

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
 Data File : BF118967.D
 Acq On : 20 Feb 2020 19:13
 Operator : CG/JU
 Sample : L1592-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-BPM-04-005-ABCD

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-BF022020.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	5.387	557	561	582	rBV	3641419	3680157	69.01%	8.217%
2	6.404	729	734	746	rBV	3261546	3576768	67.07%	7.986%
3	6.757	790	794	798	rBV	1252628	1029555	19.31%	2.299%
4	6.916	816	821	824	rBV	3647892	3312288	62.11%	7.396%
5	7.322	884	890	893	rBV	2401520	2444773	45.84%	5.459%
6	8.039	1007	1012	1015	rBV	1447089	1349320	25.30%	3.013%
7	9.116	1189	1195	1198	rBV	5238229	5081439	95.28%	11.346%
8	9.504	1257	1261	1265	rBV	357698	289945	5.44%	0.647%
9	9.727	1292	1299	1305	rBV4	34986	78621	1.47%	0.176%
10	9.786	1305	1309	1313	rVB	1742681	1639551	30.74%	3.661%
11	9.992	1340	1344	1352	rBV2	30757	55834	1.05%	0.125%
12	10.480	1423	1427	1433	rVB	37162	61392	1.15%	0.137%
13	10.574	1438	1443	1447	rBV	3328318	3319586	62.25%	7.412%
14	10.727	1465	1469	1474	rVB3	47854	74059	1.39%	0.165%
15	10.927	1498	1503	1512	rVB4	79865	156994	2.94%	0.351%
16	11.269	1557	1561	1565	rBV	1921848	1679975	31.50%	3.751%
17	11.804	1646	1652	1665	rBV	687100	975008	18.28%	2.177%
18	11.945	1672	1676	1679	rBV	142491	248459	4.66%	0.555%
19	11.974	1679	1681	1690	rVB2	174105	287426	5.39%	0.642%
