

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
 Data File : BF118231.D
 Acq On : 17 Dec 2019 17:30
 Operator : JU
 Sample : K6310-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-01

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

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

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	17	rVB	297356	383883	11.86%	1.276%
2	5.069	502	507	518	rVB	353738	424708	13.12%	1.411%
3	5.475	572	576	596	rVB	2402239	2317276	71.60%	7.701%
4	6.492	744	749	763	rBV	2516153	2549976	78.79%	8.474%
5	6.628	768	772	775	rBV	3189681	2671542	82.54%	8.878%
6	6.857	807	811	817	rBV	990291	786204	24.29%	2.613%
7	7.016	834	838	841	rBV	2400438	2060754	63.67%	6.849%
8	7.422	903	907	910	rBV	1693525	1505067	46.50%	5.002%
9	8.145	1026	1030	1045	rBV	1189127	1059874	32.75%	3.522%
10	9.222	1209	1213	1224	rBV	3507270	3236617	100.00%	10.756%
11	9.616	1277	1280	1287	rVB	289215	263568	8.14%	0.876%
12	9.904	1326	1329	1333	rBV	1391198	1243004	38.40%	4.131%
13	10.698	1460	1464	1477	rBV	2363082	2128369	65.76%	7.073%
14	11.398	1579	1583	1591	rBV	1371137	1267438	39.16%	4.212%
15	11.921	1669	1672	1681	rBV2	269915	304440	9.41%	1.012%
16	12.451	1759	1762	1765	rBV3	27152	36357	1.12%	0.121%
17	12.616	1788	1790	1795	rBV	61928	70077	2.17%	0.233%
18	12.710	1803	1806	1811	rBV3	110567	131902	4.08%	0.438%
19	12.845	1827	1829	1833	rBV	50237	54194	1.67%	0.180%
20	12.992	1849	1854	1857	rBV	3062723	2765790	85.45%	9.192%
21	13.074	1865	1868	1872	rVB	90608	75454	2.33%	0.251%
22	13.710	1973	1976	1980	rVB	231122	201412	6.22%	0.669%
23	13.886	2001	2006	2013	rBV2	286978	385087	11.90%	1.280%
