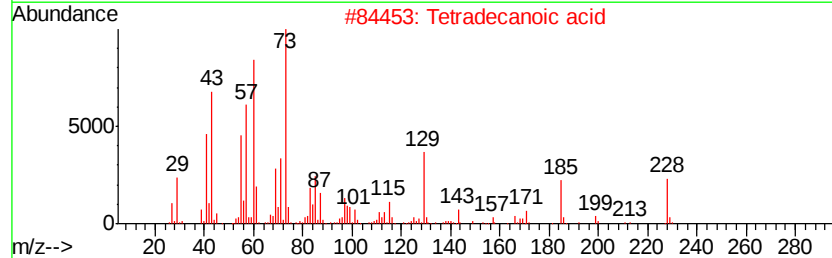
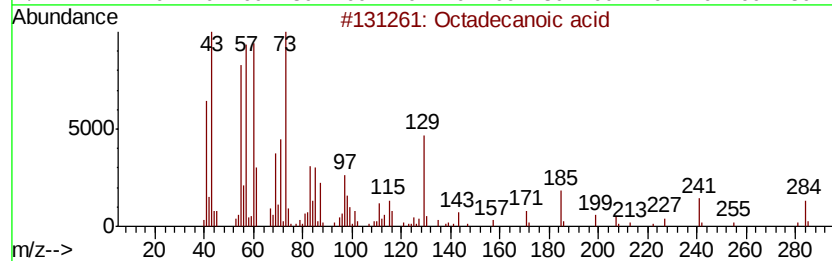
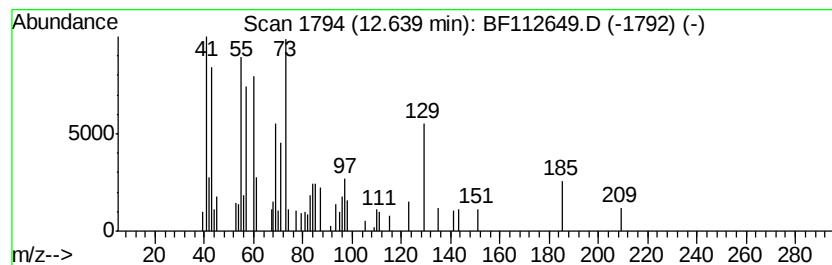
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	3.21 ng	136133	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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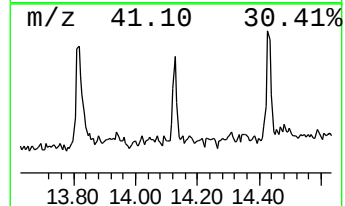
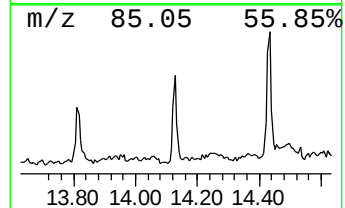
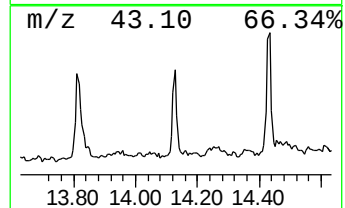
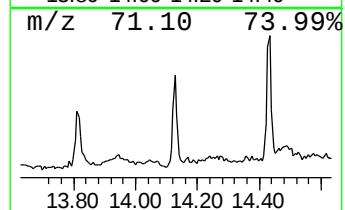
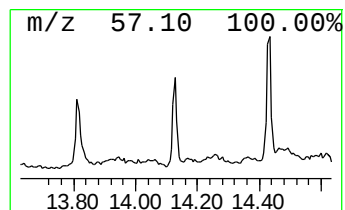
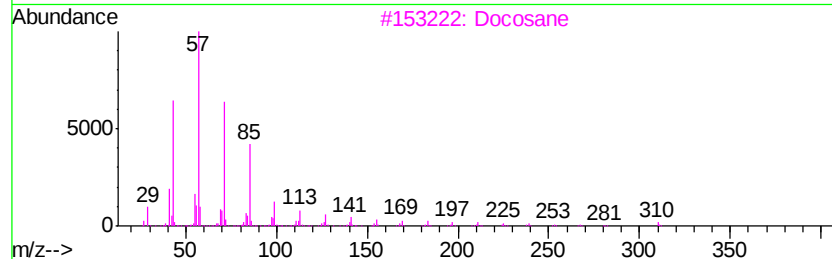
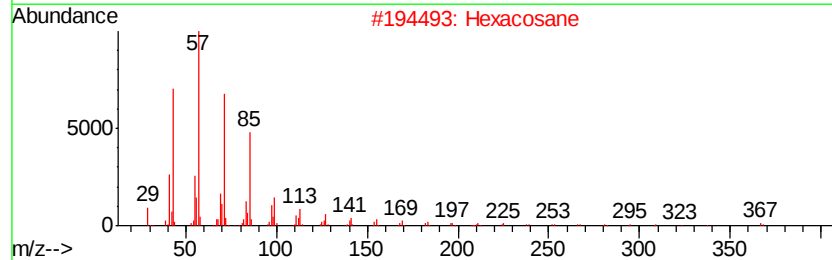
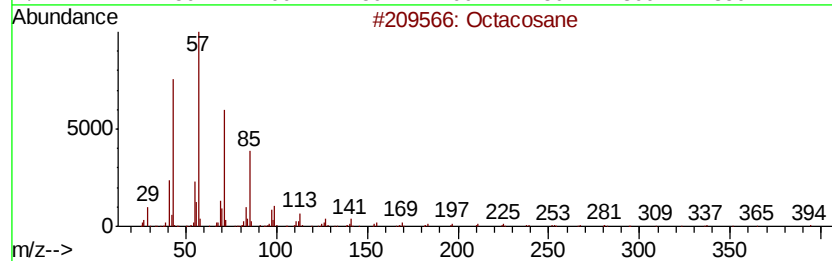
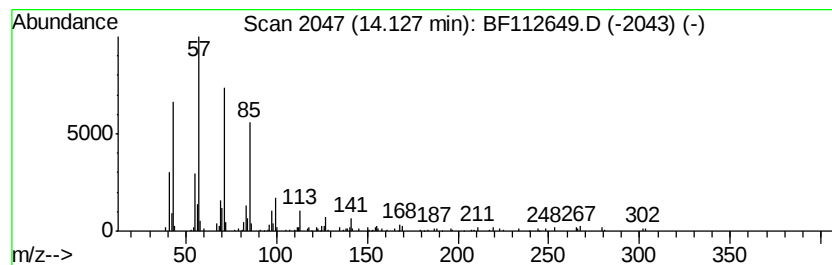
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Peak Number 7 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.66 ng	118194	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Docosane	310	C22H46	000629-97-0	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



