

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040620\
 Data File : BF119793.D
 Acq On : 7 Apr 2020 1:46
 Operator : MA/SJ
 Sample : L2101-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 239-WC-L-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-BF031820.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	4.975	488	491	496	rVB	195363	210340	3.17%	0.503%
2	5.392	558	562	566	rBV	2251618	1906073	28.77%	4.555%
3	5.722	615	618	625	rBV	126191	121621	1.84%	0.291%
4	6.404	722	734	741	rBV	1654251	1595669	24.08%	3.813%
5	6.781	794	798	801	rBV	1281489	1046057	15.79%	2.500%
6	6.845	805	809	820	rBV	331408	352661	5.32%	0.843%
7	6.939	820	825	828	rVV	4848232	4403976	66.46%	10.523%
8	7.345	888	894	897	rBV	3478324	3755924	56.68%	8.975%
9	7.445	903	911	916	rBV	140718	220838	3.33%	0.528%
10	7.969	997	1000	1005	rBV	95278	108544	1.64%	0.259%
11	8.069	1012	1017	1019	rBV	1403350	1410170	21.28%	3.370%
12	9.151	1195	1201	1204	rVB	6404345	6626050	100.00%	15.833%
13	9.539	1263	1267	1270	rBV	620312	475572	7.18%	1.136%
14	9.586	1271	1275	1280	rVV	128824	139558	2.11%	0.333%
15	9.821	1310	1315	1319	rBV	1610364	1557814	23.51%	3.722%
16	9.921	1329	1332	1339	rVB	156674	150027	2.26%	0.358%
17	10.027	1347	1350	1353	rBV	99144	87346	1.32%	0.209%
18	10.616	1444	1450	1453	rBV	2607206	2650051	39.99%	6.332%
19	10.663	1453	1458	1466	rVB2	270186	280190	4.23%	0.670%
20	11.310	1563	1568	1571	rBV	1895985	1616249	24.39%	3.862%
21	11.368	1575	1578	1582	rVB	65599	67939	1.03%	0.162%
22	11.415	1582	1586	1594	rBV4	45462	87307	1.32%	0.209%
23	11.845	1655	1659	1664	rBV	702735	639046	9.64%	1.527%