24	14.027	2026	2030	2032	rBV	1666173	1561214	48.24%	5.188%
25	14.051	2032	2034	2038	rVB	828522	723941	22.37%	2.406%
26	14.510	2110	2112	2115	rBV	63323	70212	2.17%	0.233%
27	14.821	2163	2165	2169	rVB	87493	80909	2.50%	0.269%
28	15.168	2220	2224	2228	rVB2	130241	158679	4.90%	0.527%
29	15.545	2283	2288	2297	rVB	687695	1046541	32.33%	3.478%
30	15.998	2361	2365	2372	rVB	138371	214346	6.62%	0.712%
31	16.515	2449	2453	2458	rBV2	101478	187726	5.80%	0.624%
32	17.127	2552	2557	2566	rVB2	57469	123873	3.83%	0.412%

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

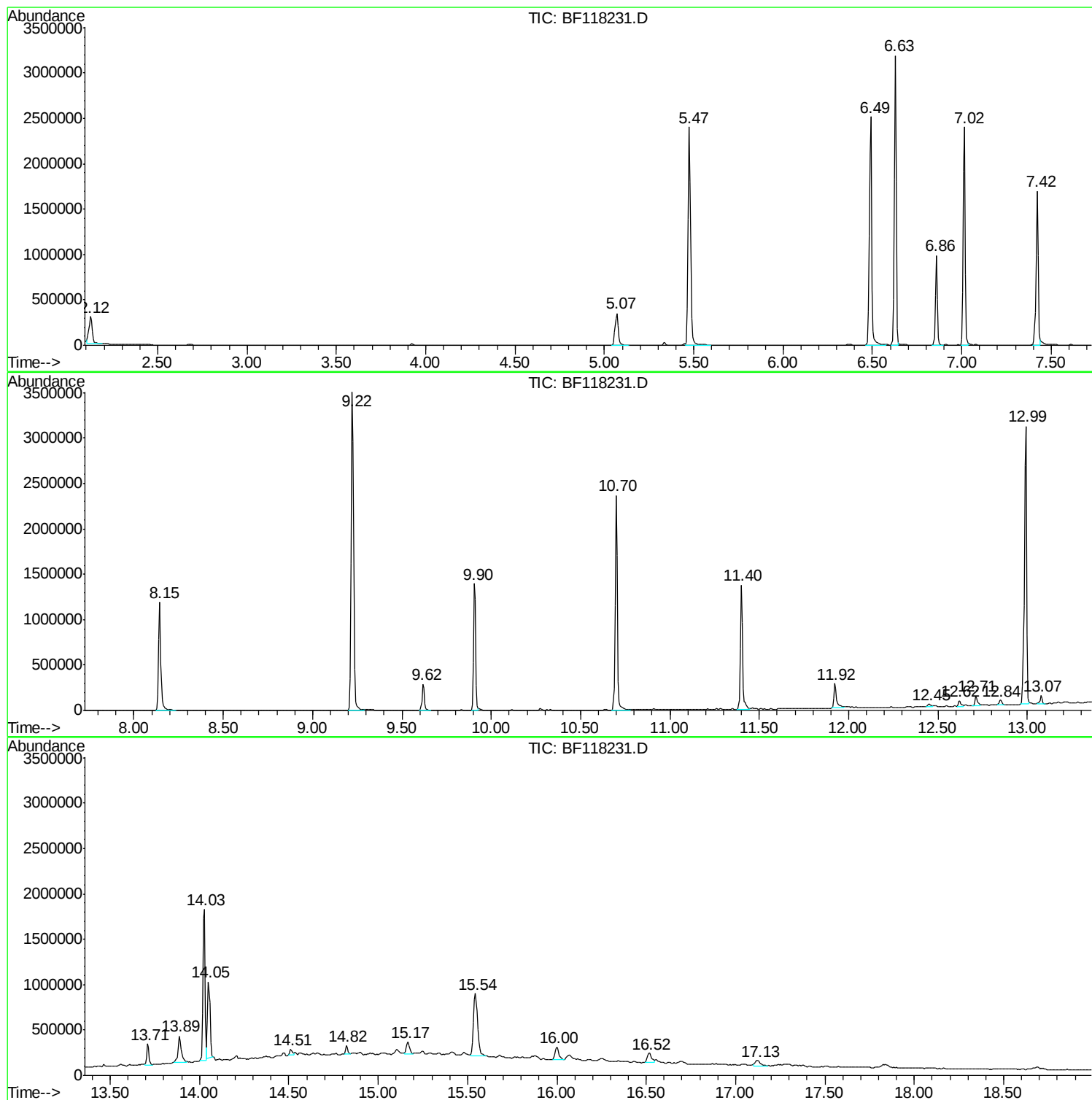
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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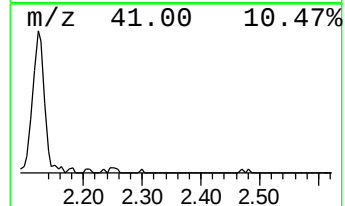
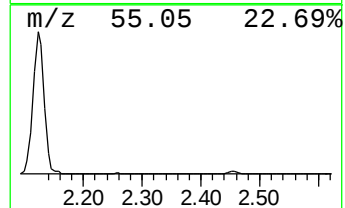
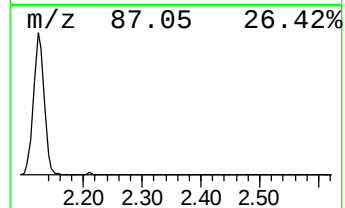
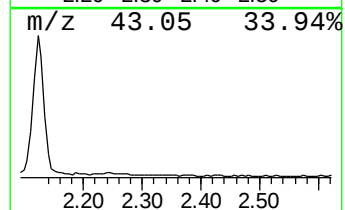
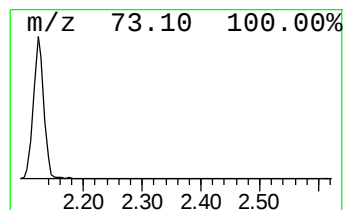
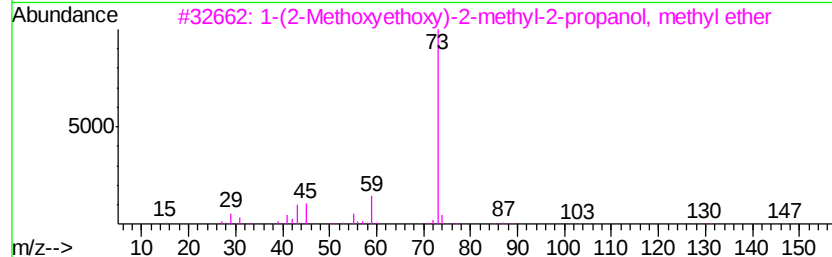
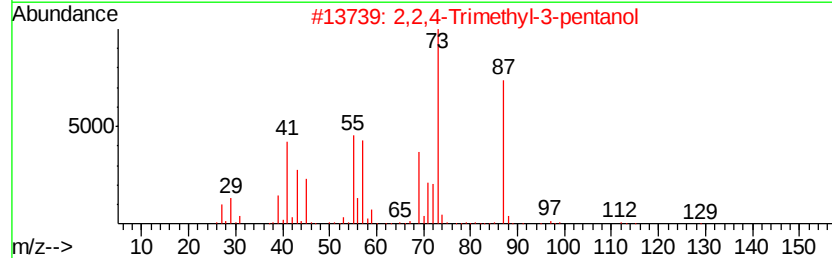
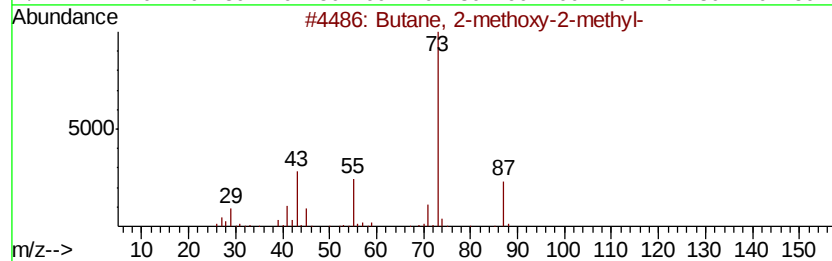
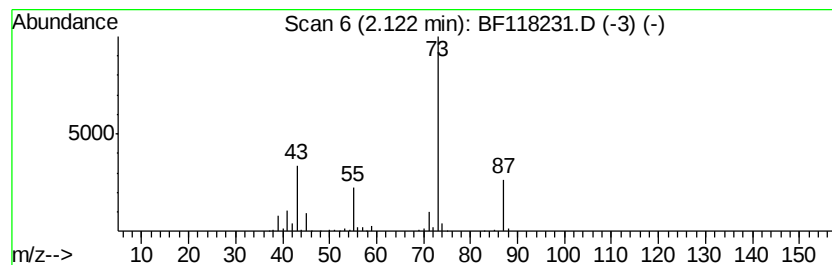
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	9.77 ng	383883	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		1-(2-Methoxyethoxy)-2-methyl-2-propanol	162	C8H18O3	1000364-24-4	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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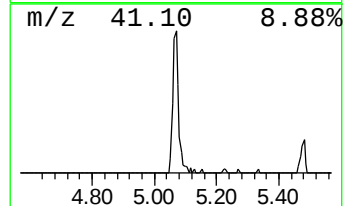
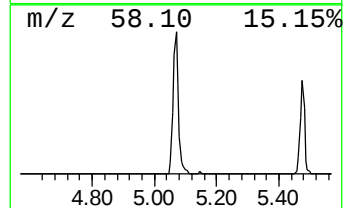
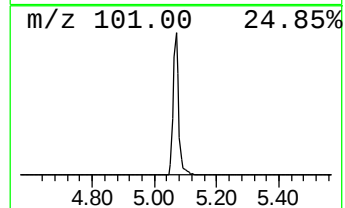
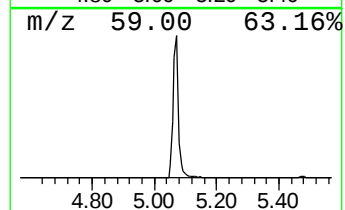
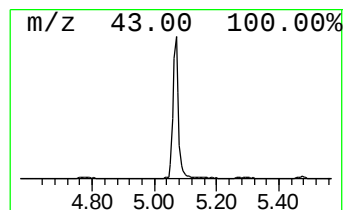
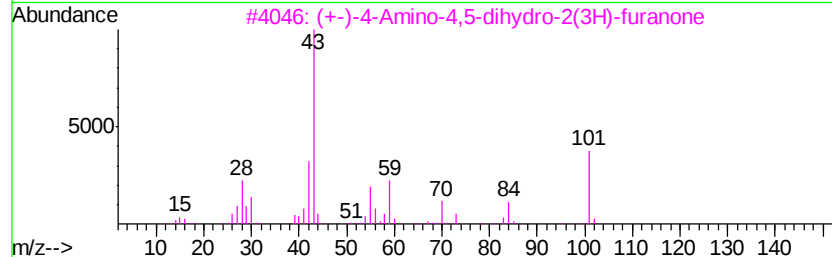
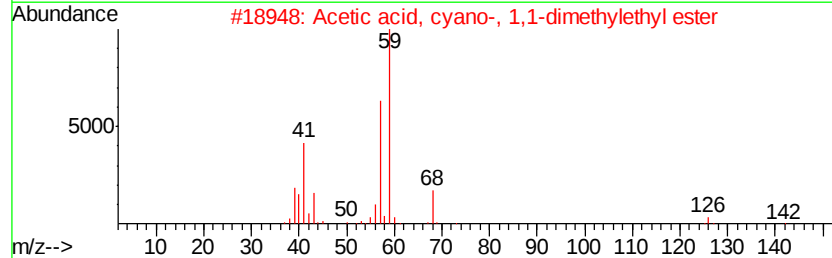