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ClientSampleId :
M-11-A-S

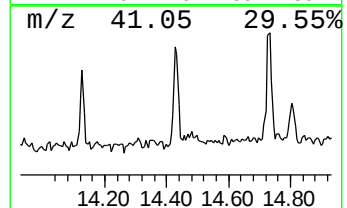
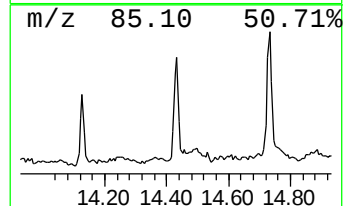
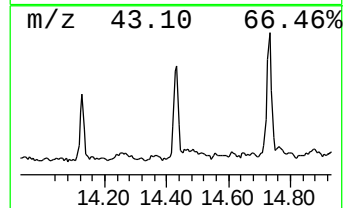
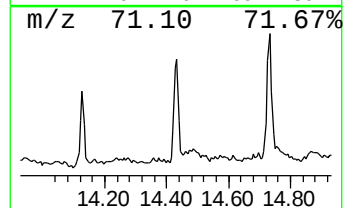
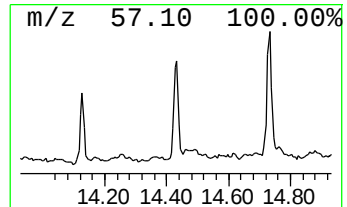
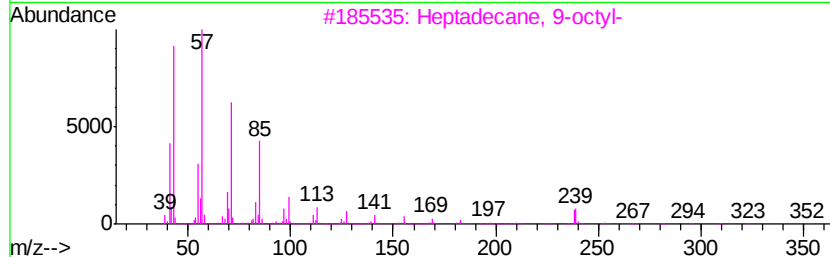
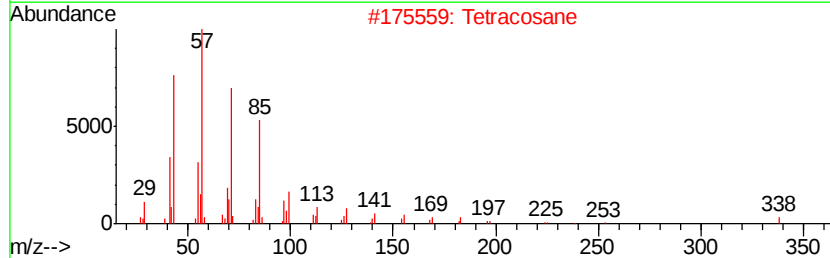
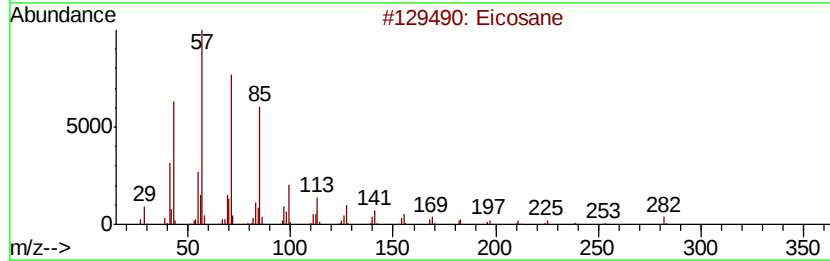
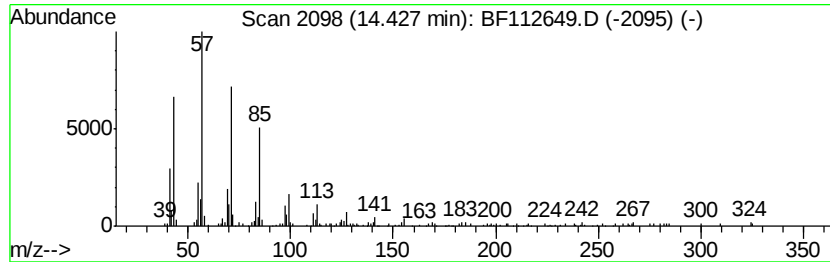
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	6.31 ng	203701	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	98
2	Tetracosane		338	C24H50	000646-31-1	94
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Heptadecane		240	C17H36	000629-78-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