20	12.504	1766	1771	1779	rVB9	29728	63032	1.18%	0.141%
21	12.586	1779	1785	1794	rBV	330693	490621	9.20%	1.095%
22	12.857	1826	1831	1834	rBV	5463078	5332985	100.00%	11.907%
23	13.086	1868	1870	1876	rVB2	58464	58048	1.09%	0.130%
24	13.427	1922	1928	1931	rBV2	98129	112078	2.10%	0.250%
25	13.751	1977	1983	1992	rBV4	573220	870255	16.32%	1.943%
26	13.874	1999	2004	2005	rBV3	85155	118640	2.22%	0.265%
27	13.904	2005	2009	2017	rVB	1454203	1419127	26.61%	3.169%
28	14.074	2033	2038	2047	rVB	349503	428669	8.04%	0.957%
29	14.374	2084	2089	2101	rVB	633671	710094	13.32%	1.585%
30	14.674	2134	2140	2148	rBV	904515	1089874	20.44%	2.433%
31	14.992	2188	2194	2200	rBV	898120	1132344	21.23%	2.528%
32	15.327	2246	2251	2253	rBV	1029362	1300608	24.39%	2.904%
33	15.351	2253	2255	2263	rVB	820120	992710	18.61%	2.216%
34	15.762	2318	2325	2330	rBV	504741	791902	14.85%	1.768%

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

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

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35	16.233	2399	2405	2414	rvB	214558	418080	7.84%	0.933%
36	16.792	2496	2500	2509	rvB4	58506	117622	2.21%	0.263%

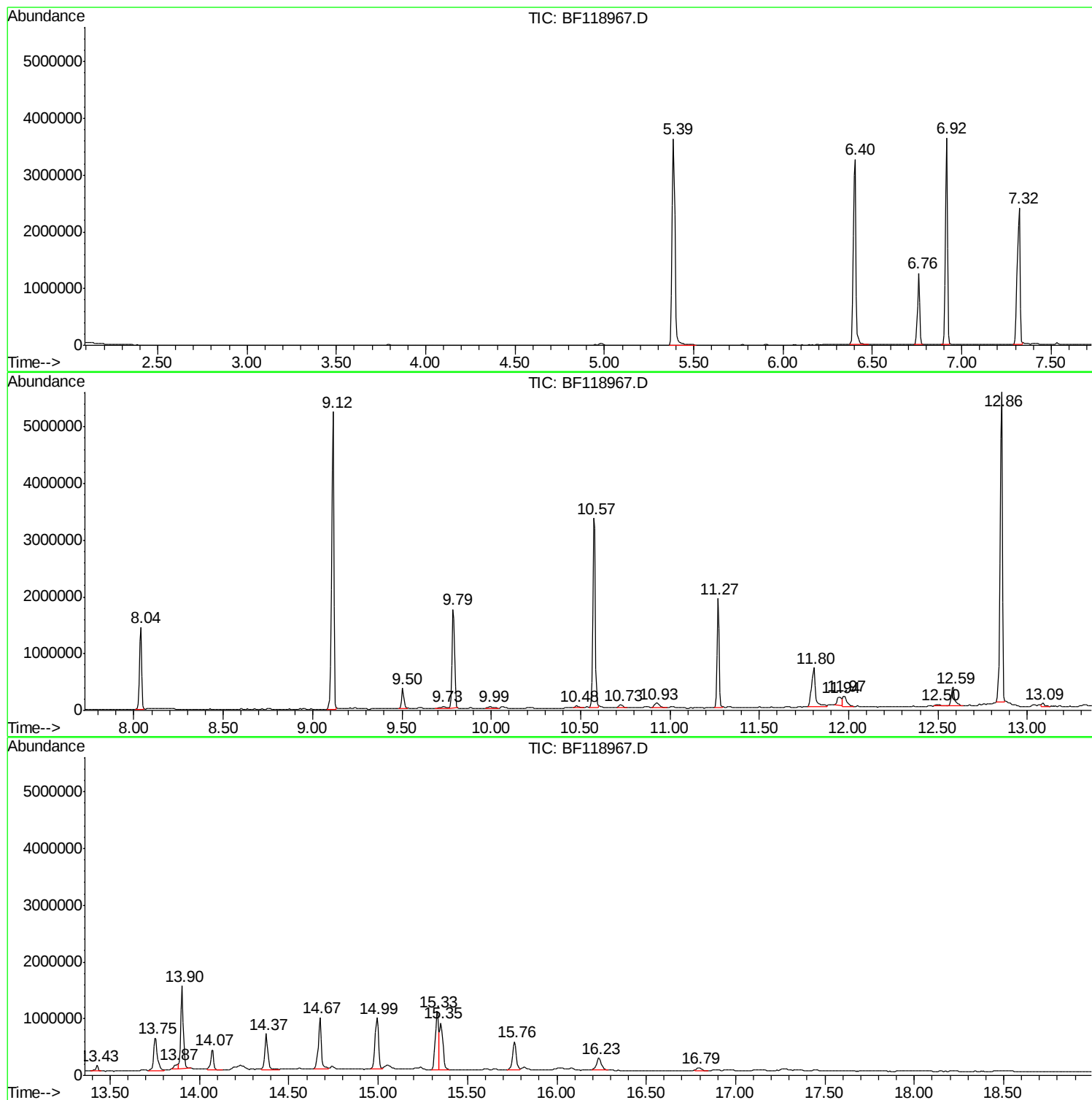
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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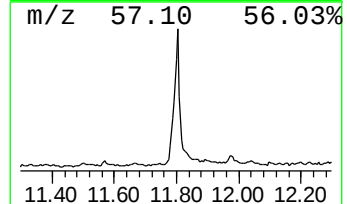
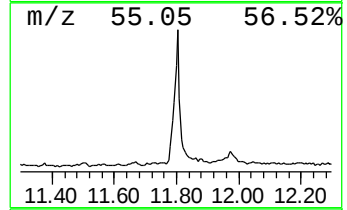
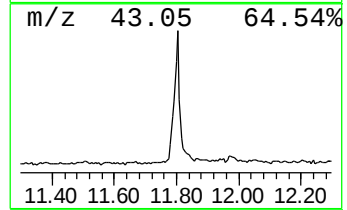