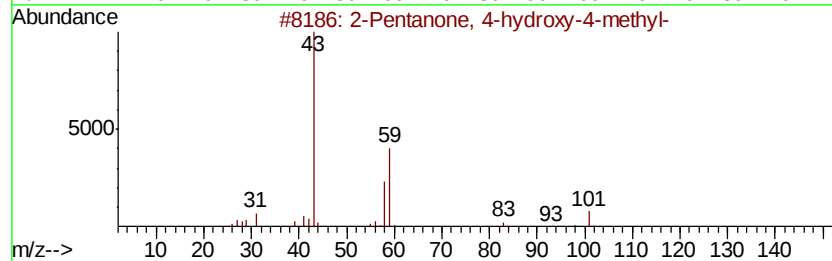
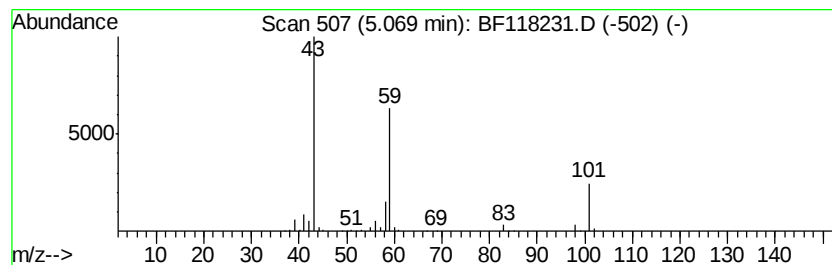
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	10.80 ng	424708	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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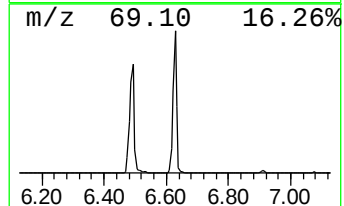
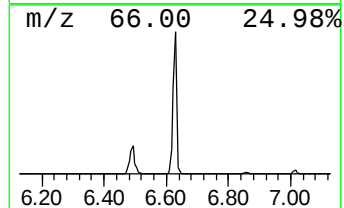
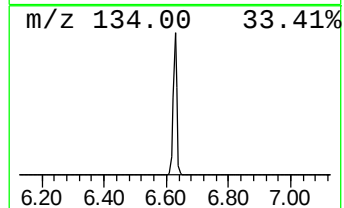
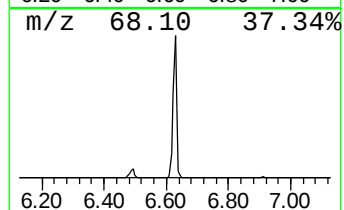
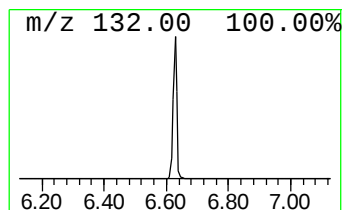
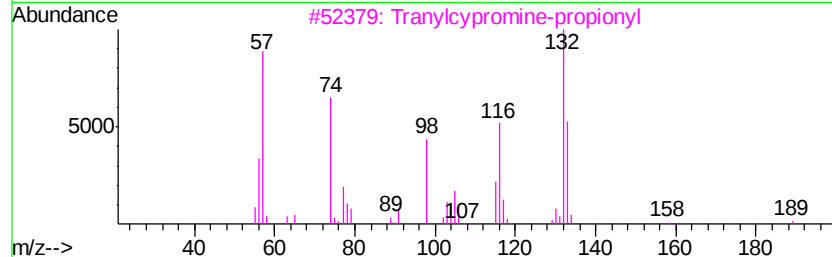
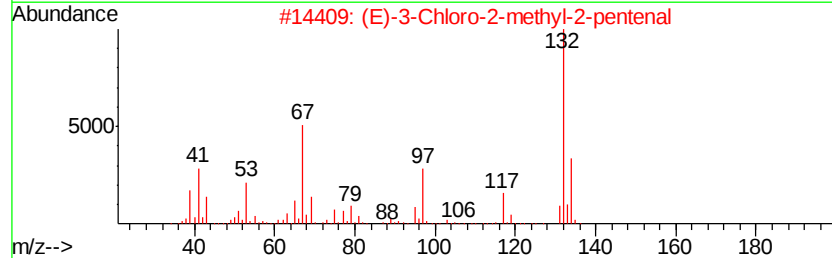
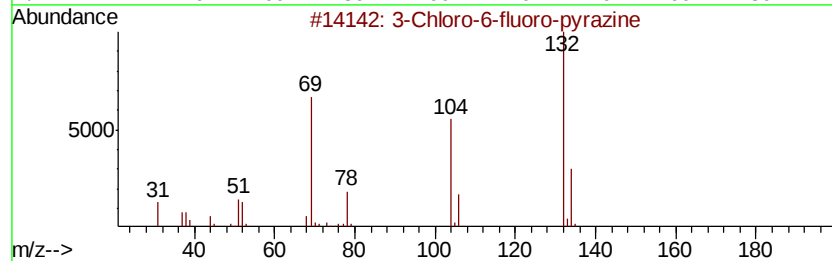
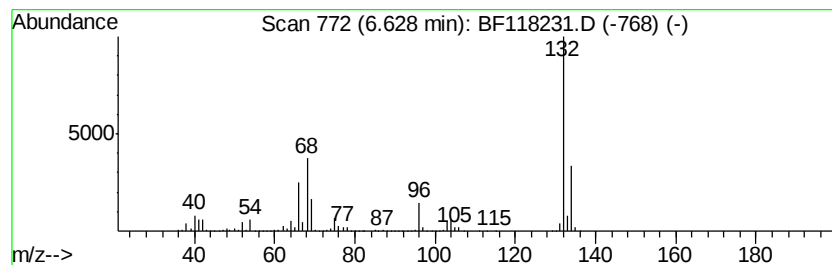
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	67.96 ng	2671540	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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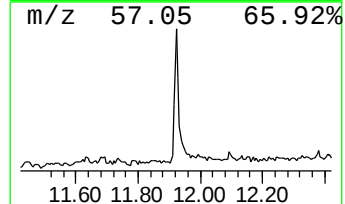
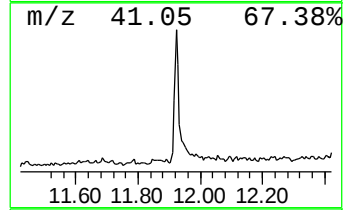
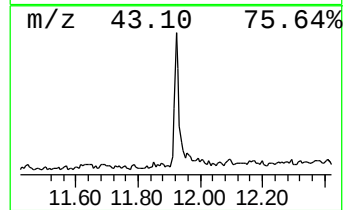
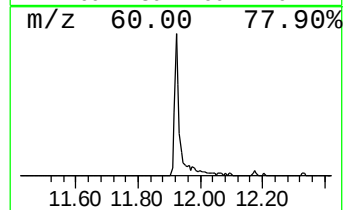
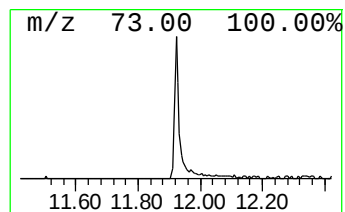
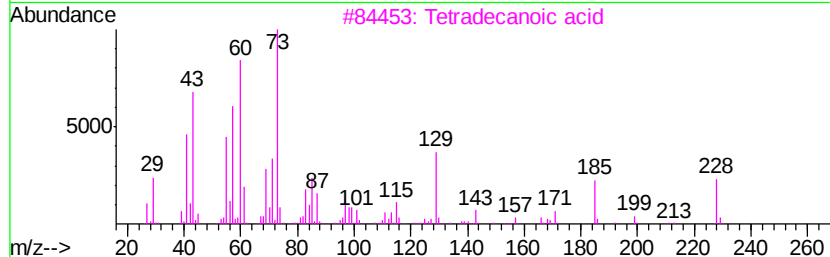
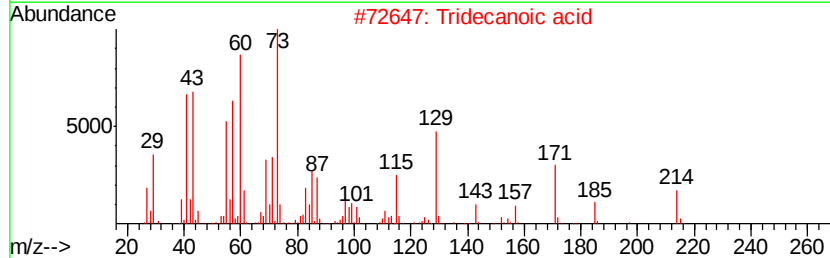
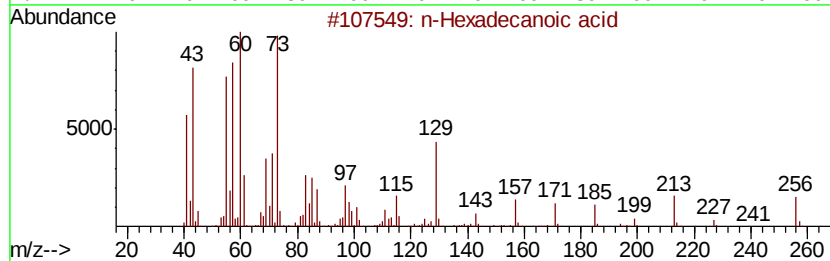
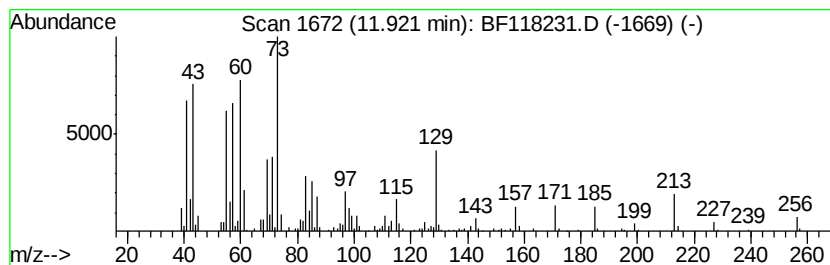
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.80 ng	304440	Phenanthrene-d10	11.40

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	93
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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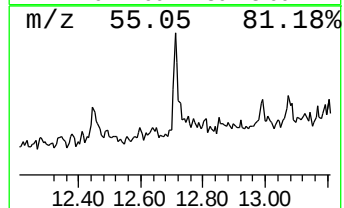
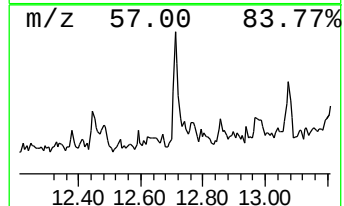
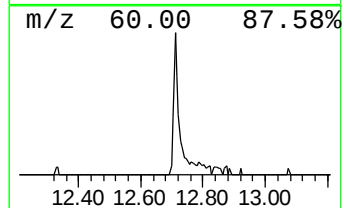
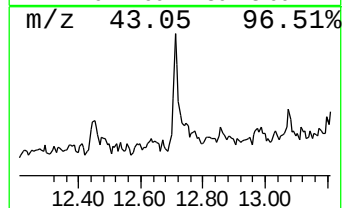
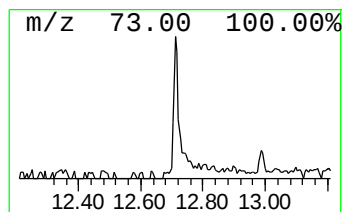