24	12.633	1789	1793	1800	rBV	296640	354055	5.34%	0.846%
25	12.904	1834	1839	1842	rBV	5982360	6145799	92.75%	14.685%
26	13.139	1874	1879	1881	rBV	73376	82373	1.24%	0.197%
27	13.386	1913	1921	1925	rBV6	66339	102465	1.55%	0.245%
28	13.480	1935	1937	1940	rVB	103431	81906	1.24%	0.196%
29	13.809	1989	1993	2002	rBV	647470	770961	11.64%	1.842%
30	13.951	2012	2017	2021	rBV	1569533	1510303	22.79%	3.609%
31	14.127	2043	2047	2052	rBV	218150	216290	3.26%	0.517%
32	14.433	2095	2099	2105	rBV	276864	307488	4.64%	0.735%
33	14.733	2147	2150	2154	rVB	348011	304697	4.60%	0.728%
34	15.062	2202	2206	2210	rBV	303250	341359	5.15%	0.816%

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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	15.398	2257	2263	2266	rBV	1108026	1286747	19.42%	3.075%
36	15.439	2266	2270	2277	rVB	252436	333938	5.04%	0.798%
37	15.862	2336	2342	2347	rBV	176257	254877	3.85%	0.609%
38	15.927	2348	2353	2358	rBV6	43243	84325	1.27%	0.201%
39	16.356	2420	2426	2433	rBV	85857	162882	2.46%	0.389%

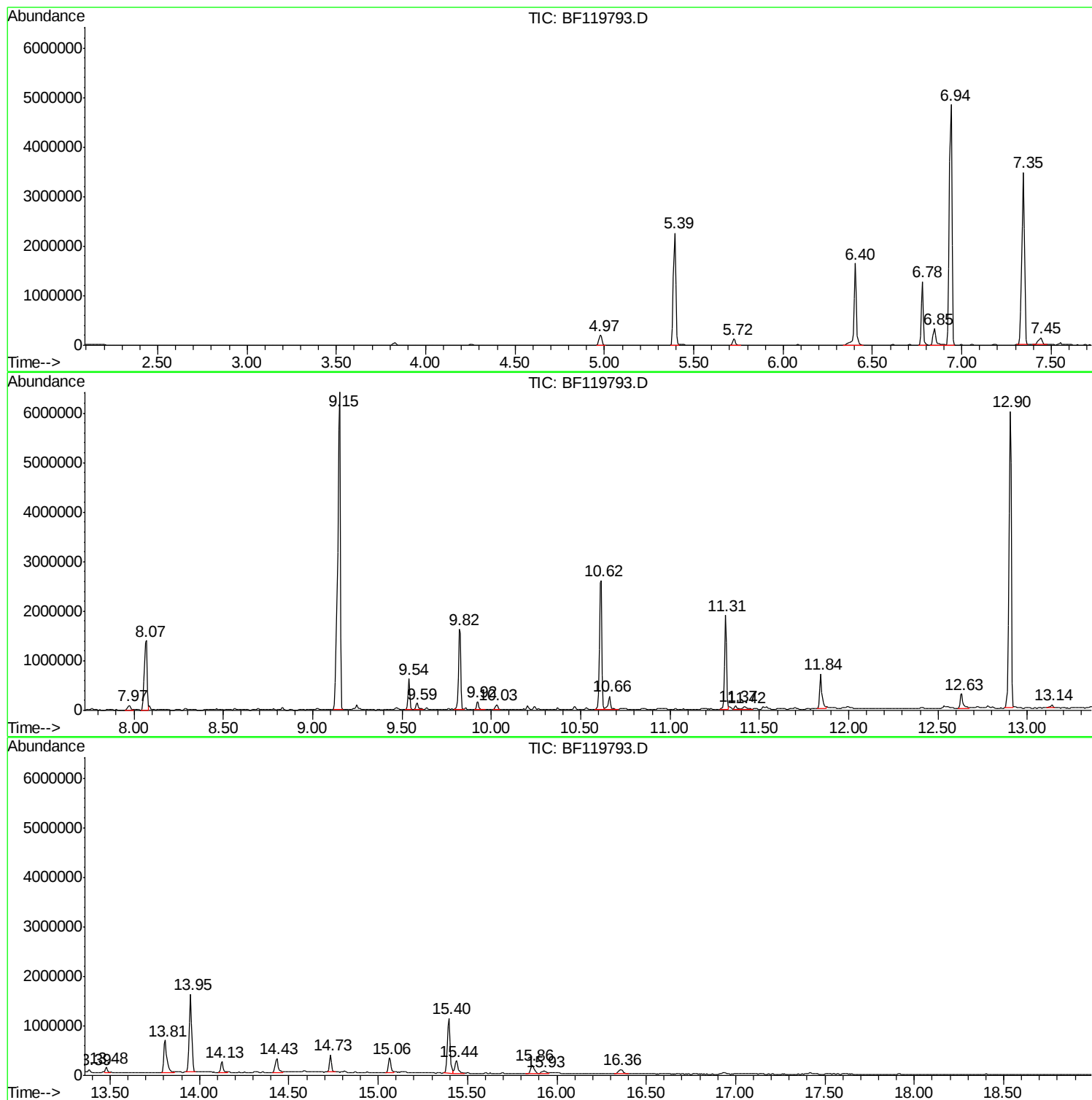
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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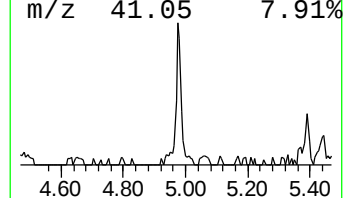
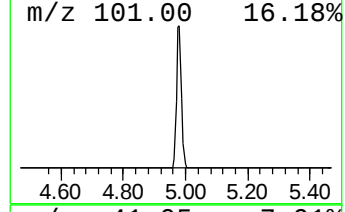
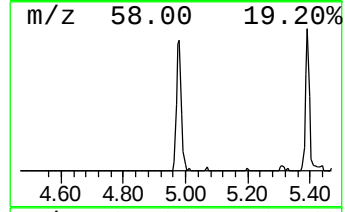
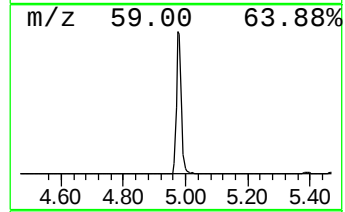
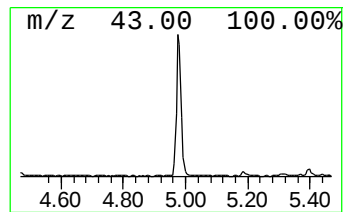
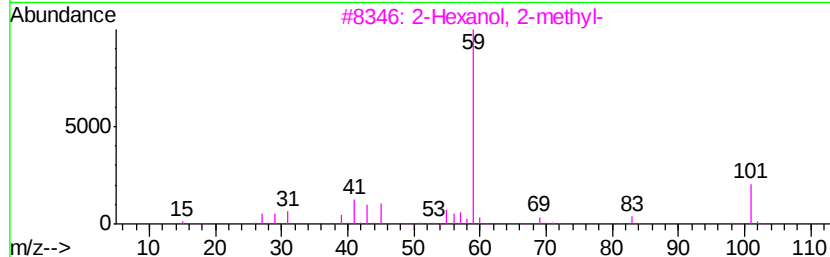
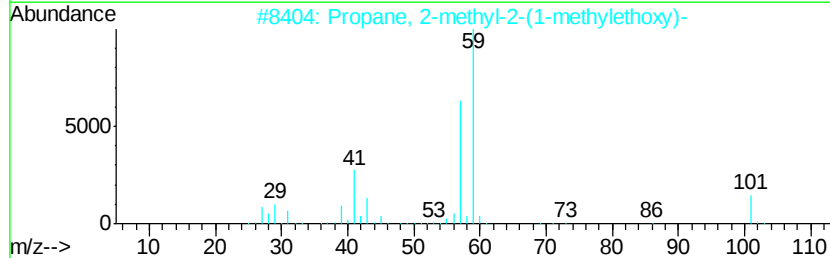
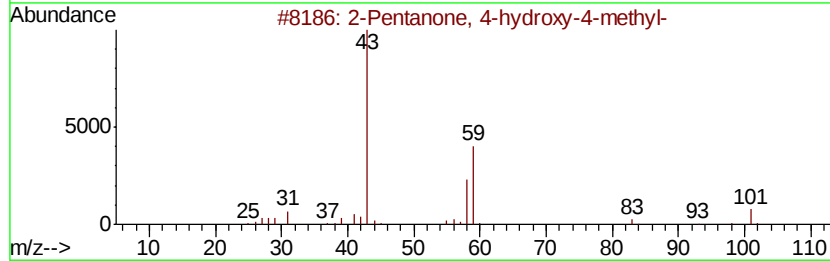
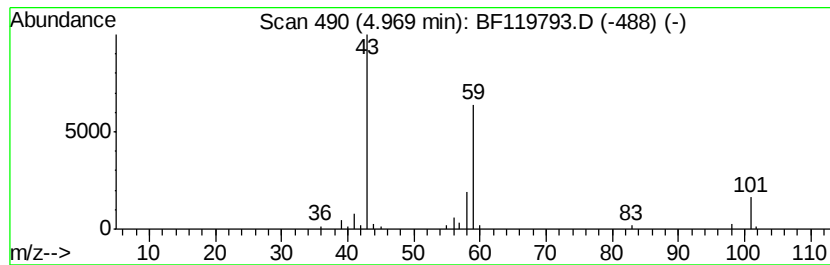