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 Acq On : 21 Feb 2019 13:41
 Operator : JU/SJ
 Sample : K1538-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 M-11-A-S

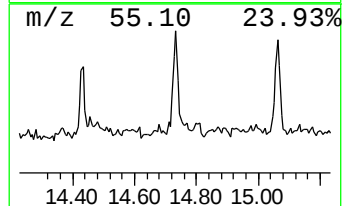
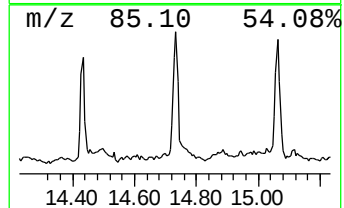
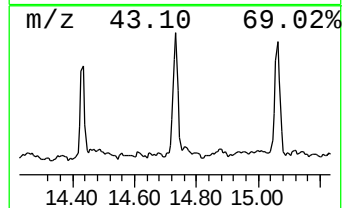
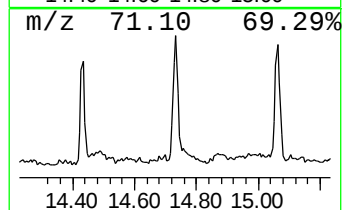
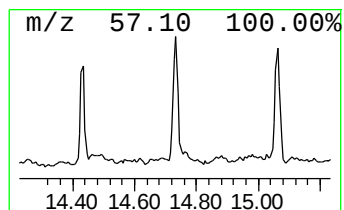
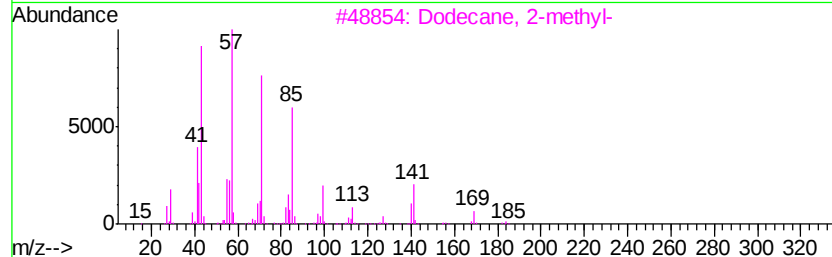
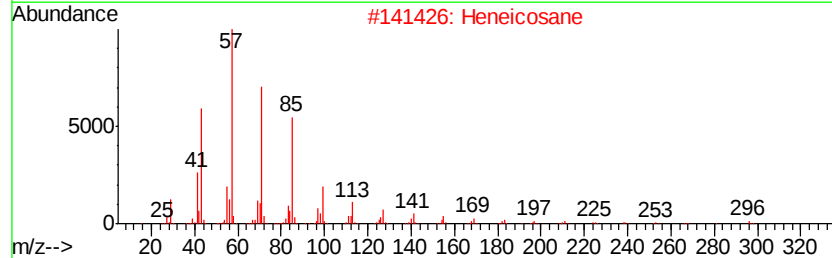
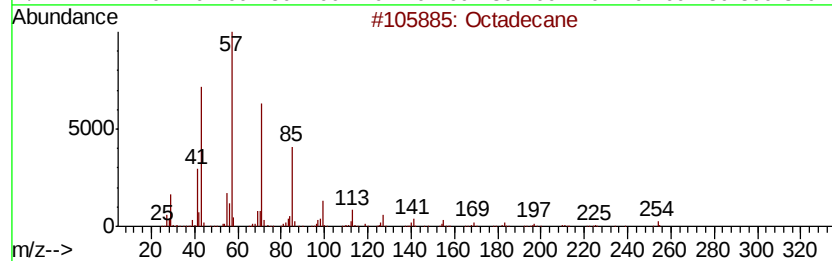
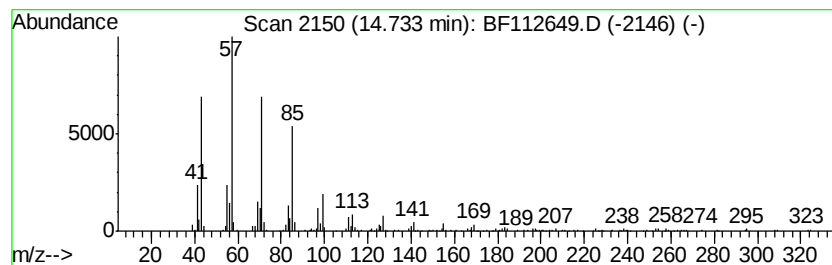
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.73	7.32 ng	236357	Chrysene-d12		14.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	94
2			Heneicosane	296	C21H44	000629-94-7	90
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