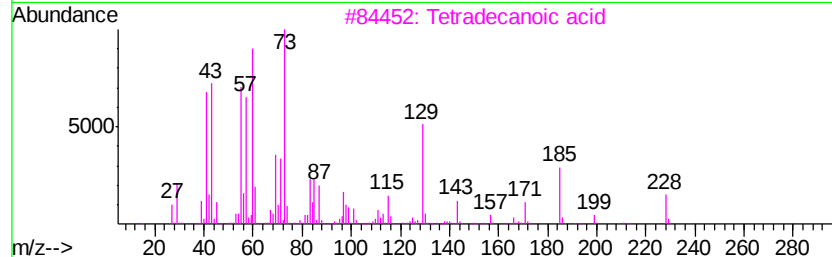
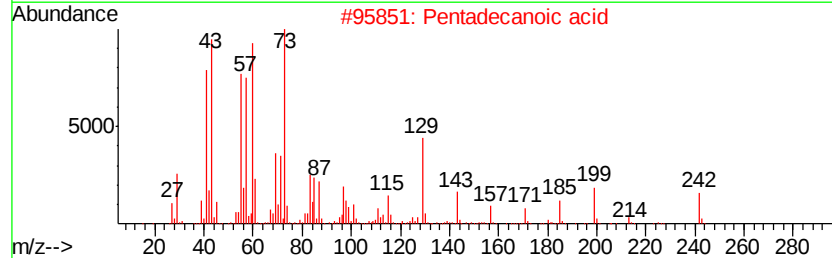
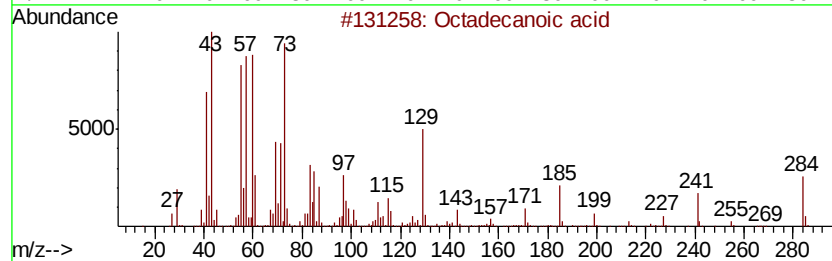
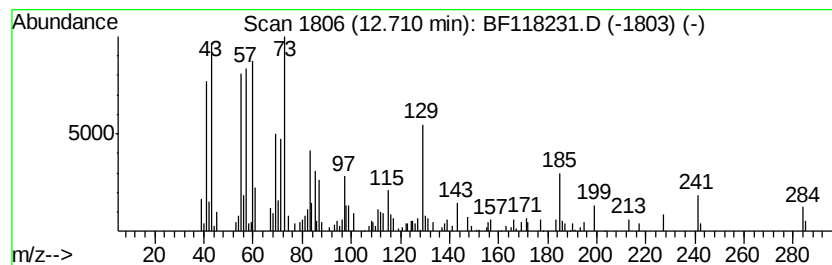
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Peak Number 6 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.08 ng	131902	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-Decanoic acid	172	C10H20O2	000334-48-5	83
5		Tridecanoic acid	214	C13H26O2	000638-53-9	68



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Instrument :
BNA_F
ClientSampleId :
SP-01

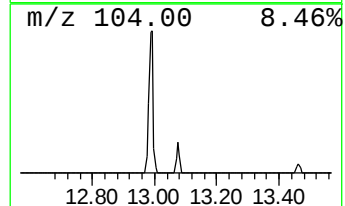
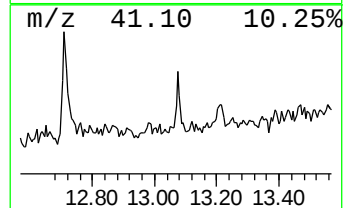
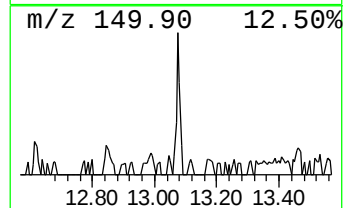
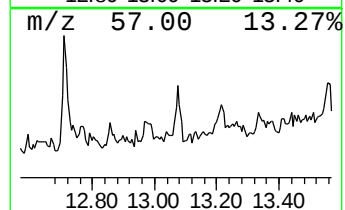
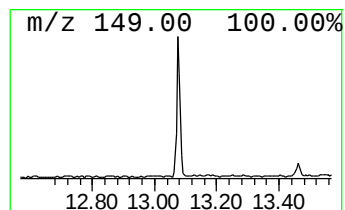
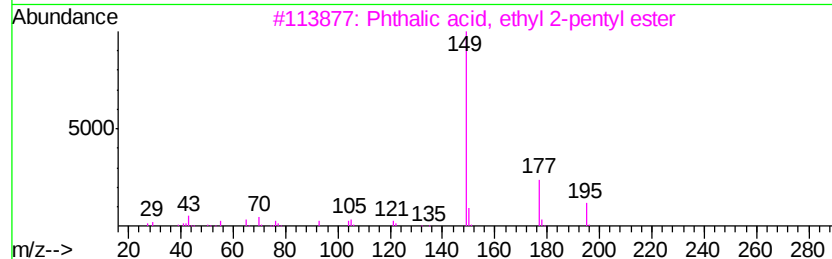
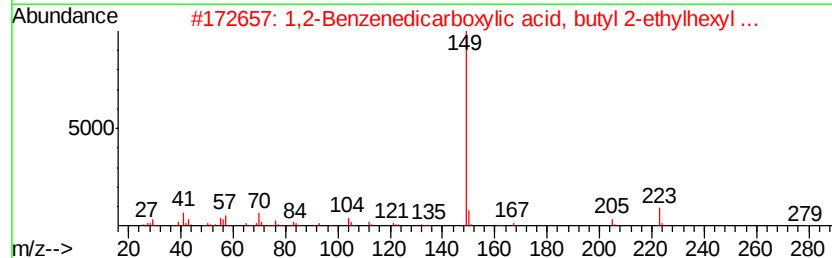
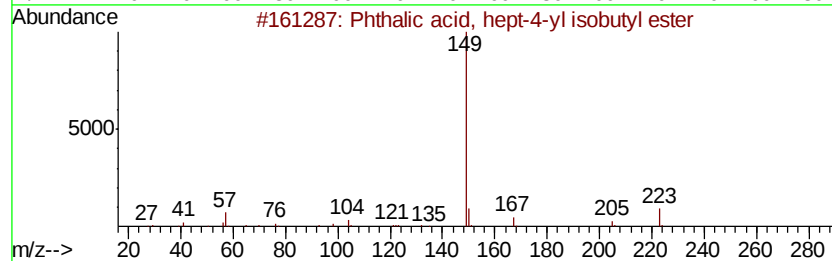
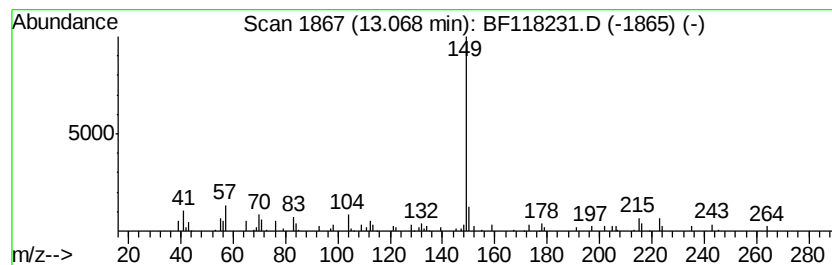
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phthalic acid, hept-4-yl is... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	2.08 ng	75454	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hept-4-yl isobutyl...	320	C19H28O4	1000356-78-3	80
2		1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	78
3		Phthalic acid, ethyl 2-pentyl ester	264	C15H20O4	1000315-47-4	72
4		Phthalic acid, isobutyl 3-methyl...	290	C17H22O4	1000357-10-1	72
5		Phthalic acid, cycloheptyl isobu...	318	C19H26O4	1000322-82-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118231.D
Acq On : 17 Dec 2019 17:30
Operator : JU
Sample : K6310-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