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	4.02 ng	210340	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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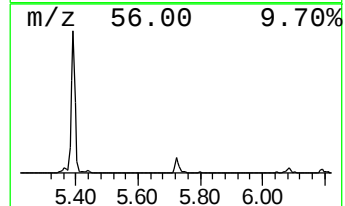
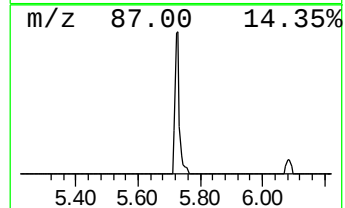
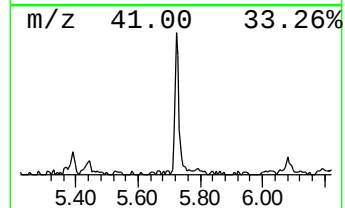
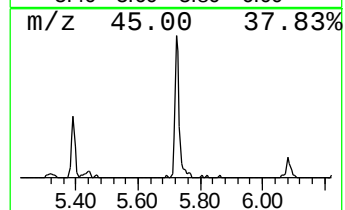
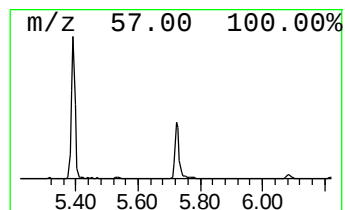
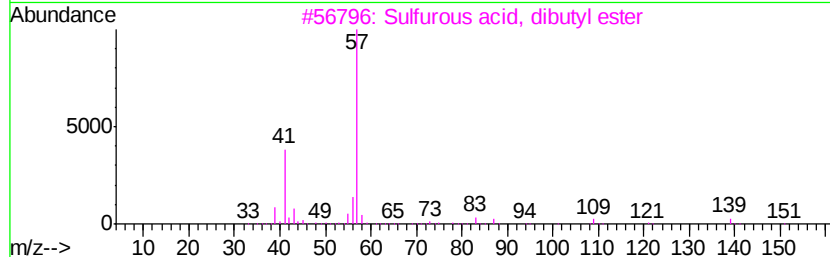
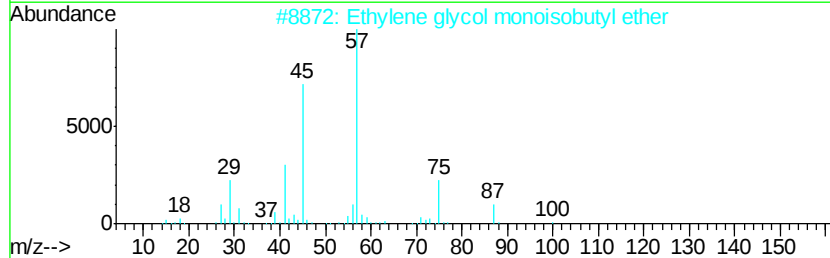
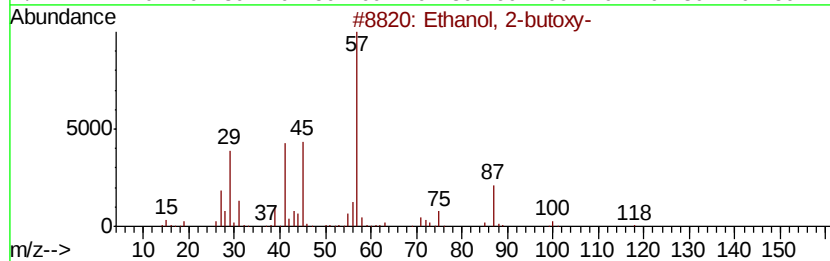
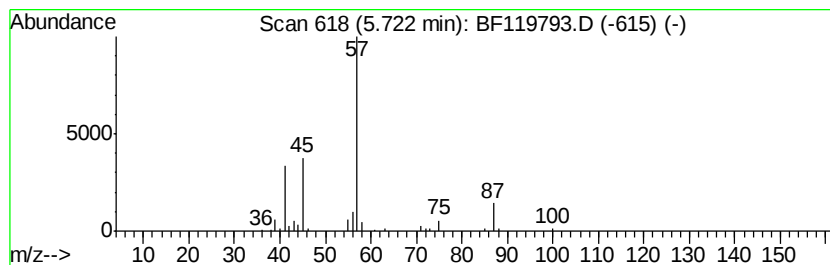
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.33 ng	121621	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
2		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38
3		Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	35
4		1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	25
5		Isobutyl ether	130	C8H18O	000628-55-7	25



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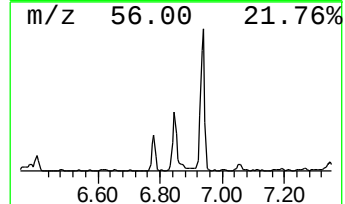
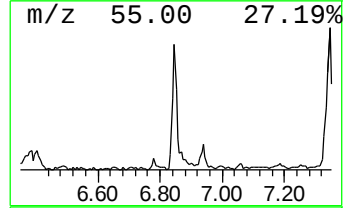
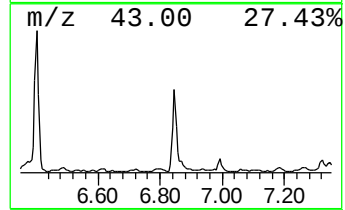
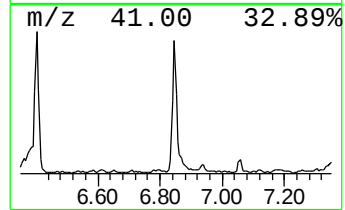
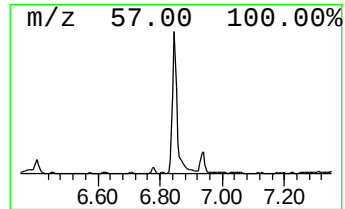
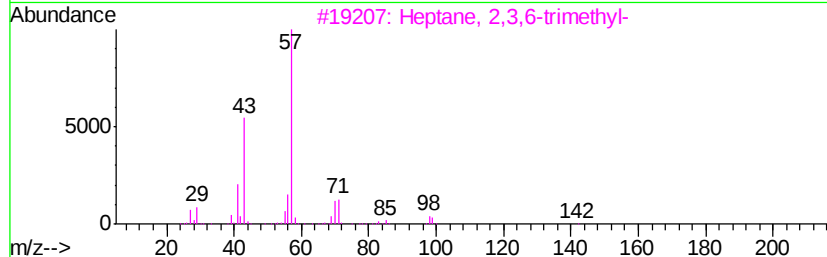
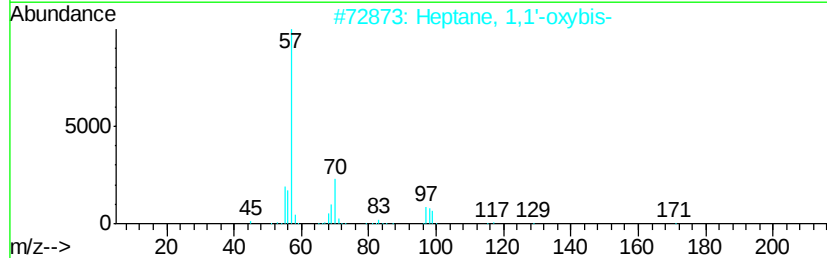
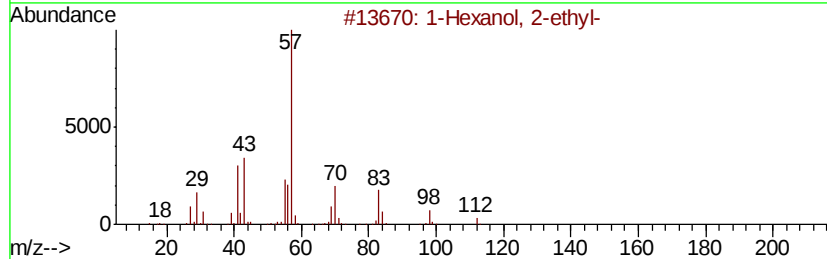
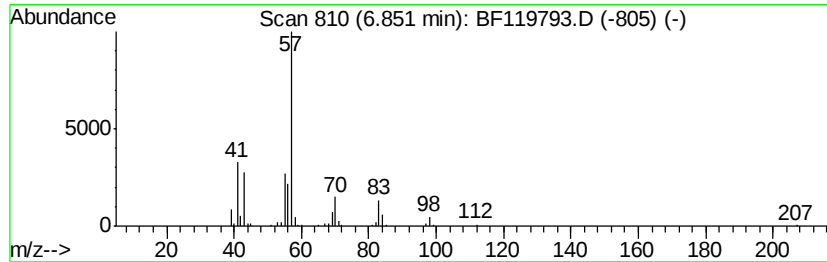
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	6.74 ng	352661	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
4			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	45
5			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	45



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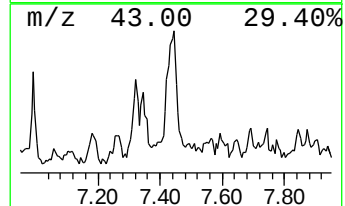
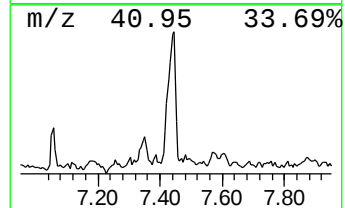