4			Heptadecane	240	C17H36	000629-78-7	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
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Acq On : 21 Feb 2019 13:41
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ClientSampleId :
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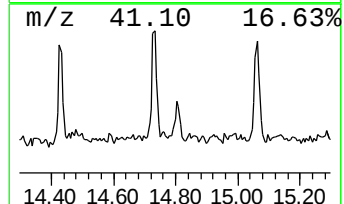
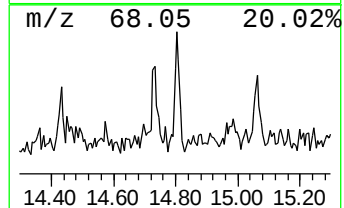
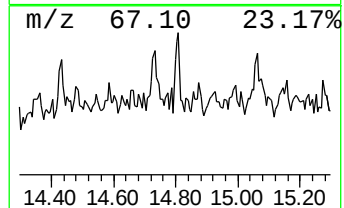
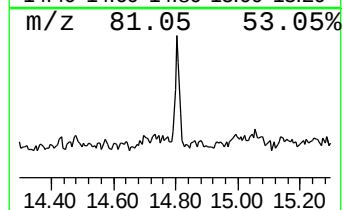
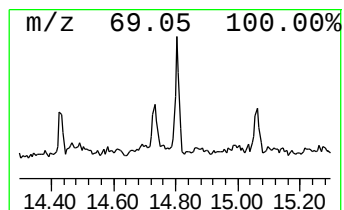
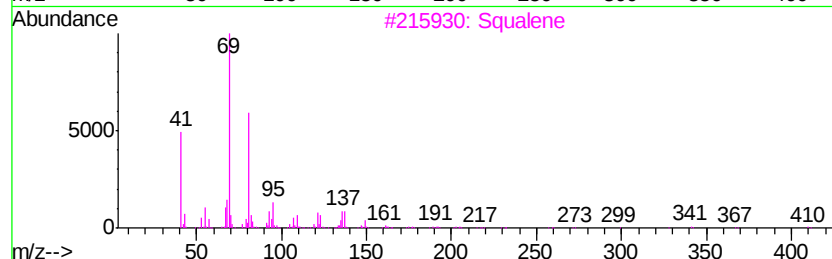
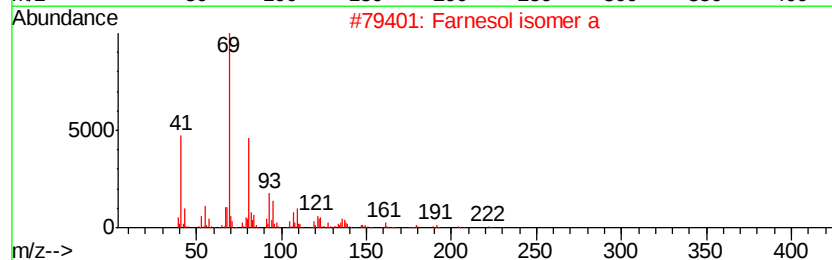
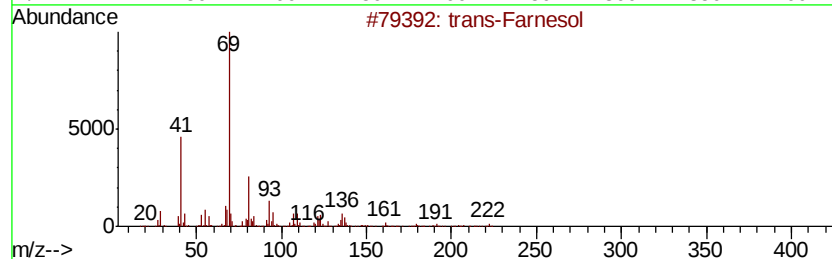
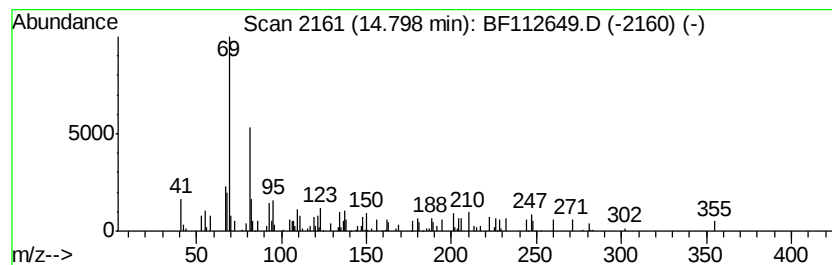
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 trans-Farnesol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.45 ng	73316	Perylene-d12	15.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Farnesol	222	C15H26O	000106-28-5	87