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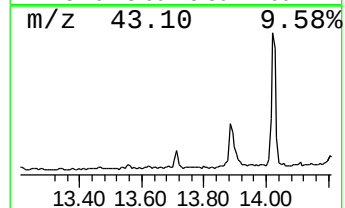
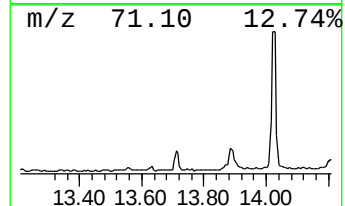
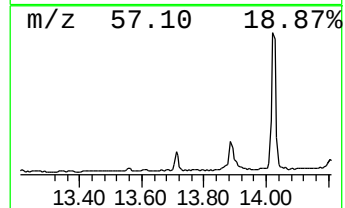
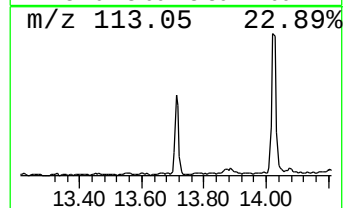
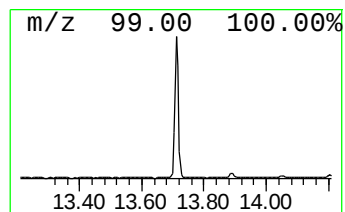
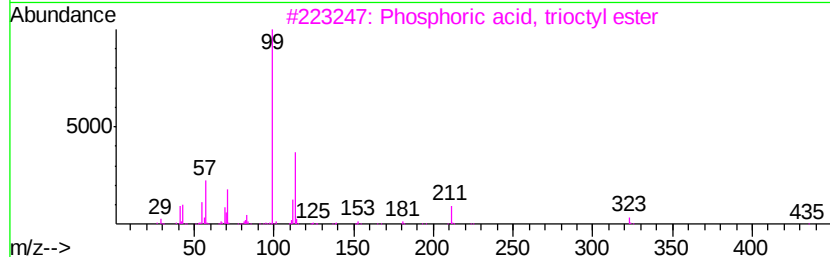
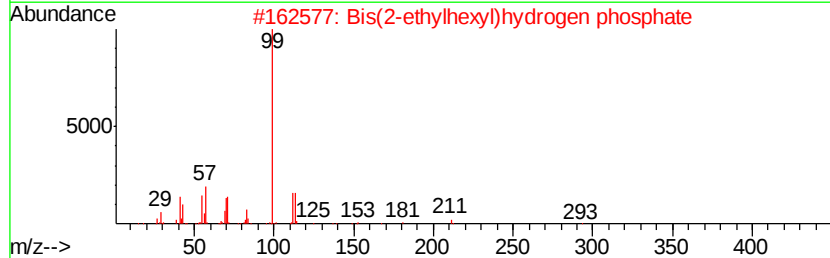
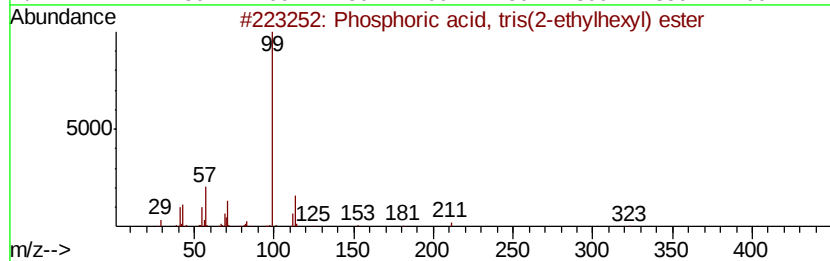
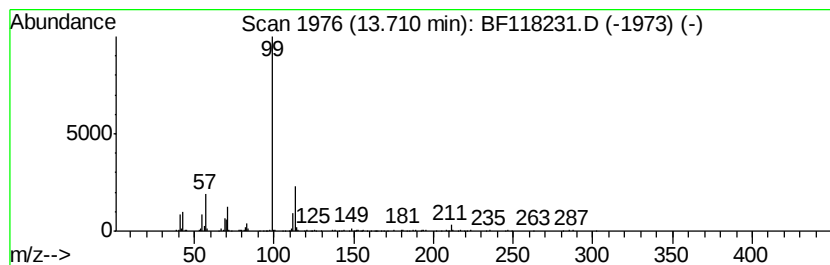
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phosphoric acid, tris(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	5.56 ng	201412	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphoric acid, tris(2-ethylhex...	434	C24H51O4P	000078-42-2	80
2			Bis(2-ethylhexyl)hydrogen phosphate	322	C16H35O4P	000298-07-7	72
3			Phosphoric acid, trioctyl ester	434	C24H51O4P	001806-54-8	50
4			n-Hexyl methylphosphonofluoridate	182	C7H16F02P	113548-89-3	43
5			n-Heptyl methylphosphonofluoridate	196	C8H18F02P	162085-82-7	37



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
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Acq On : 17 Dec 2019 17:30
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Sample : K6310-03
Misc :
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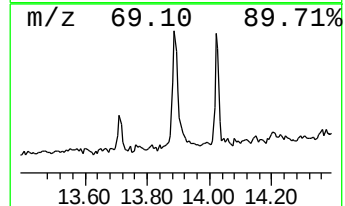
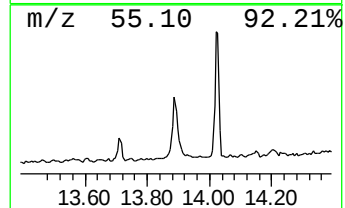
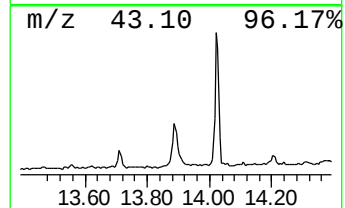
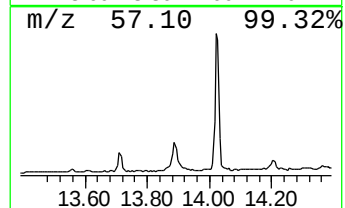
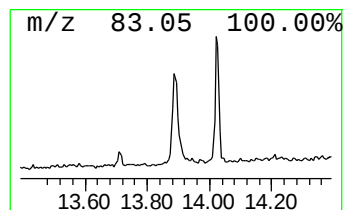
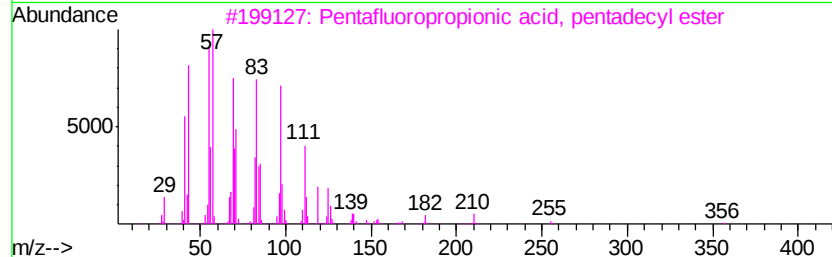
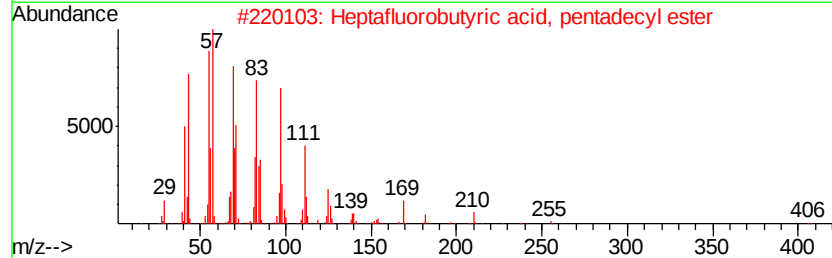
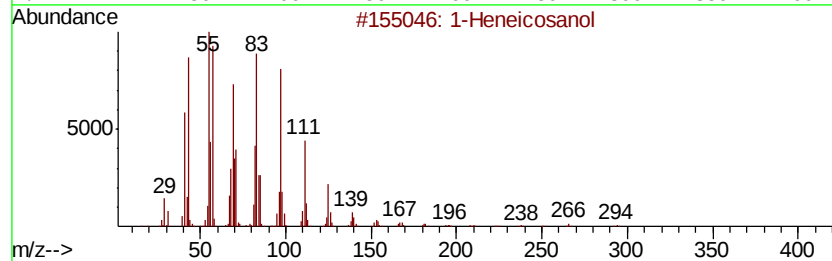
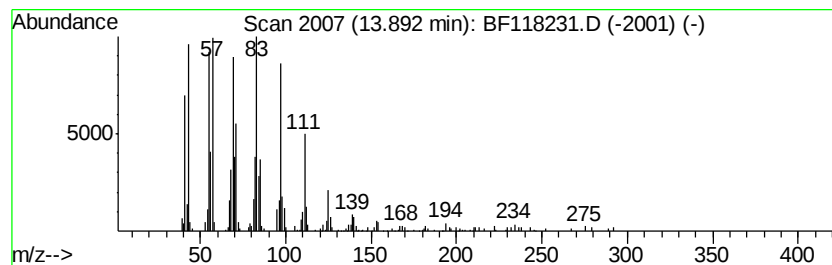
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	10.64 ng	385087	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 95