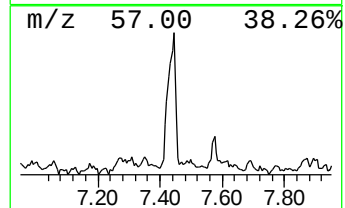
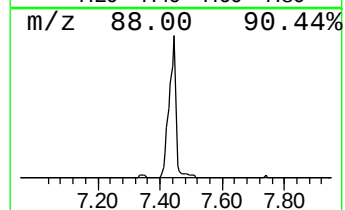
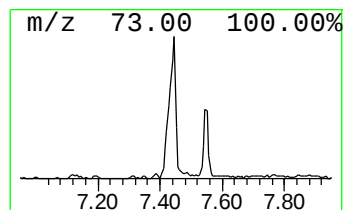
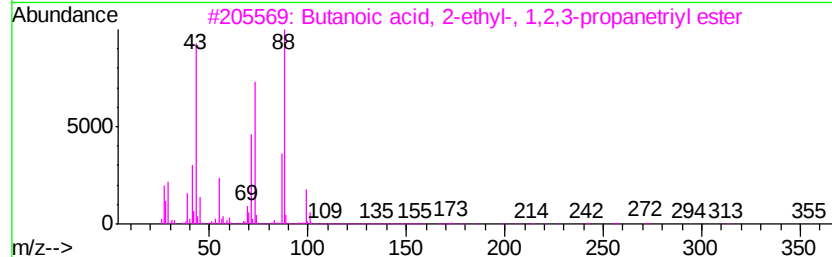
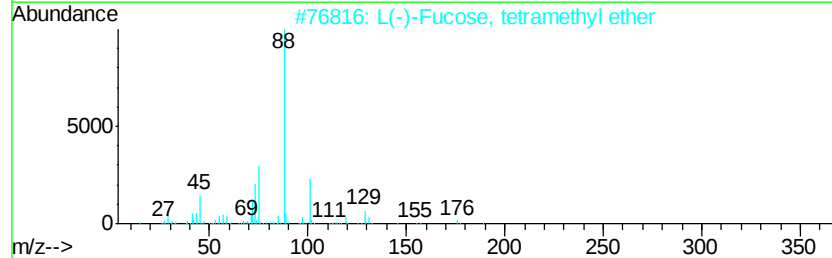
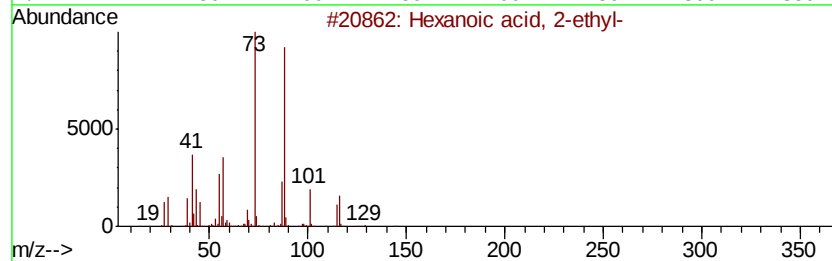
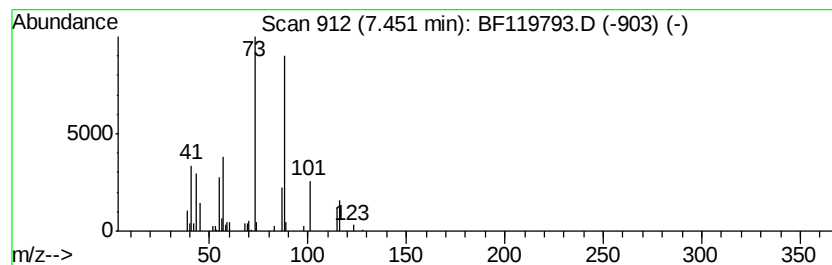
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	3.13 ng	220838	Naphthalene-d8	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2		L(-)-Fucose, tetramethyl ether	220	C10H20O5	1000332-75-0	50
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4		1,4-Dioxane	88	C4H8O2	000123-91-1	38
5		Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	36



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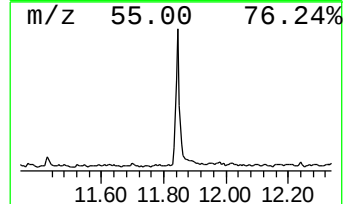
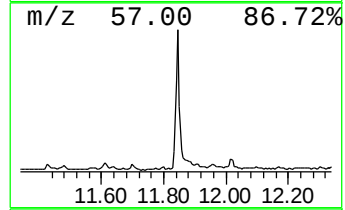
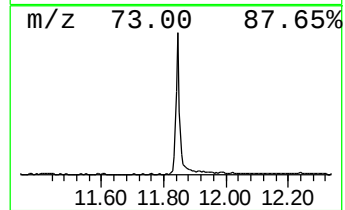
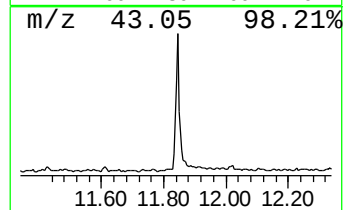
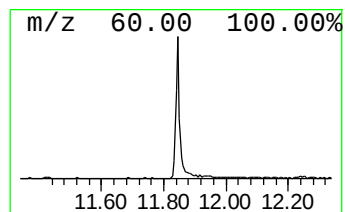
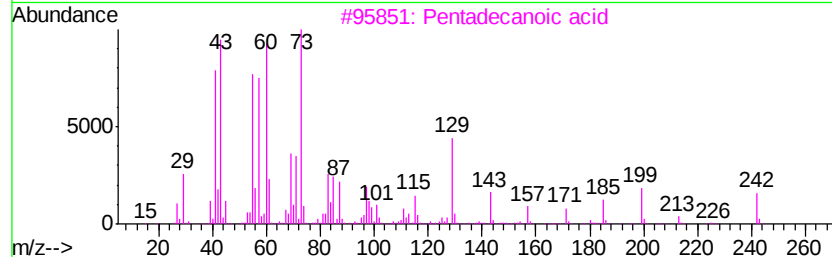
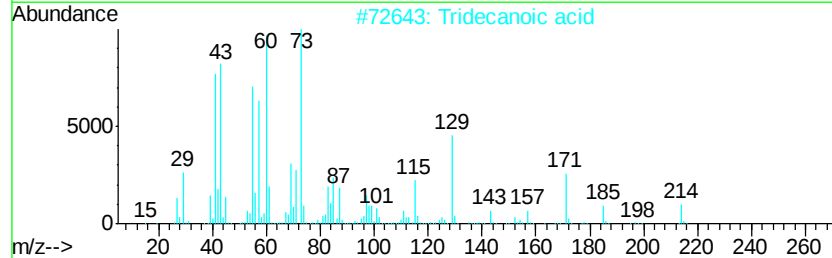
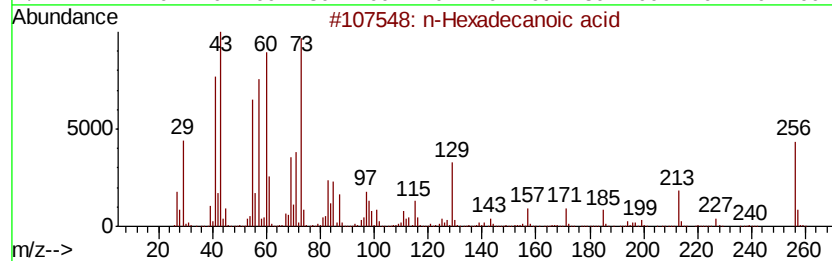
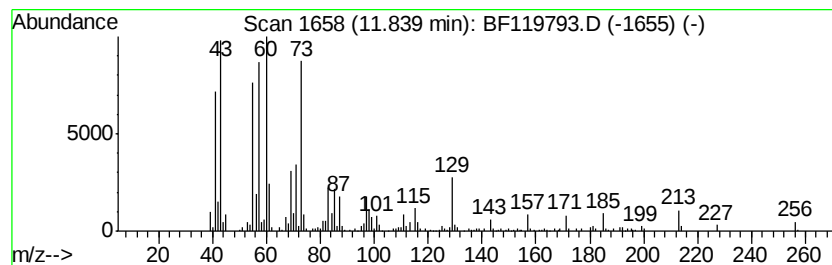
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TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	7.91 ng	639046	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119793.D
Acq On : 7 Apr 2020 1:46
Operator : MA/SJ
Sample : L2101-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
239-WC-L-01

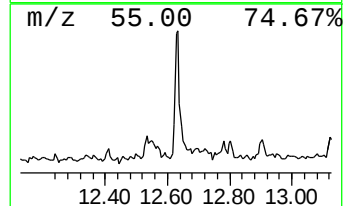
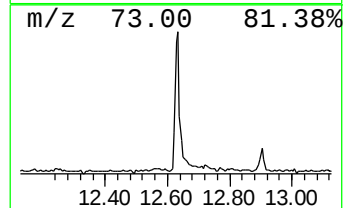
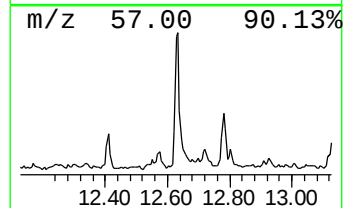
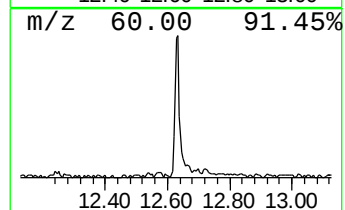
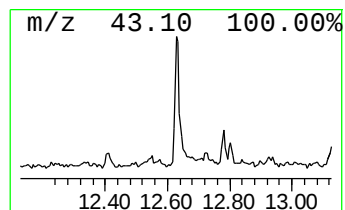