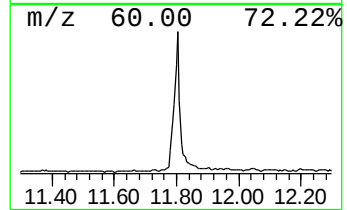
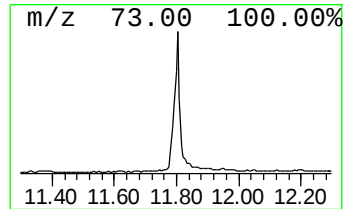
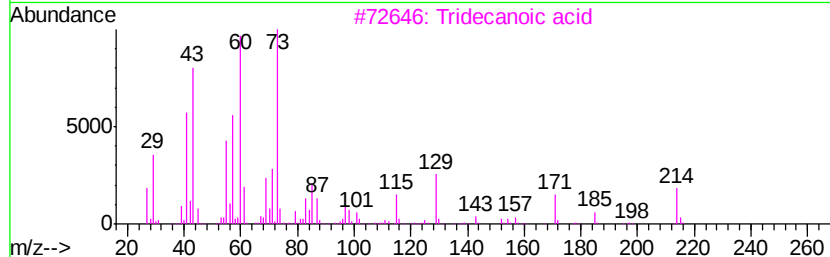
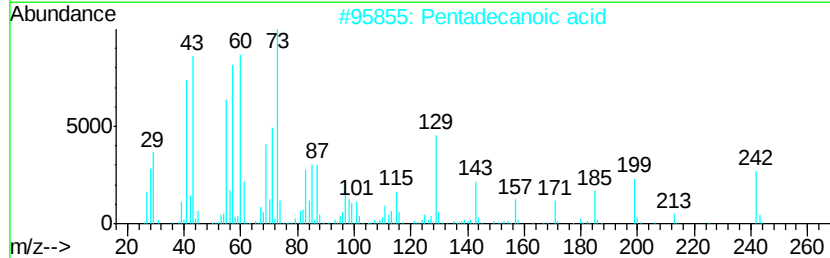
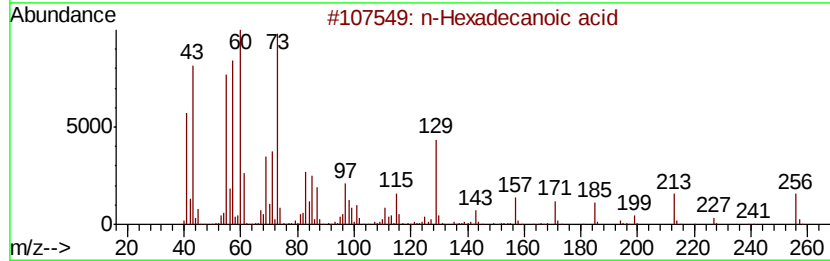
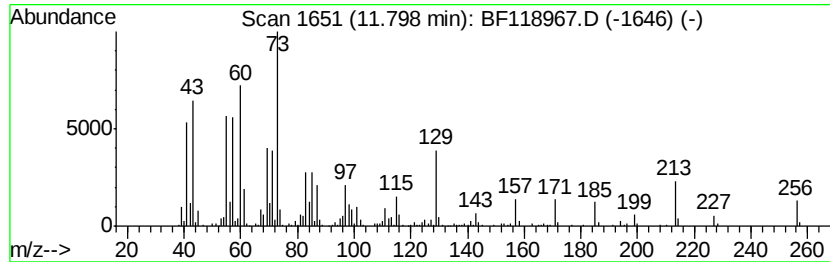
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	11.61 ng	975008	Phenanthrene-d10	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		Tridecanoic acid	214	C13H26O2	000638-53-9	55
4		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	25
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	25



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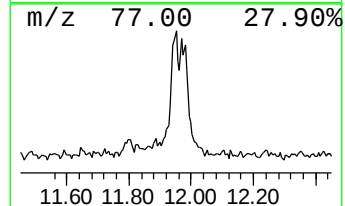
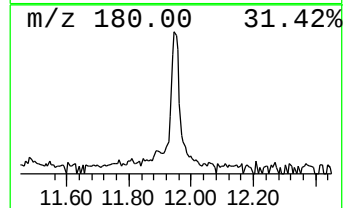
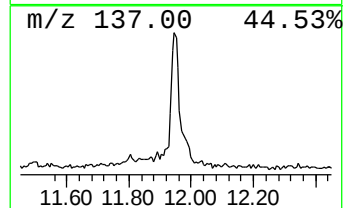
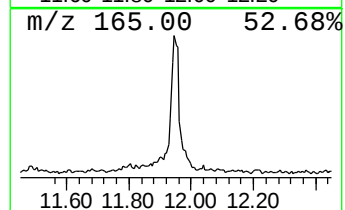
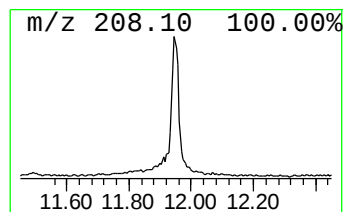
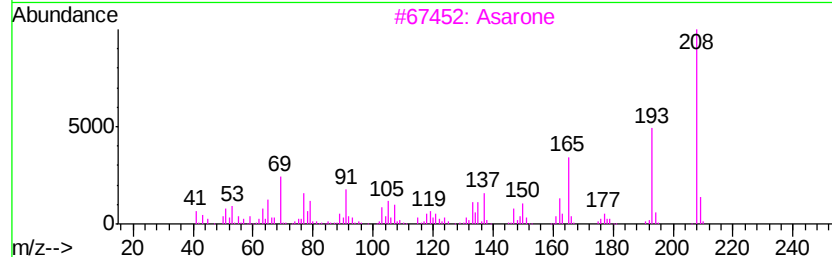
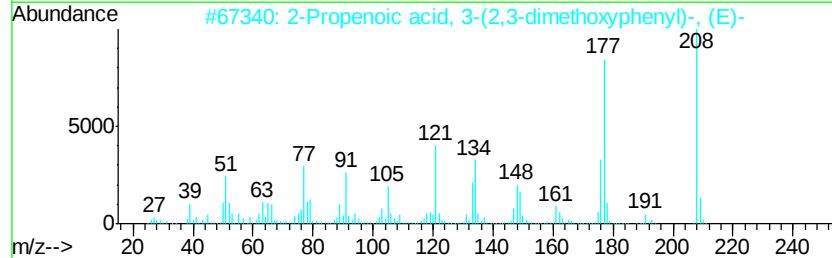
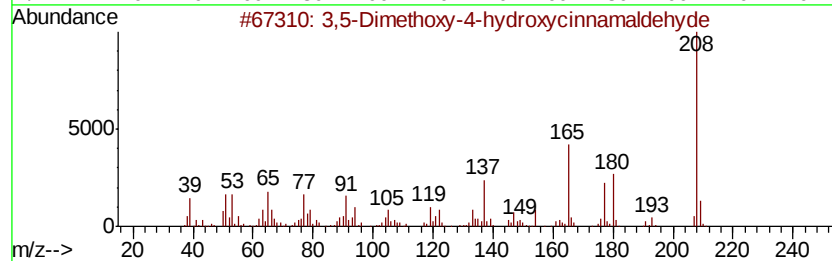
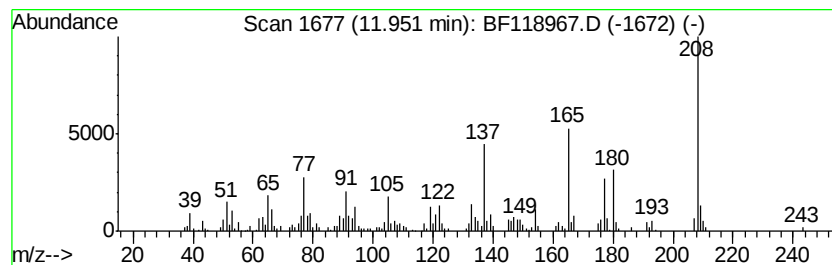
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.95	2.96 ng	248459	Phenanthrene-d10	11.27		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamaldehyde	208	C11H12O4	087345-53-7	93	
2	2-Propenoic acid, 3-(2,3-dimethoxyphenyl)-, (E)-	208	C11H12O4	007345-82-6	46	
3	Asarone	208	C12H16O3	002883-98-9	46	
4	3,4-Dimethoxycinnamic acid	208	C11H12O4	002316-26-9	42	
5	trans-2,5-Dimethoxycinnamic acid	208	C11H12O4	038489-74-6	41	