2		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 94
3		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 94
4		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 94
5		n-Tetracosanol-1	354 C24H50O	000506-51-4 94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
 Data File : BF118231.D
 Acq On : 17 Dec 2019 17:30
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 Misc :
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Instrument :
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 ClientSampleId :
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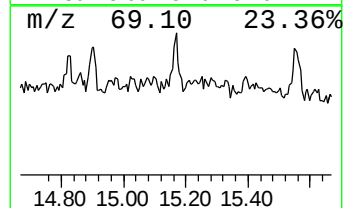
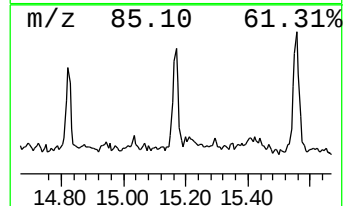
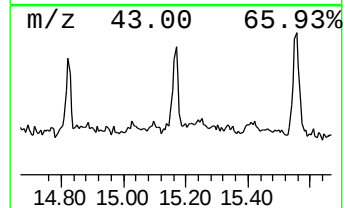
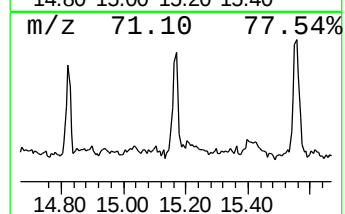
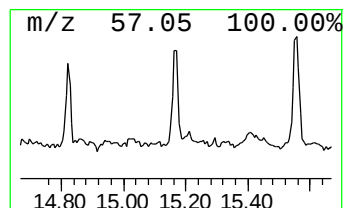
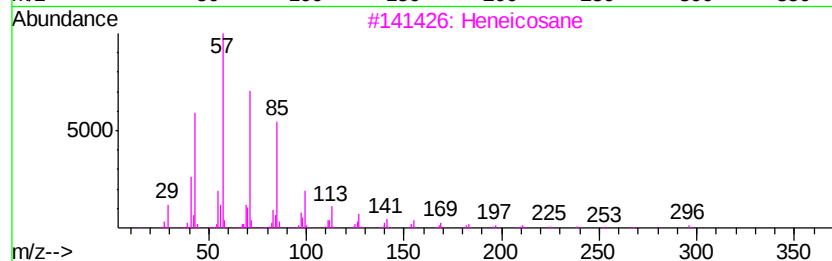
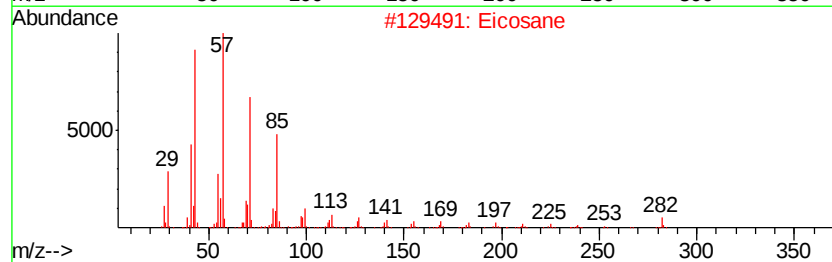
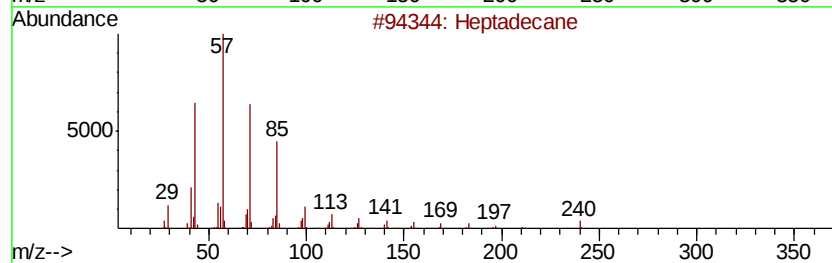
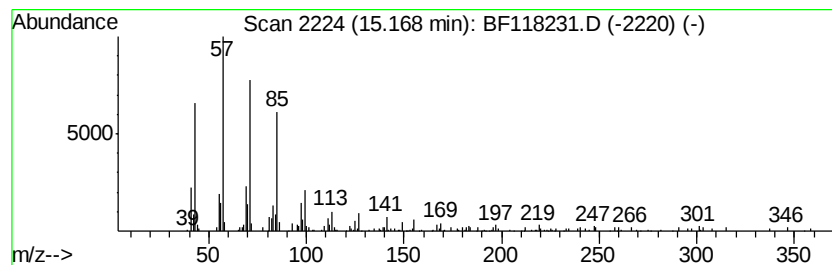
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.03 ng	158679	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	93
2		Eicosane	282	C20H42	000112-95-8	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118231.D
Acq On : 17 Dec 2019 17:30
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Sample : K6310-03
Misc :
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Instrument :
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ClientSampleId :
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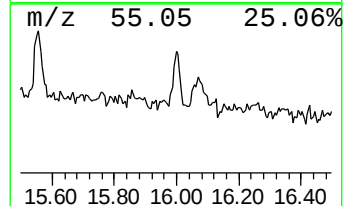
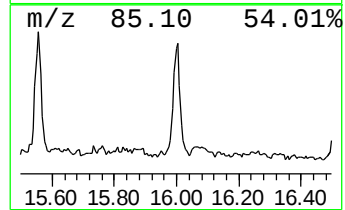
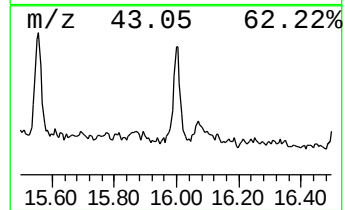
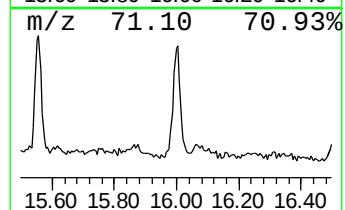