2			Farnesol isomer a	222	C15H26O	1000108-92-4	87
3			Squalene	410	C30H50	000111-02-4	87
4			Supraene	410	C30H50	007683-64-9	86
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112649.D
Acq On : 21 Feb 2019 13:41
Operator : JU/SJ
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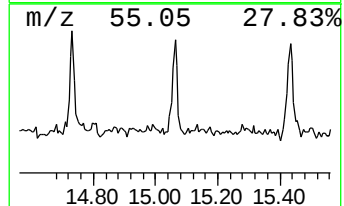
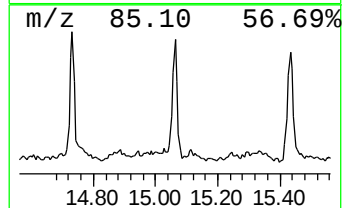
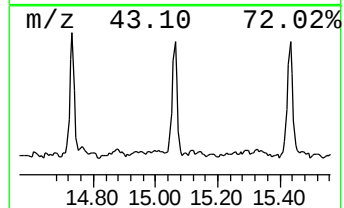
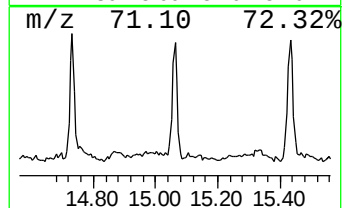
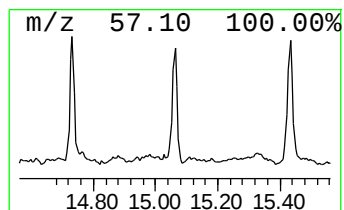
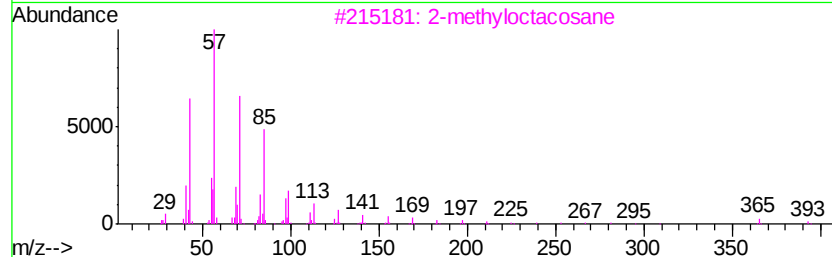
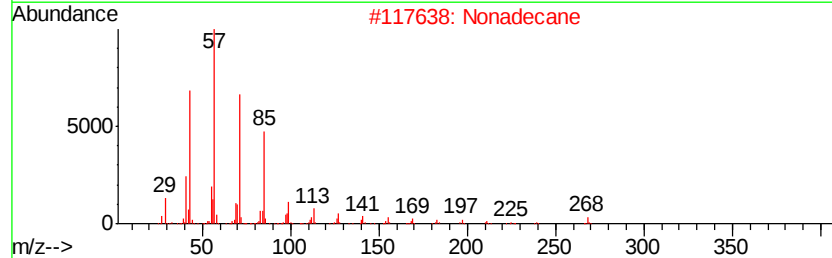
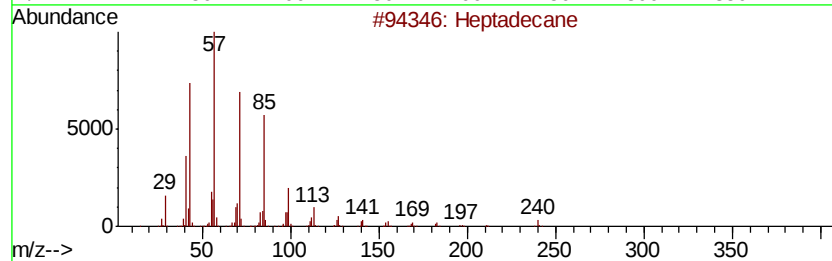
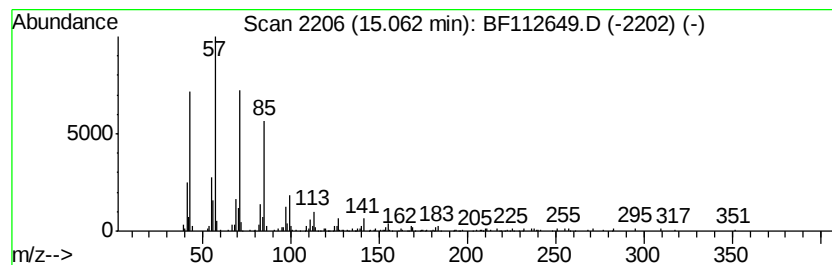
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	9.00 ng	269363	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	93