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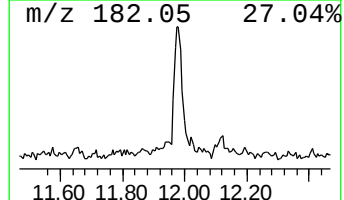
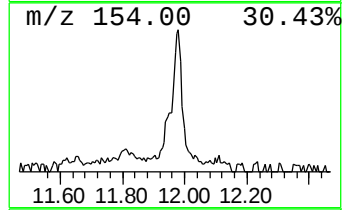
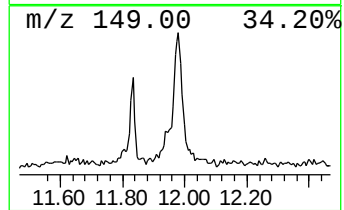
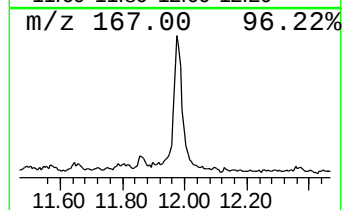
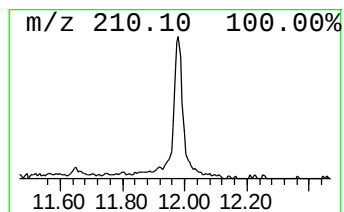
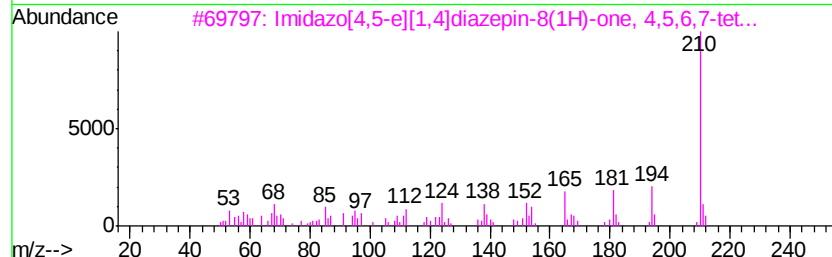
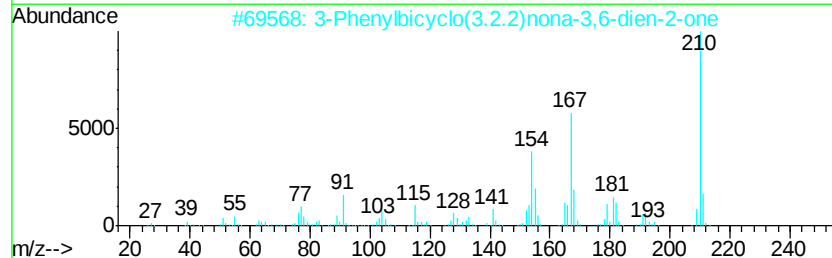
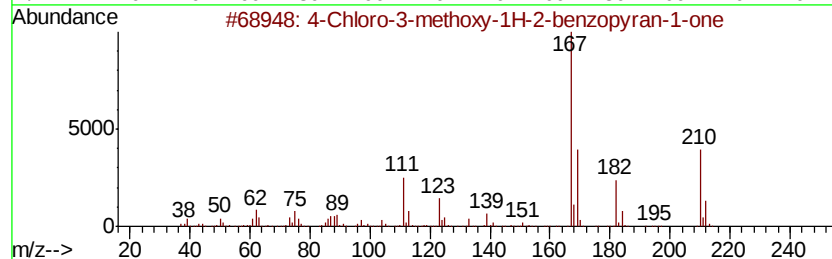
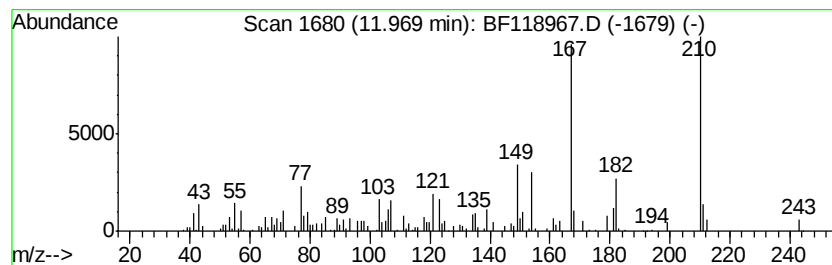
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Chloro-3-methoxy-1H-2-ben... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.97	3.42 ng	287426	Phenanthrene-d10	11.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-3-methoxy-1H-2-benzopyr...	210	C10H7ClO3	024672-89-7	59
2	3-Phenylbicyclo(3.2.2)nona-3,6-d...	210	C15H14O	073830-83-8	50
3	Imidazo[4,5-e][1,4]diazepin-8(1H...	210	C8H10N4OS	1000142-41-3	35
4	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	35
5	6-Methoxy-4-piperidin-1-yl-1H-[1...	210	C9H14N4O2	1000300-24-3	30



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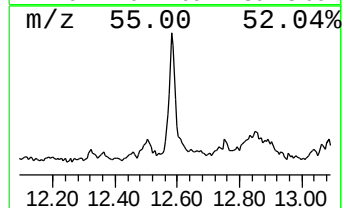
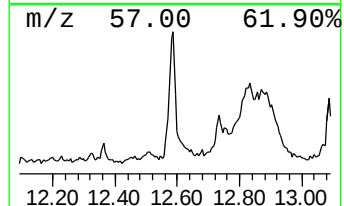
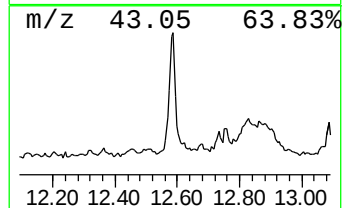
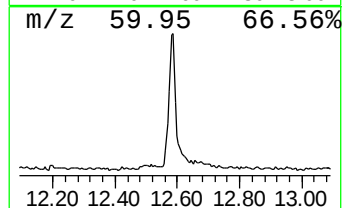
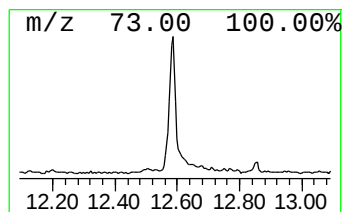
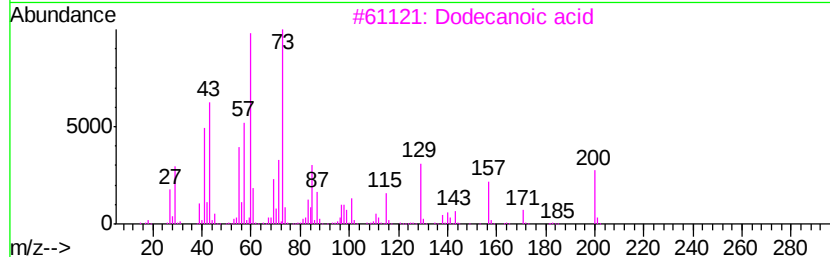
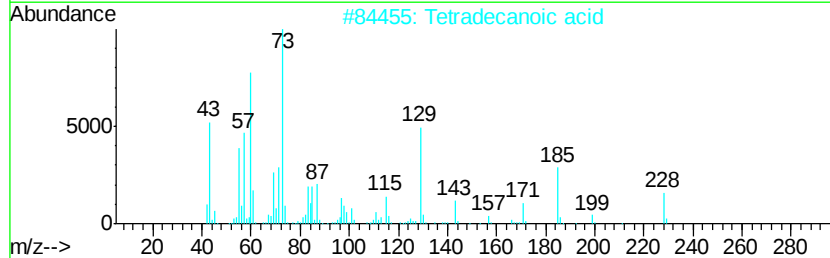
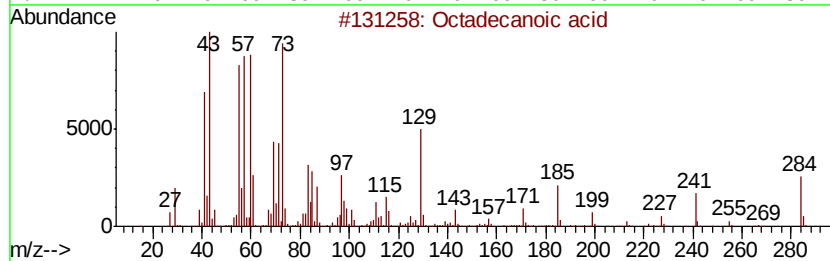
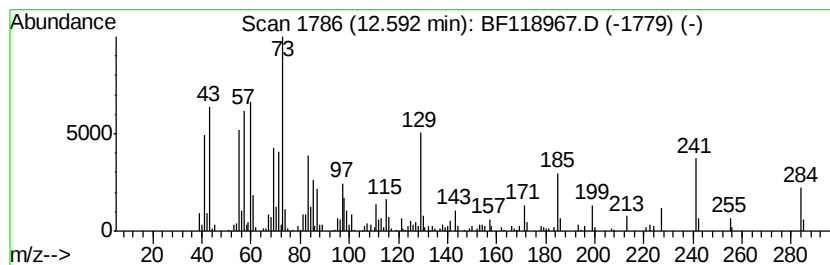