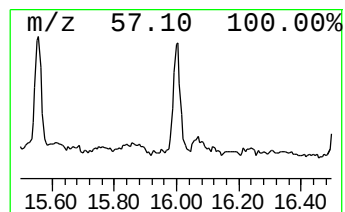
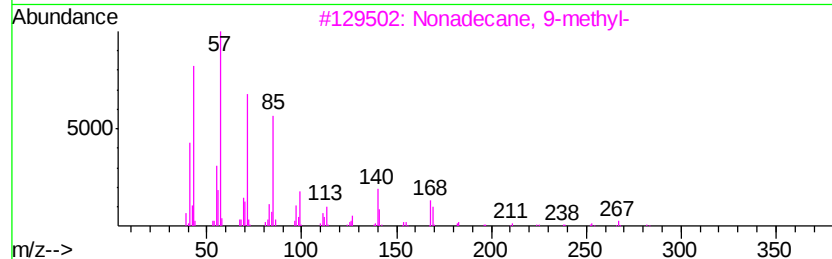
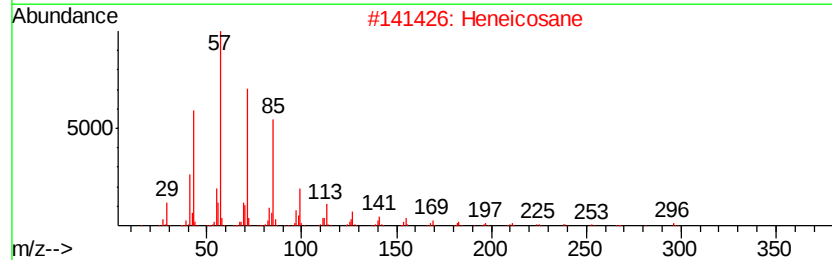
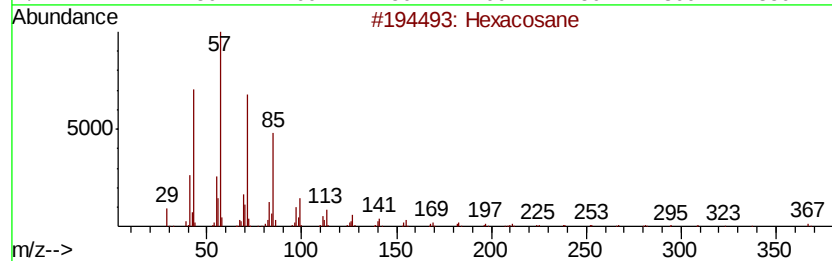
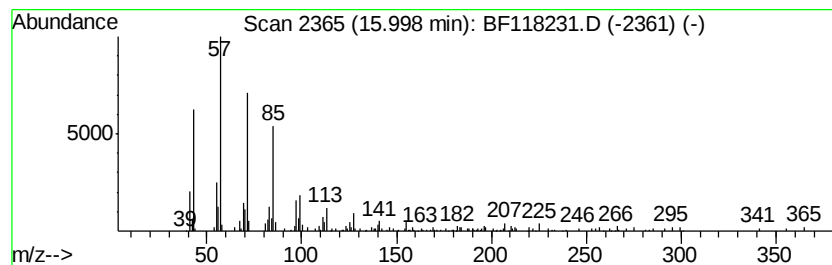
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	4.10 ng	214346	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
4		Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118231.D
Acq On : 17 Dec 2019 17:30
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Sample : K6310-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

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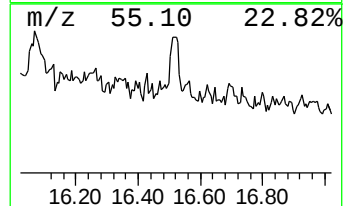
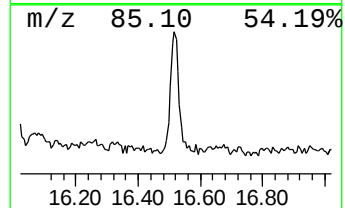
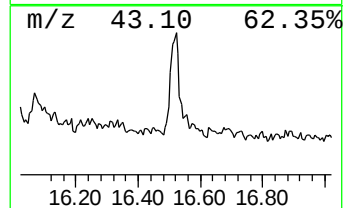
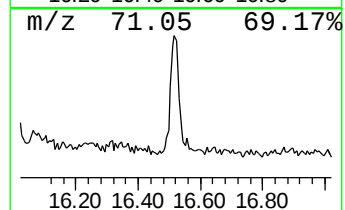
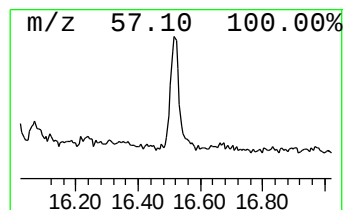
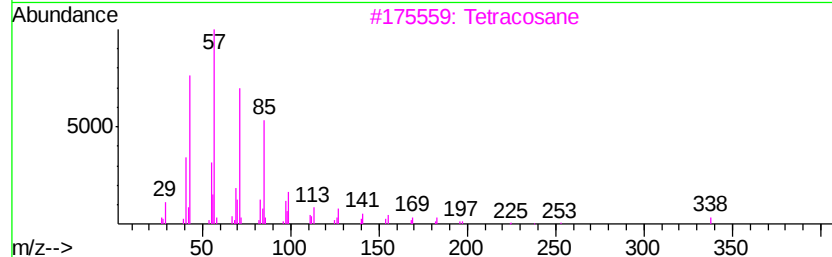
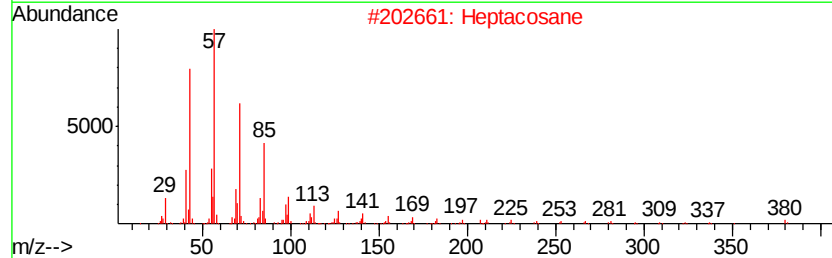
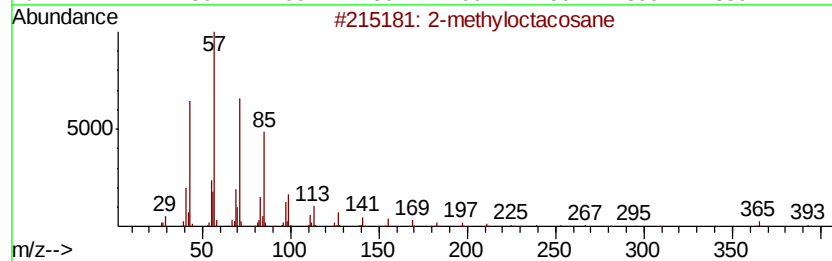
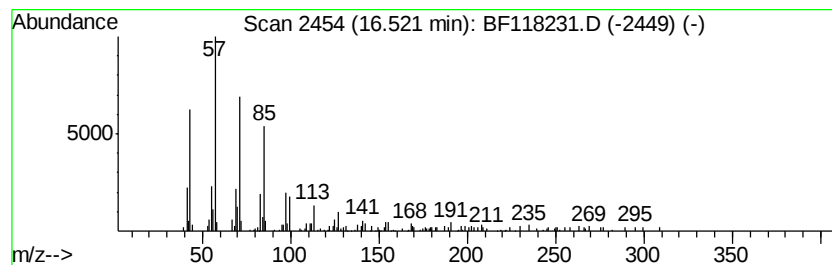
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	3.59 ng	187726	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	87
2		Heptacosane	380	C27H56	000593-49-7	83
3		Tetracosane	338	C24H50	000646-31-1	83
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
5		Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
 Data File : BF118231.D
 Acq On : 17 Dec 2019 17:30
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 Misc :
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Instrument :
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 ClientSampleId :
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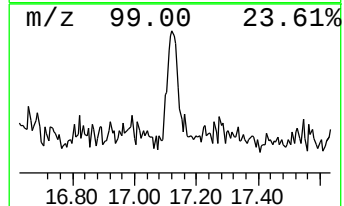