2		Nonadecane	268	C19H40	000629-92-5	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Eicosane	282	C20H42	000112-95-8	90
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112649.D
Acq On : 21 Feb 2019 13:41
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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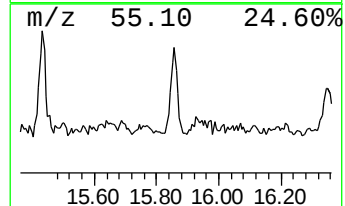
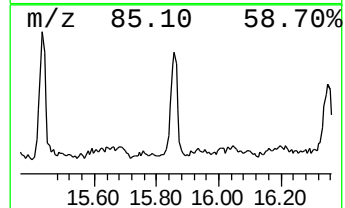
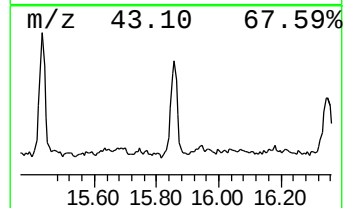
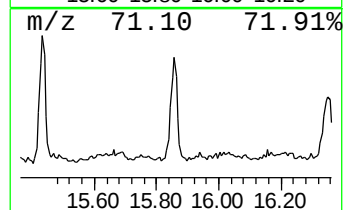
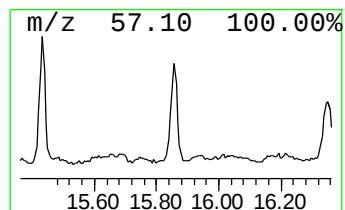
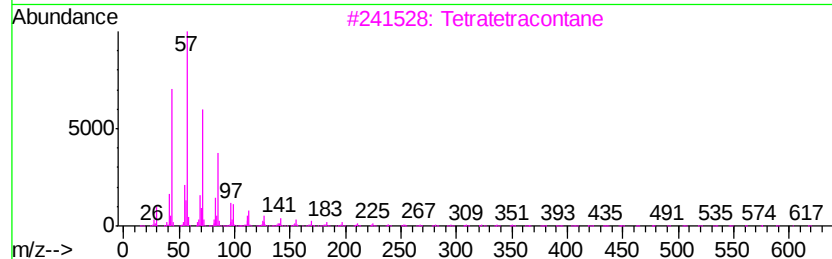
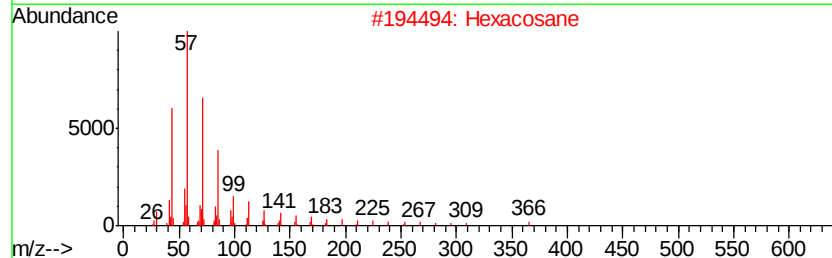
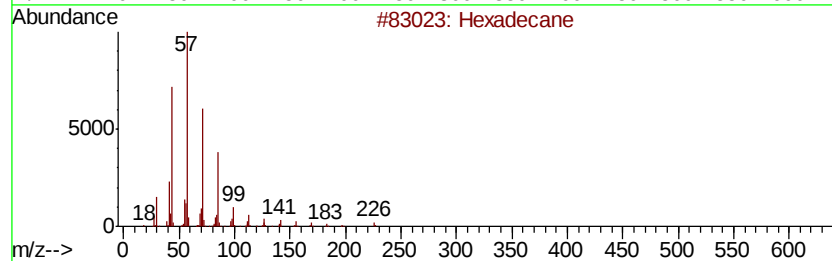
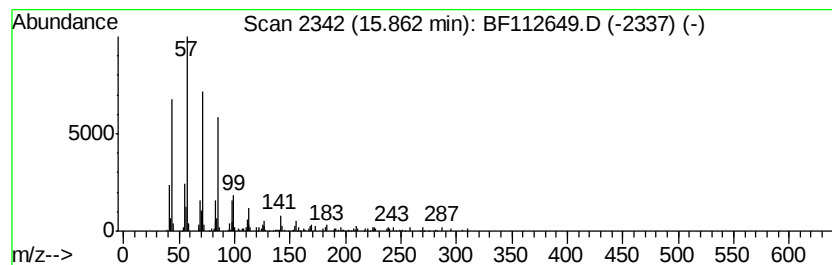
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	8.05 ng	241167	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	94
2		Hexacosane	366	C26H54	000630-01-3	91