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.59	6.91 ng	490621	Chrysene-d12	13.90	
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	62
3	Dodecanoic acid	200	C12H24O2	000143-07-7	62
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



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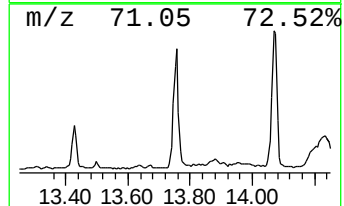
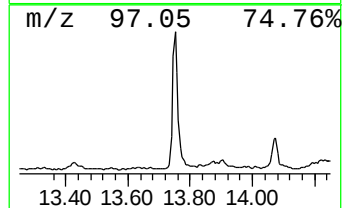
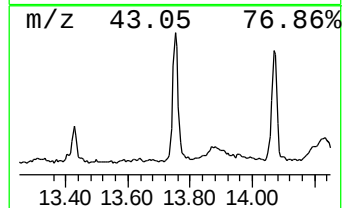
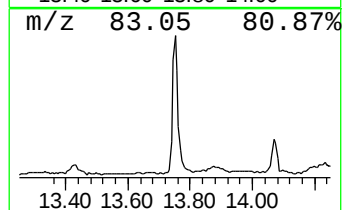
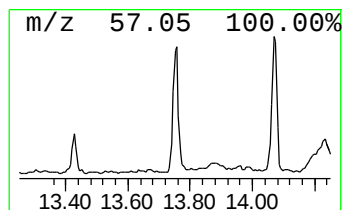
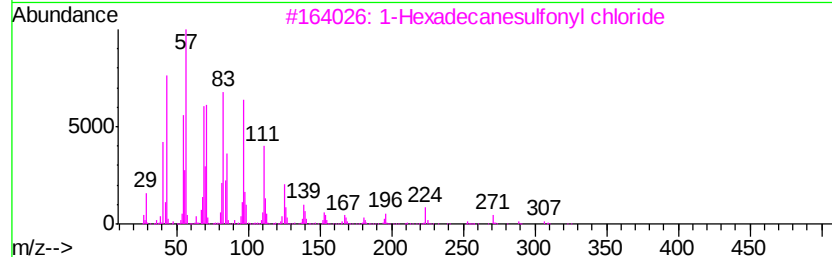
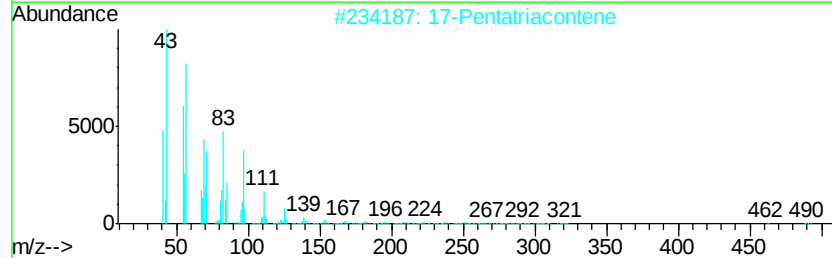
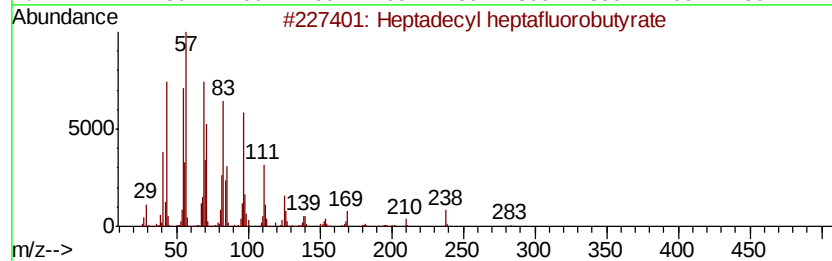
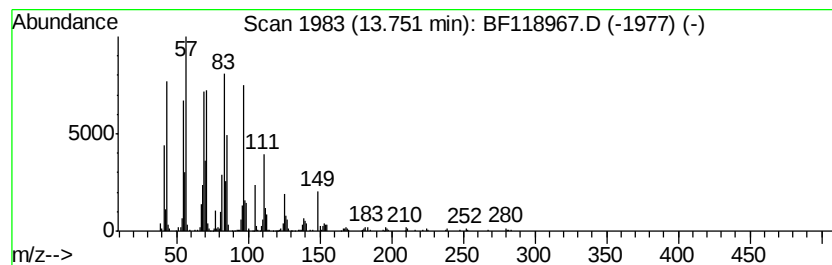
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.75	12.26 ng	870255	Chrysene-d12	13.90		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2		17-Pentatriacontene	491	C35H70	006971-40-0	90
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
4		1-Octadecene	252	C18H36	000112-88-9	90
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118967.D
Acq On : 20 Feb 2020 19:13
Operator : CG/JU
Sample : L1592-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-BPM-04-005-ABCD

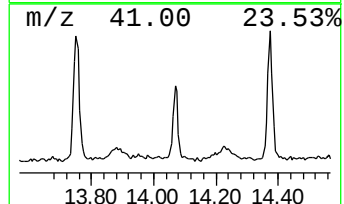
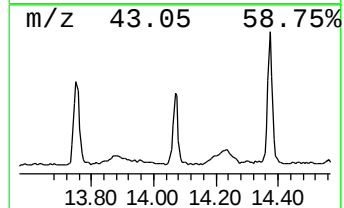
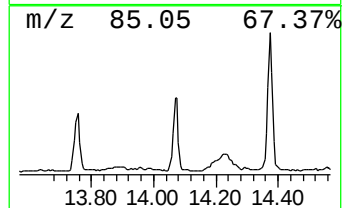
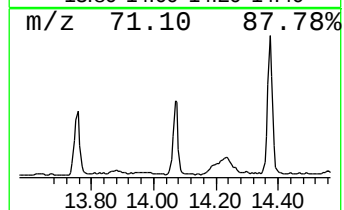
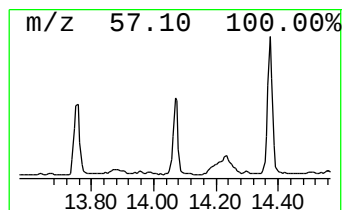