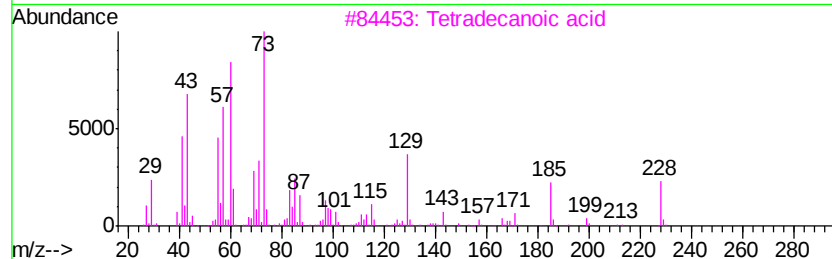
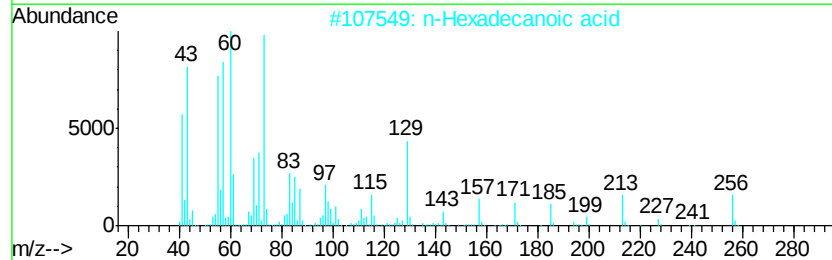
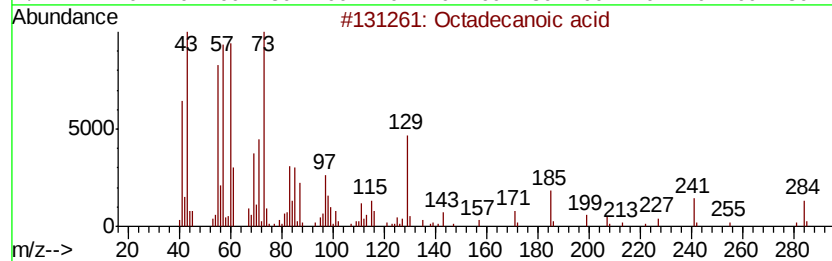
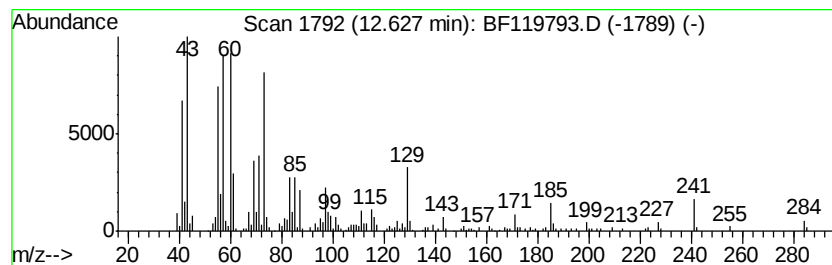
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	4.69 ng	354055	Chrysene-d12	13.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
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ClientSampleId :
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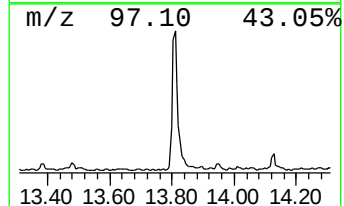
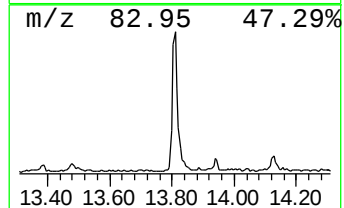
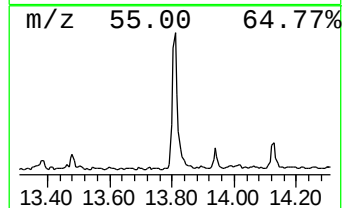
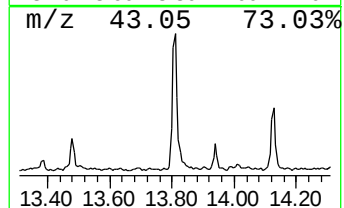
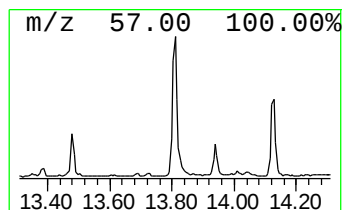
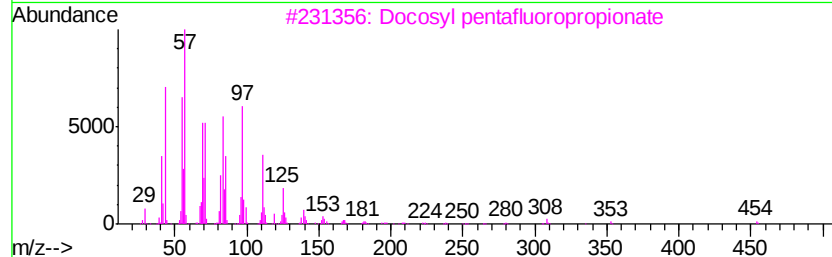
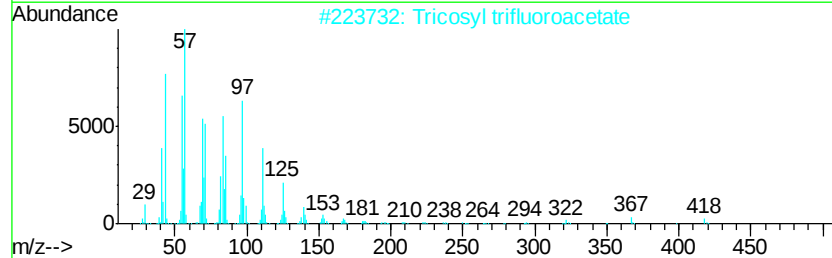
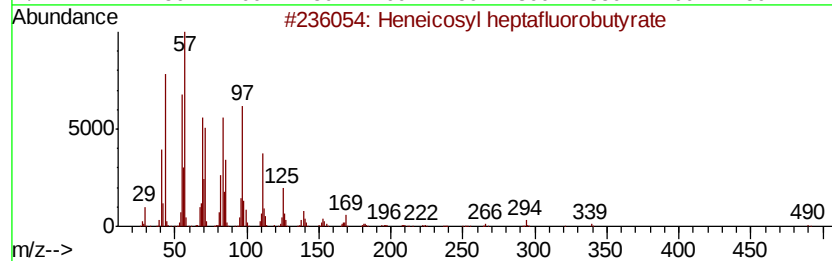
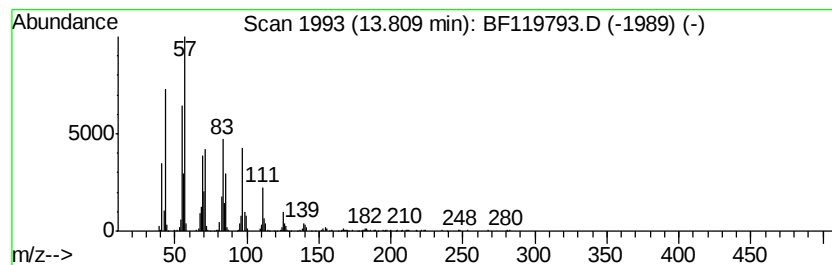
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	10.21 ng	770961	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
5		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119793.D
Acq On : 7 Apr 2020 1:46
Operator : MA/SJ
Sample : L2101-04
Misc :
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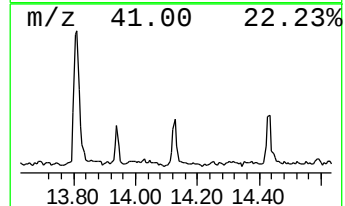
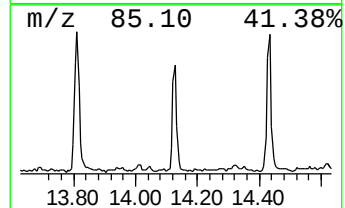
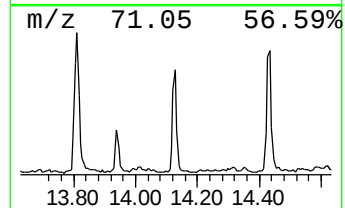
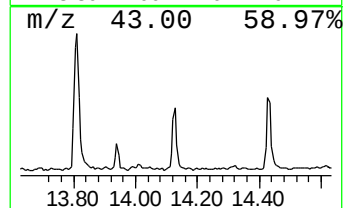
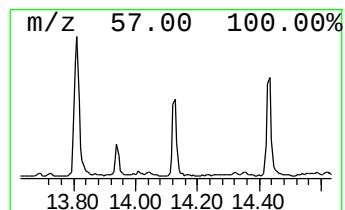
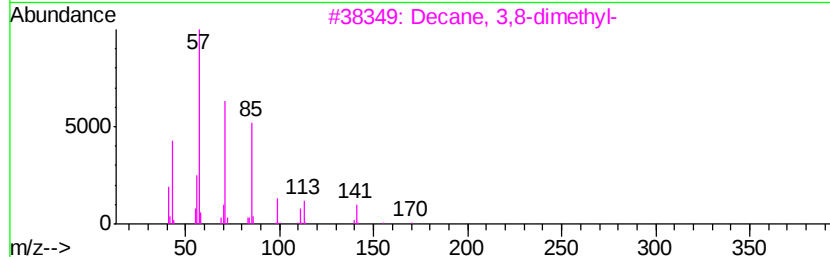
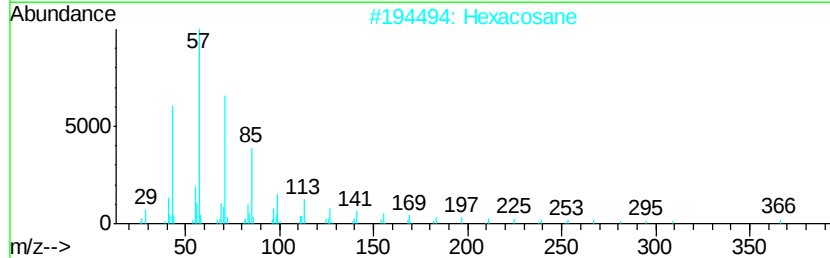
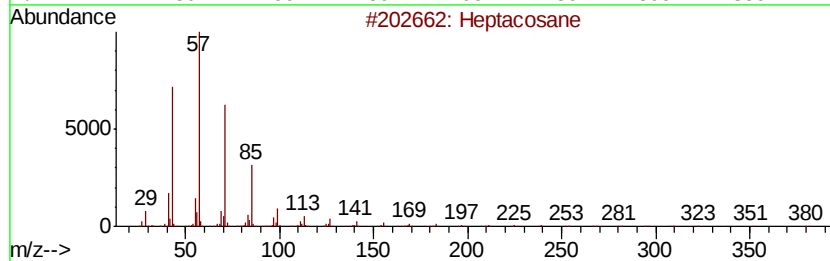
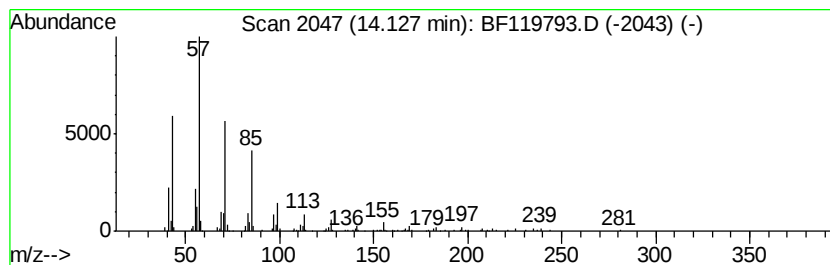
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	2.86 ng	216290	Chrysene-d12	13.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	87