3		Tetratetracontane	619	C44H90	007098-22-8	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112649.D
Acq On : 21 Feb 2019 13:41
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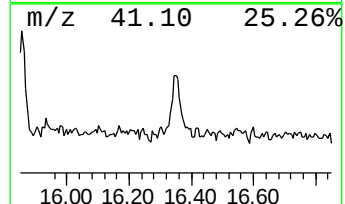
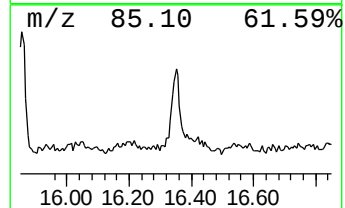
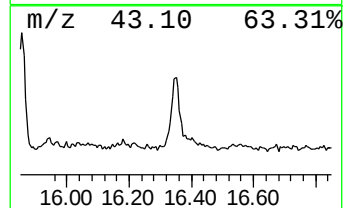
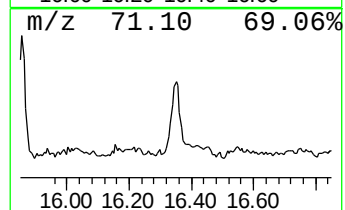
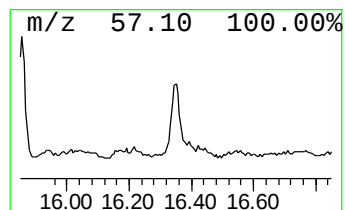
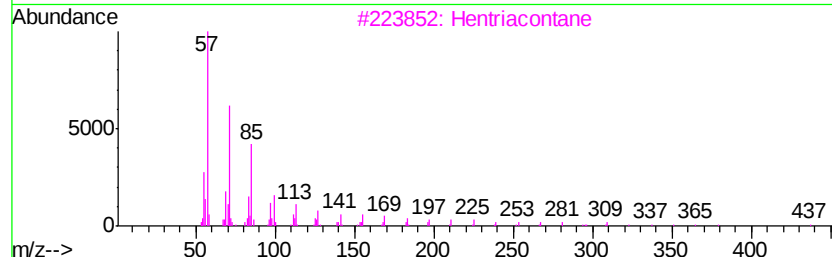
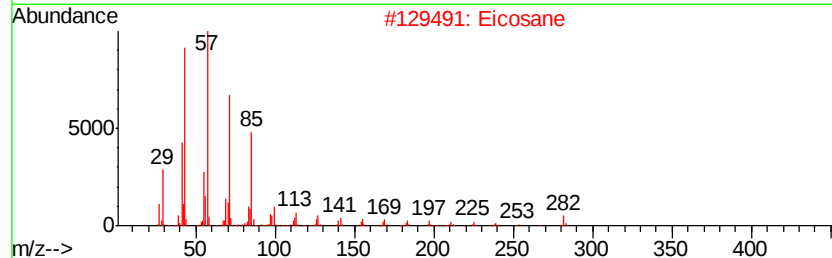
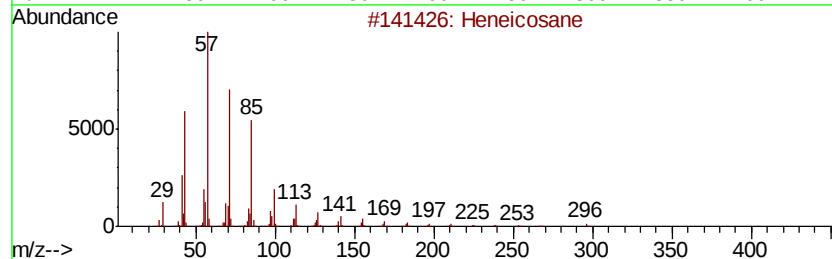
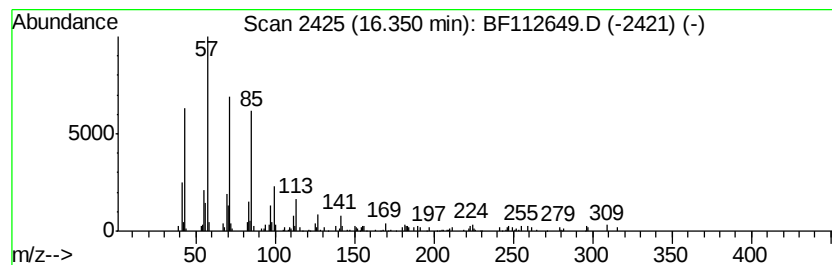
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	7.09 ng	212315	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	94
2	Eicosane		282	C20H42	000112-95-8	91
3	Hentriacontane		437	C31H64	000630-04-6	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	87
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022119\
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 Sample : K1538-03
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 ALS Vial : 6 Sample Multiplier: 1

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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.60	6.60	75.3	ng	1928960	1	6.82	512388	20.0
n-Hexadecanoic acid	11.86	7.2	ng	302902	4	11.34	847192	20.0
Octadecanoic acid	12.64	3.2	ng	136133	4	11.34	847192	20.0
Octacosane	14.13	3.7	ng	118194	5	14.00	646154	20.0
Eicosane	14.43	6.3	ng	203701	5	14.00	646154	20.0
Octadecane	14.73	7.3	ng	236357	5	14.00	646154	20.0
trans-Farnesol	14.80	2.5	ng	73316	6	15.47	598846	20.0
Heptadecane	15.06	9.0	ng	269363	6	15.47	598846	20.0
Hexadecane	15.86	8.1	ng	241167	6	15.47	598846	20.0
Heneicosane	16.35	7.1	ng	212315	6	15.47	598846	20.0