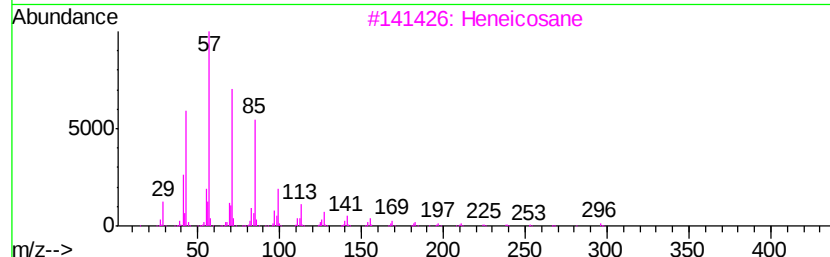
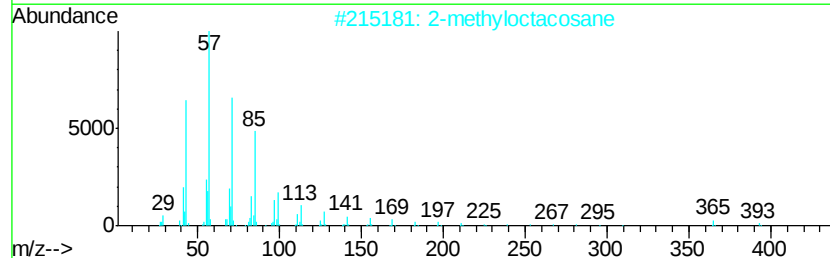
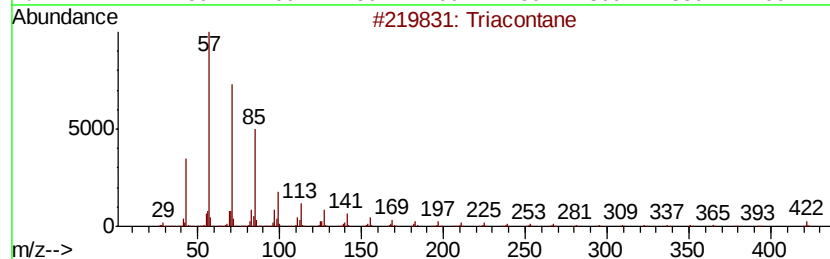
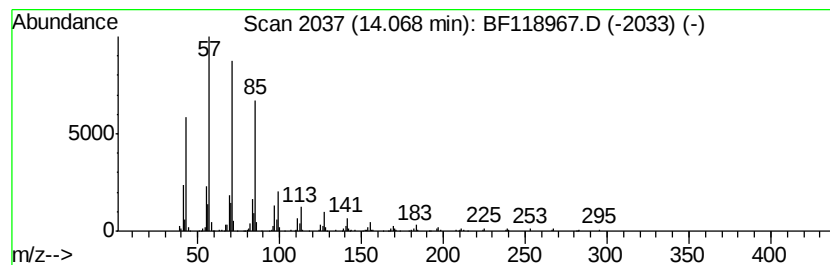
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	6.04 ng	428669	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118967.D
Acq On : 20 Feb 2020 19:13
Operator : CG/JU
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ClientSampleId :
FK-BPM-04-005-ABCD

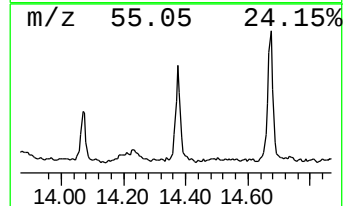
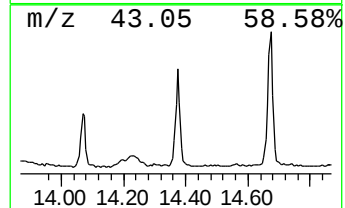
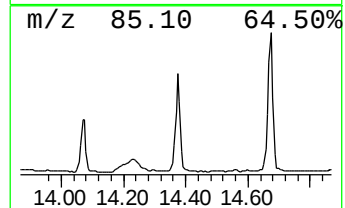
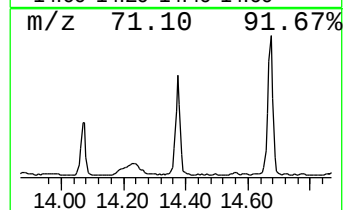
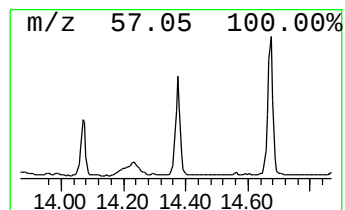
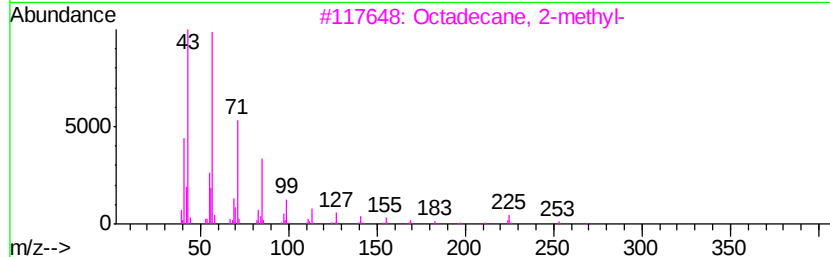
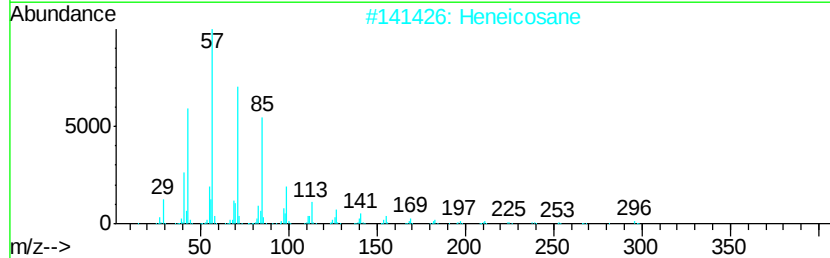
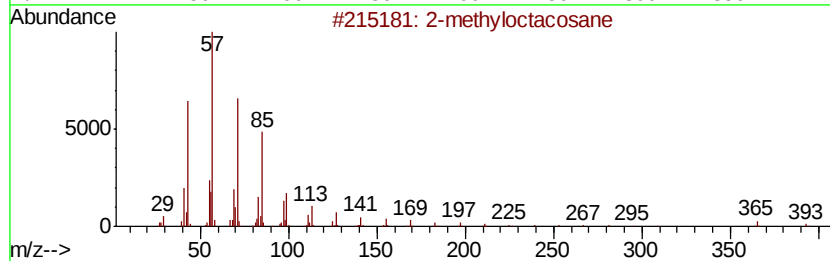
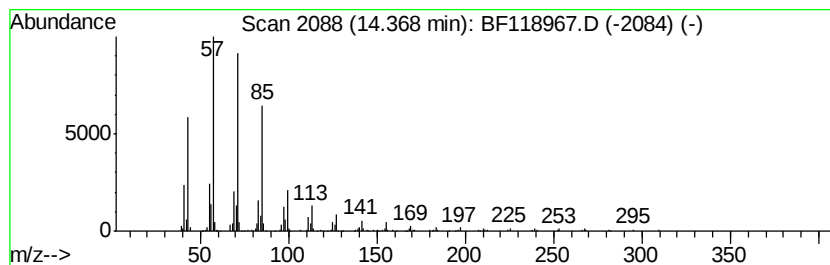
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	10.01 ng	710094	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octadecane, 2-methyl-		268	C19H40	001560-88-9	91
4	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	91
5	Eicosane		282	C20H42	000112-95-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118967.D
Acq On : 20 Feb 2020 19:13
Operator : CG/JU
Sample : L1592-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-BPM-04-005-ABCD

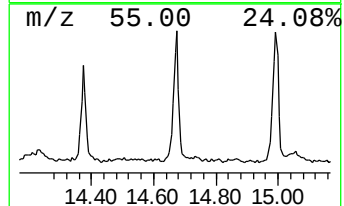
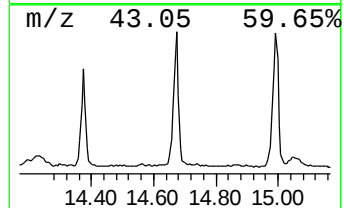
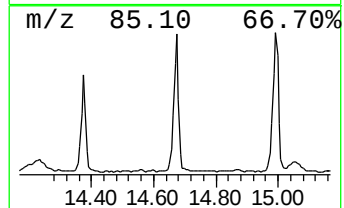
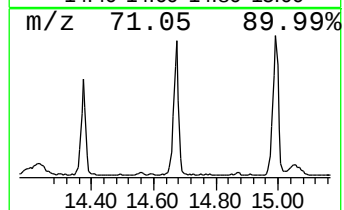