4	Hentriacontane		437	C31H64	000630-04-6	87
5	Hexadecane		226	C16H34	000544-76-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119793.D
Acq On : 7 Apr 2020 1:46
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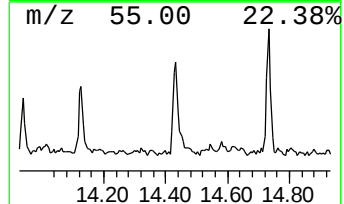
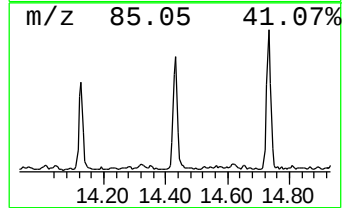
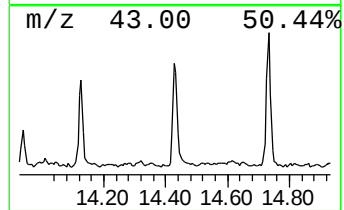
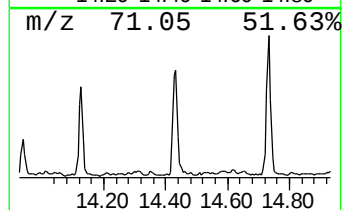
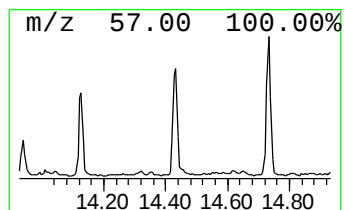
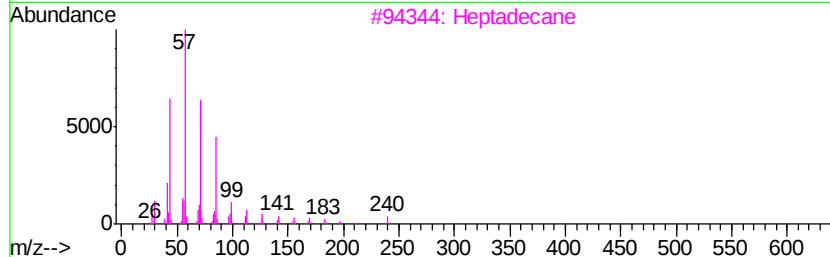
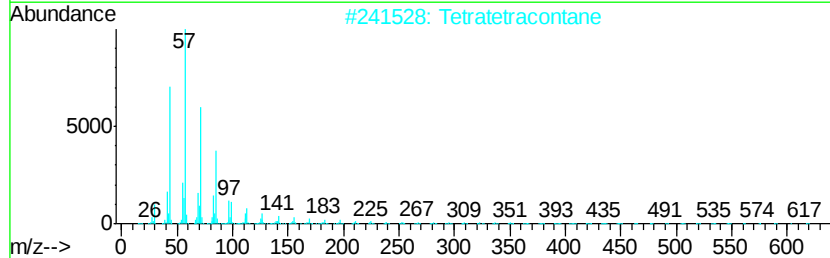
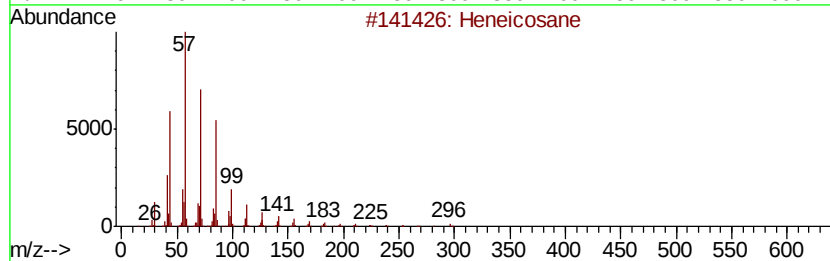
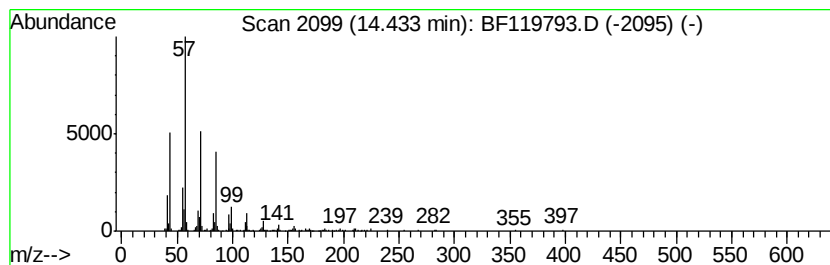
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	4.07 ng	307488	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Tetratetracontane	619	C44H90	007098-22-8	90
3		Heptadecane	240	C17H36	000629-78-7	87
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119793.D
Acq On : 7 Apr 2020 1:46
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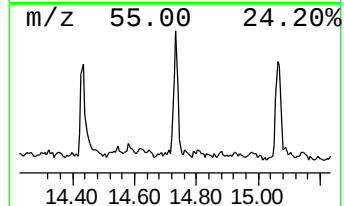
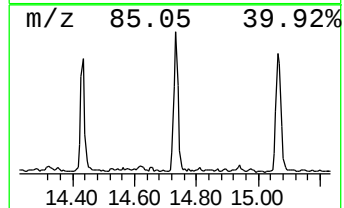
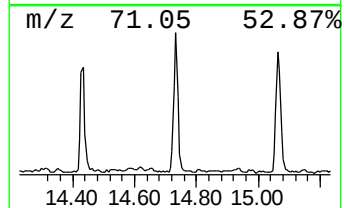
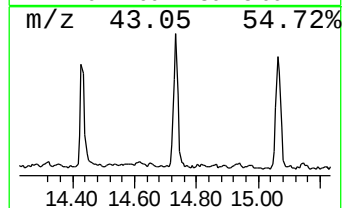
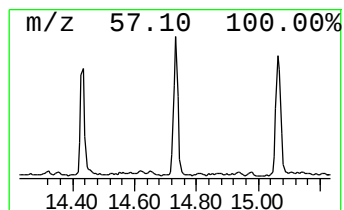
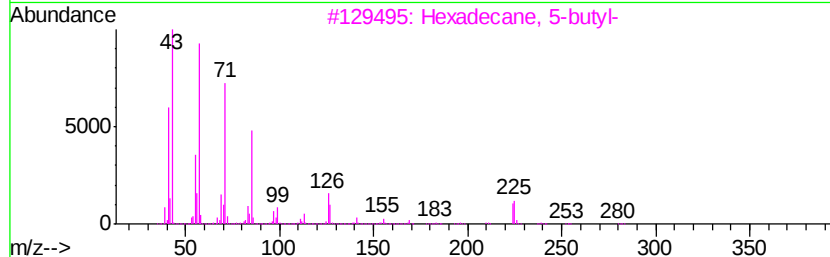
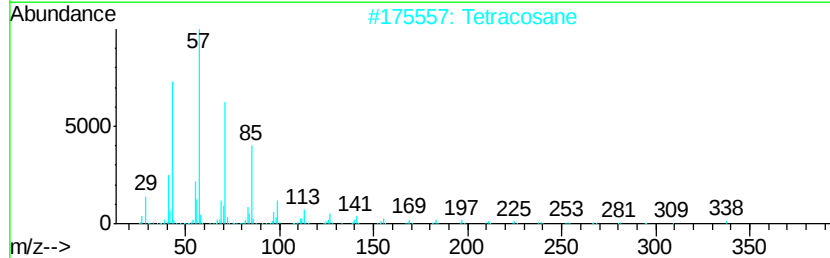
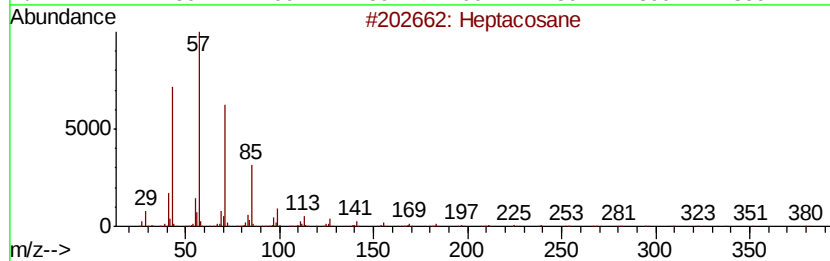
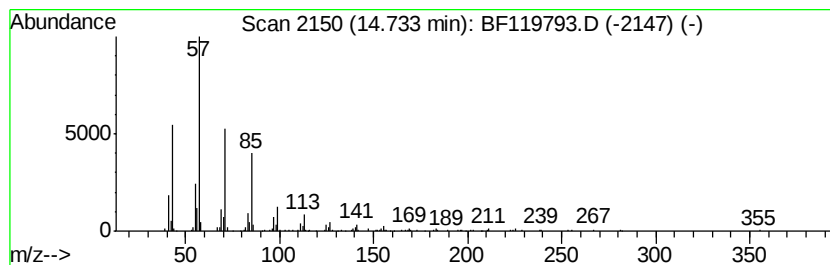
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.74 ng	304697	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Hexadecane, 5-butyl-	282	C20H42	006912-07-8	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
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Acq On : 7 Apr 2020 1:46