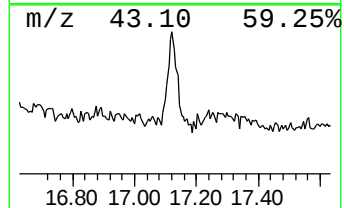
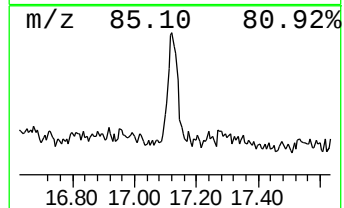
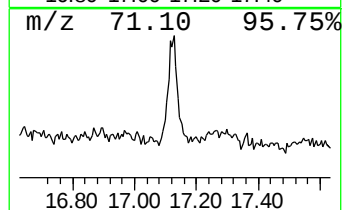
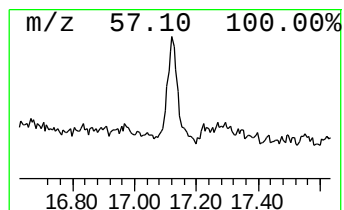
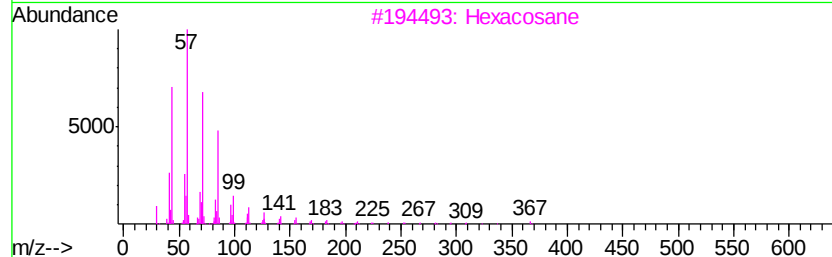
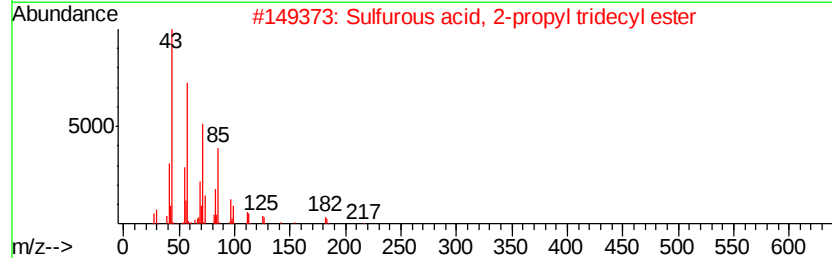
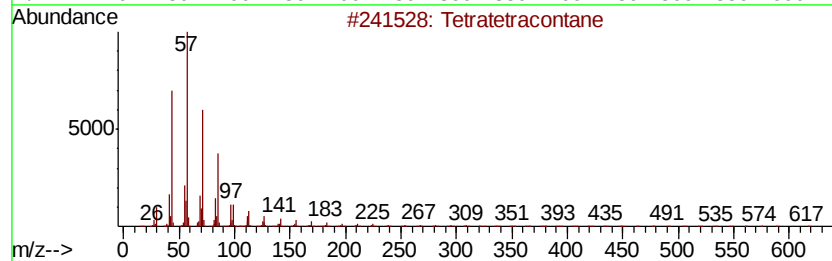
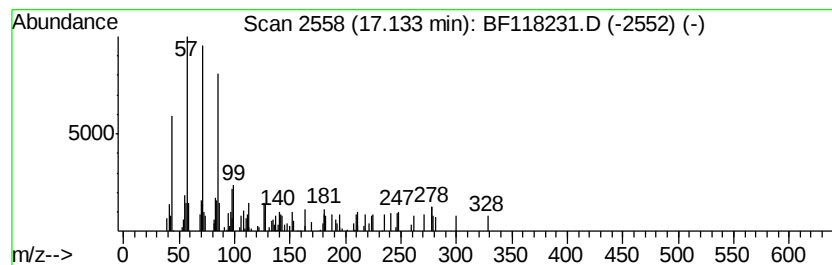
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 13 Tetratetracontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.37 ng	123873	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	74
2		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72
3		Hexacosane	366	C26H54	000630-01-3	68
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	68
5		Tetracosane	338	C24H50	000646-31-1	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
 Data File : BF118231.D
 Acq On : 17 Dec 2019 17:30
 Operator : JU
 Sample : K6310-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-01

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	9.8	ng	383883	1	6.86	786204	20.0
2-Pentanone, 4-hy...	5.07	10.8	ng	424708	1	6.86	786204	20.0
unknown6.63	6.63	68.0	ng	2671540	1	6.86	786204	20.0
n-Hexadecanoic acid	11.92	4.8	ng	304440	4	11.40	1267440	20.0
Octadecanoic acid	12.71	2.1	ng	131902	4	11.40	1267440	20.0
Phthalic acid, he...	13.07	2.1	ng	75454	5	14.05	723941	20.0
Phosphoric acid, ...	13.71	5.6	ng	201412	5	14.05	723941	20.0
1-Heneicosanol	13.89	10.6	ng	385087	5	14.05	723941	20.0
Heptadecane	15.17	3.0	ng	158679	6	15.54	1046540	20.0
Hexacosane	16.00	4.1	ng	214346	6	15.54	1046540	20.0
2-methyloctacosane	16.52	3.6	ng	187726	6	15.54	1046540	20.0
Tetratetracontane	17.13	2.4	ng	123873	6	15.54	1046540	20.0