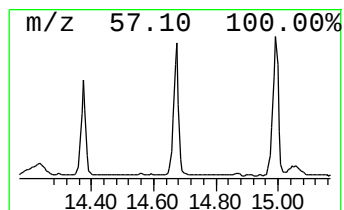
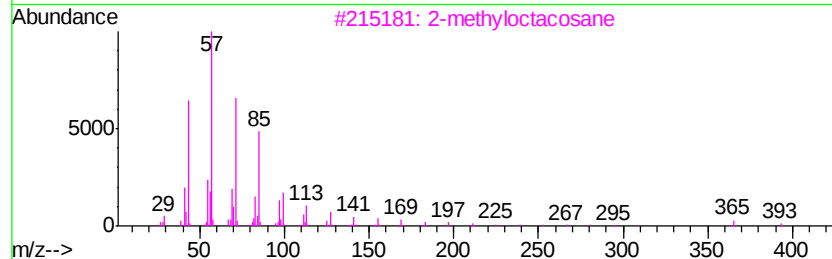
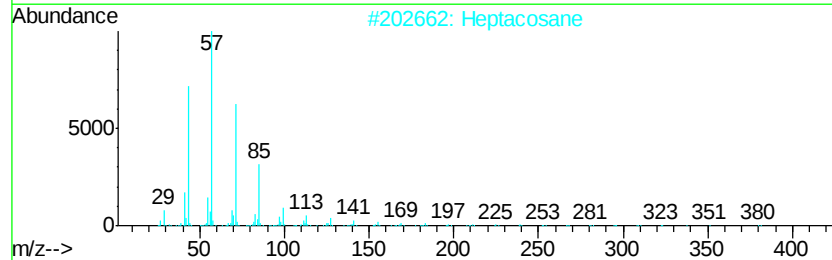
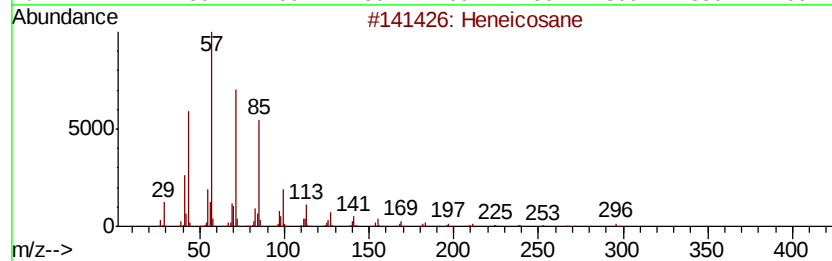
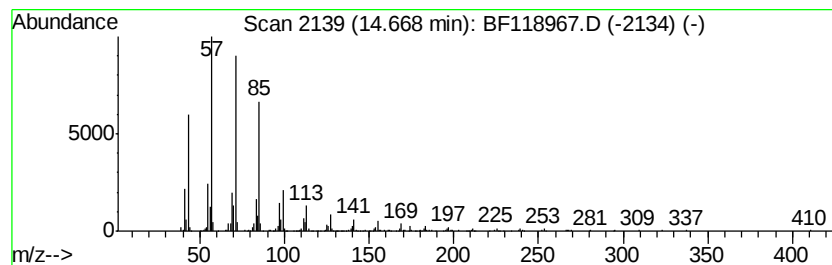
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	16.76 ng	1089870	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptacosane		380	C27H56	000593-49-7	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	triacontane		422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118967.D
Acq On : 20 Feb 2020 19:13
Operator : CG/JU
Sample : L1592-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

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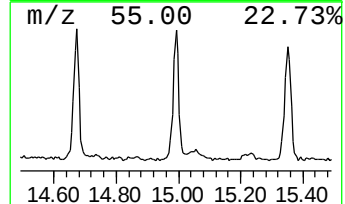
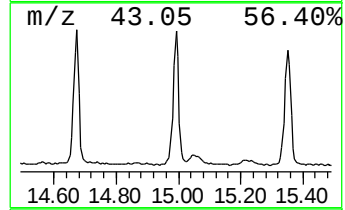
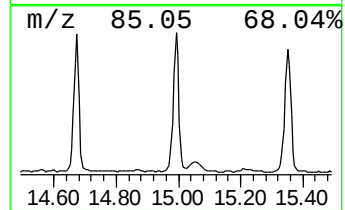
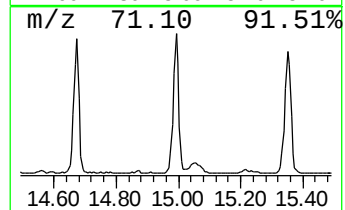
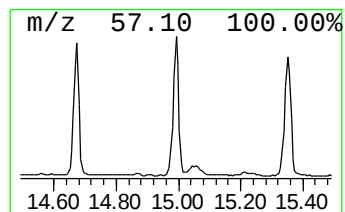
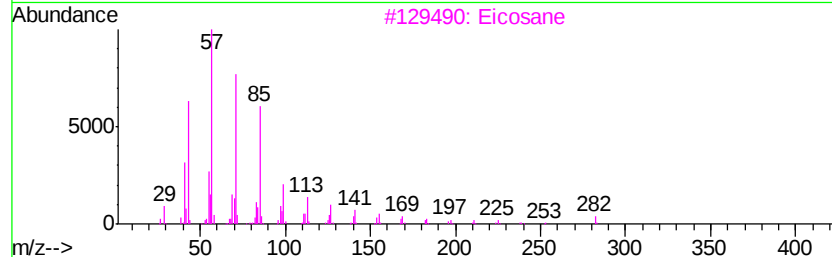
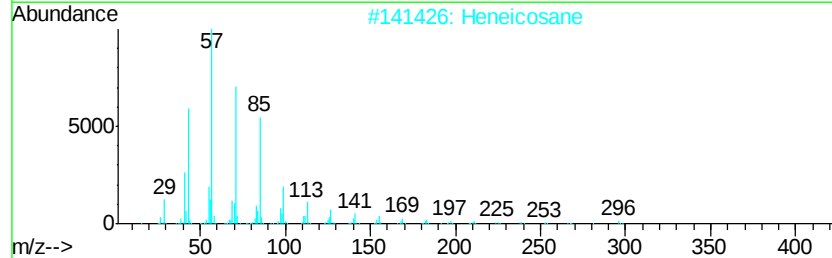
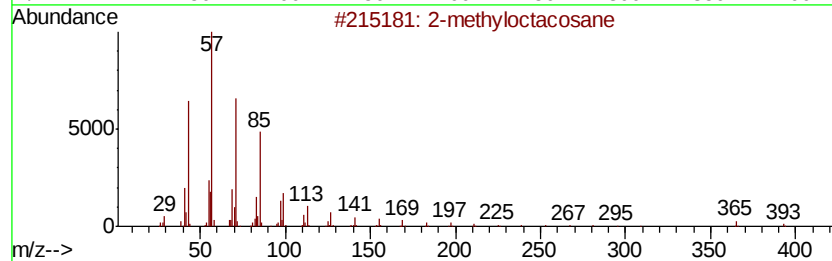
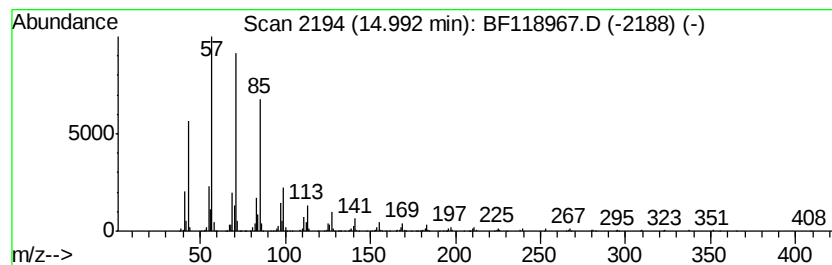
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	17.41 ng	1132340	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Eicosane	282	C20H42	000112-95-8	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118967.D
Acq On : 20 Feb 2020 19:13
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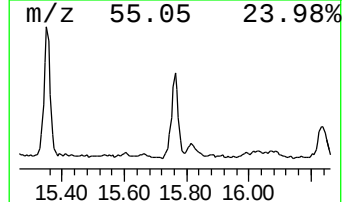