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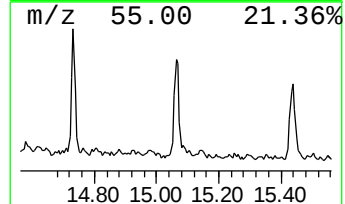
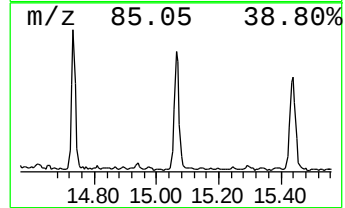
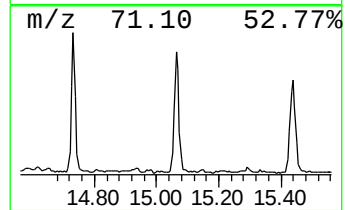
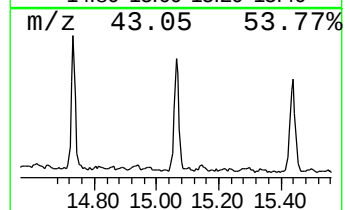
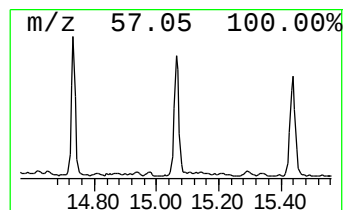
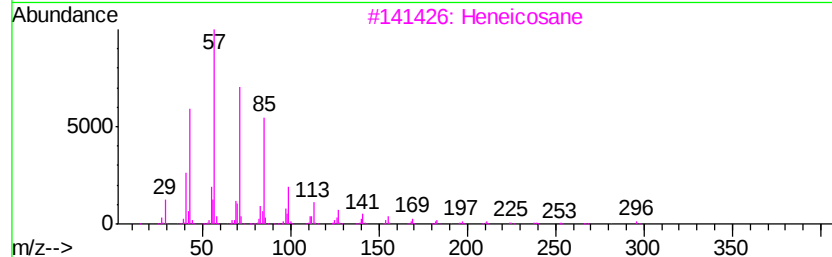
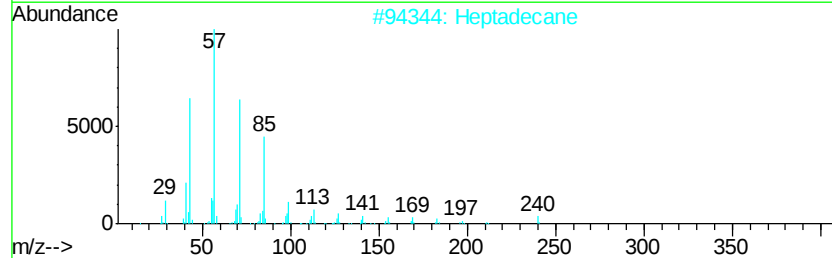
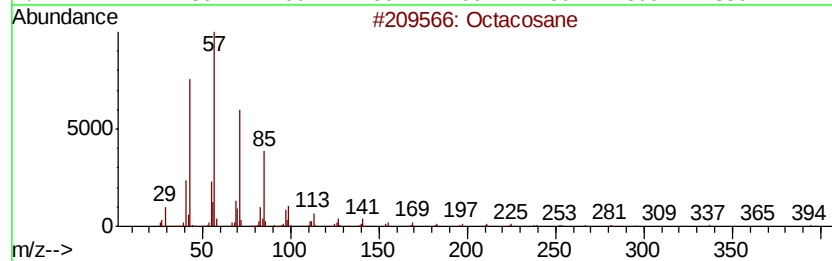
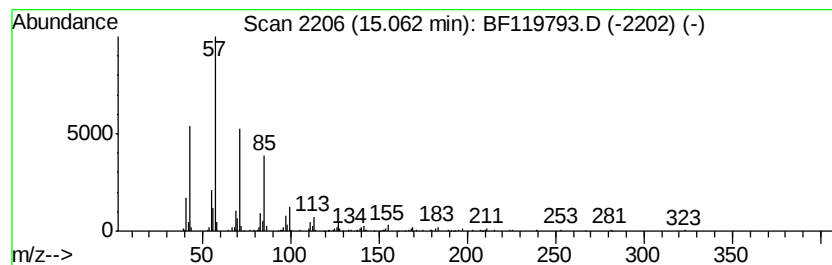
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	5.31 ng	341359	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octadecane	254	C18H38	000593-45-3	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119793.D
Acq On : 7 Apr 2020 1:46
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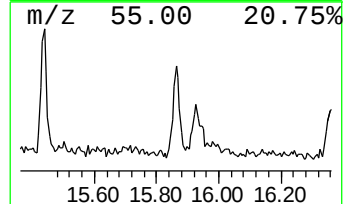
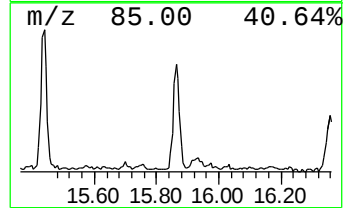
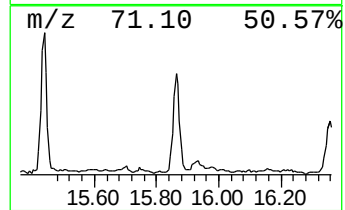
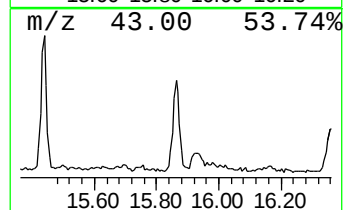
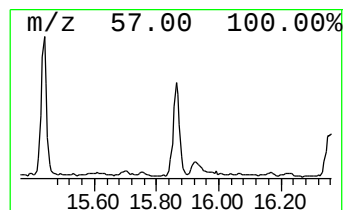
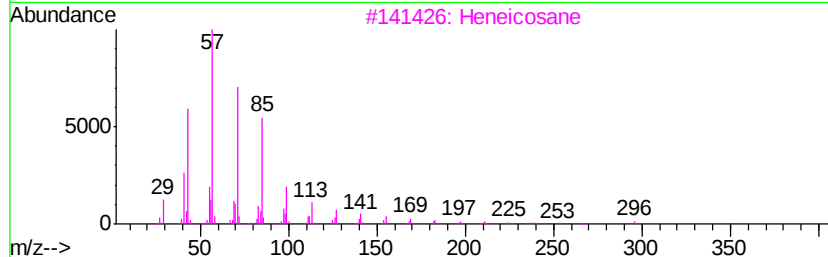
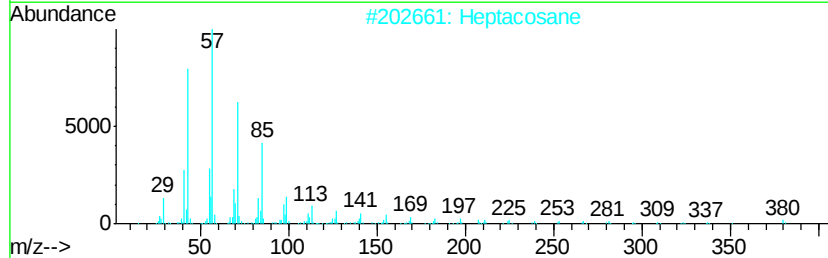
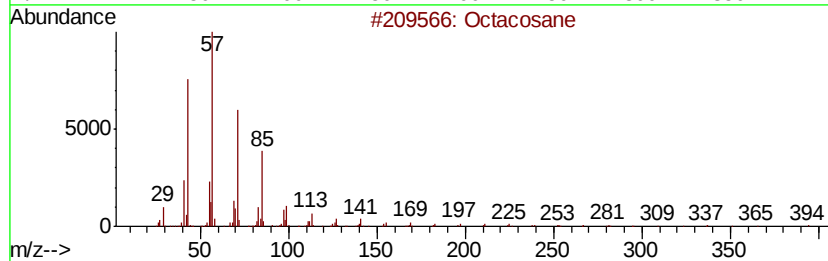
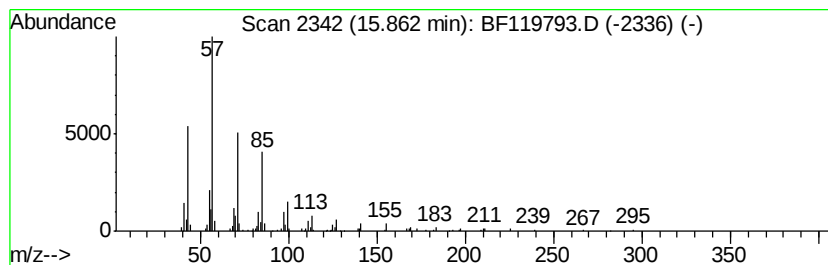
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.96 ng	254877	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Tetracosane	338	C24H50	000646-31-1	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119793.D
Acq On : 7 Apr 2020 1:46
Operator : MA/SJ
Sample : L2101-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

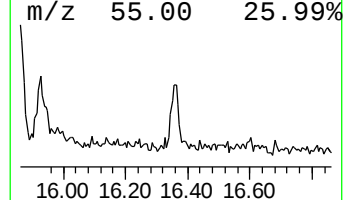
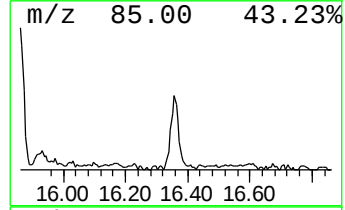
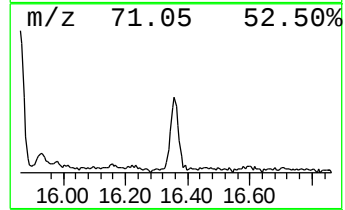
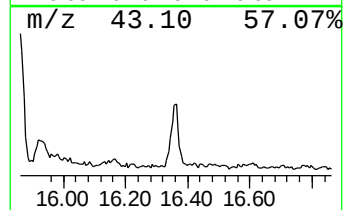
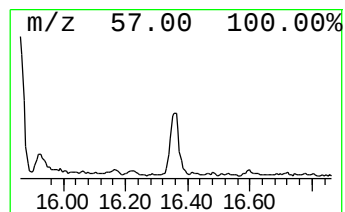
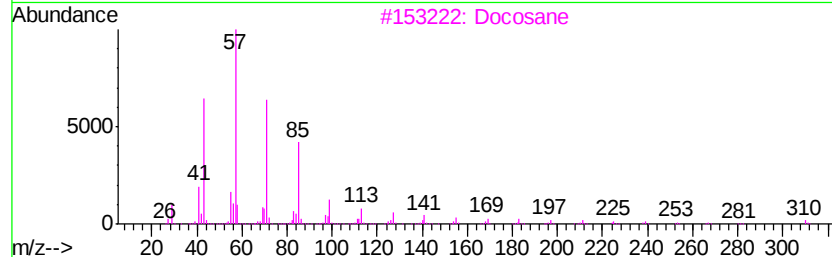
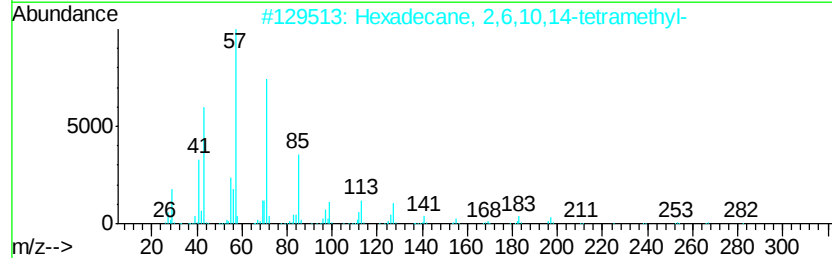
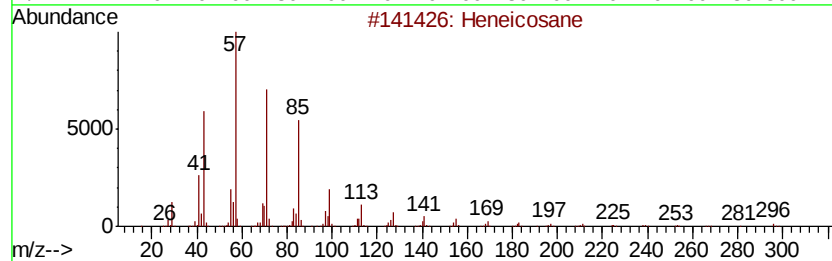
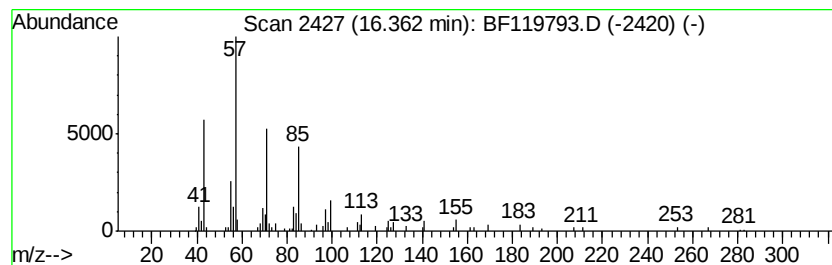
Instrument :
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ClientSampleId :
239-WC-L-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexadecane, 2,6,10,14-tetra... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.36	2.53 ng	162882	Perylene-d12	15.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
3	Docosane	310	C22H46	000629-97-0	80
4	Triacontane	422	C30H62	000638-68-6	80
5	Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040620\
 Data File : BF119793.D
 Acq On : 7 Apr 2020 1:46
 Operator : MA/SJ
 Sample : L2101-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 239-WC-L-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	4.0	ng	210340	1	6.78	1046060	20.0
Ethanol, 2-butoxy-	5.72	2.3	ng	121621	1	6.78	1046060	20.0
1-Hexanol, 2-ethyl-	6.85	6.7	ng	352661	1	6.78	1046060	20.0
Hexanoic acid, 2-...	7.45	3.1	ng	220838	2	8.07	1410170	20.0
n-Hexadecanoic acid	11.84	7.9	ng	639046	4	11.31	1616250	20.0
Octadecanoic acid	12.63	4.7	ng	354055	5	13.95	1510300	20.0
Heneicosyl hepta...	13.81	10.2	ng	770961	5	13.95	1510300	20.0
Heptacosane	14.13	2.9	ng	216290	5	13.95	1510300	20.0
Heneicosane	14.43	4.1	ng	307488	5	13.95	1510300	20.0
Tetracosane	14.73	4.7	ng	304697	6	15.40	1286750	20.0
Octacosane	15.06	5.3	ng	341359	6	15.40	1286750	20.0
2-methyloctacosane	15.86	4.0	ng	254877	6	15.40	1286750	20.0
Hexadecane, 2,6,1...	16.36	2.5	ng	162882	6	15.40	1286750	20.0