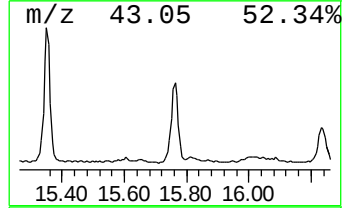
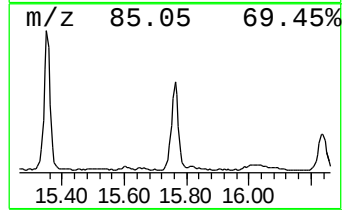
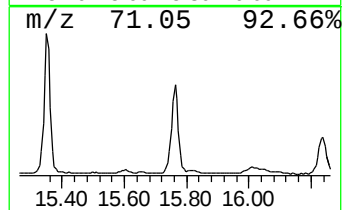
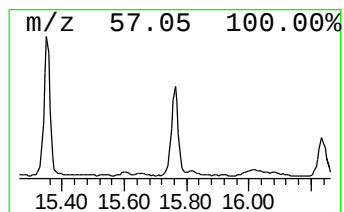
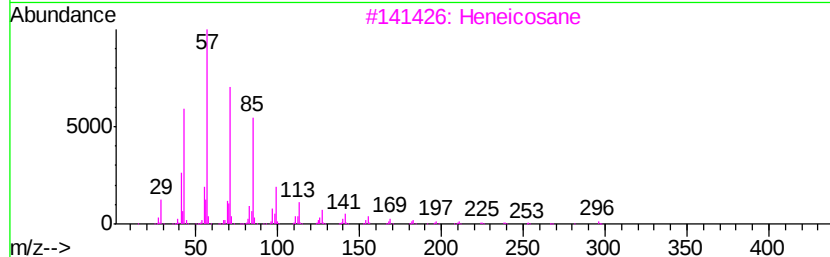
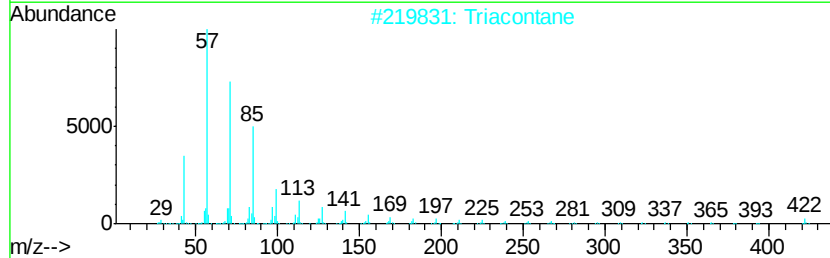
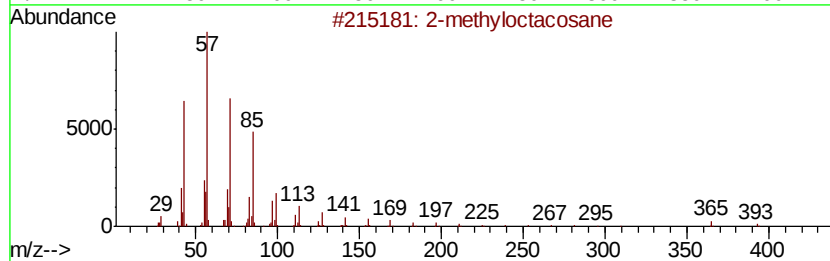
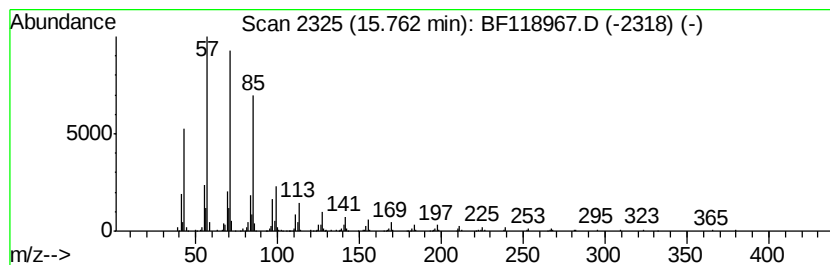
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	12.18 ng	791902	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118967.D
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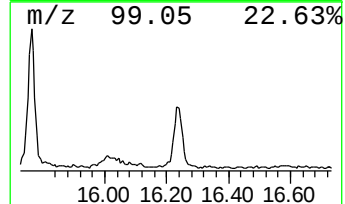
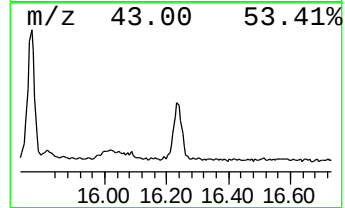
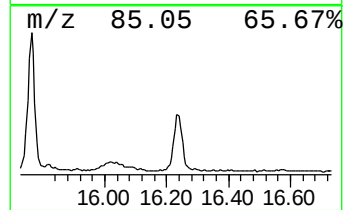
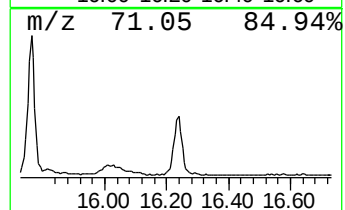
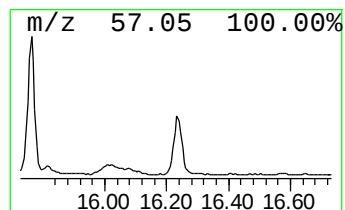
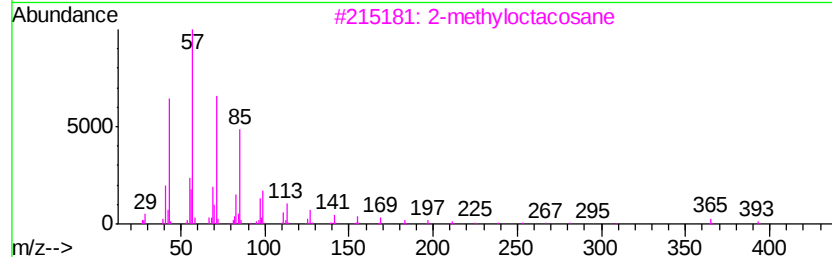
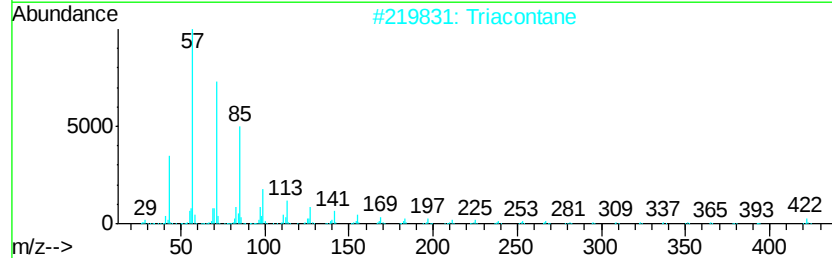
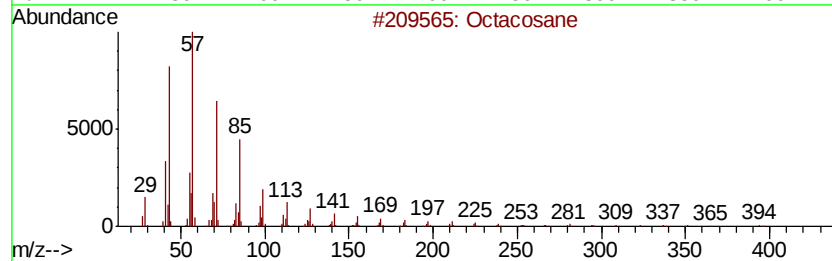
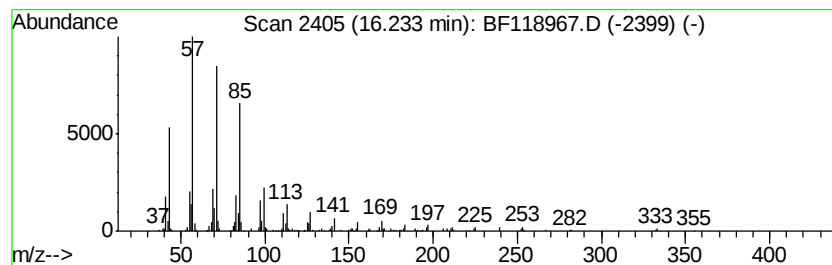
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	6.43 ng	418080	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Triacontane	422	C30H62	000638-68-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022020\
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 Sample : L1592-01
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 ClientSampleId :
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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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3,5-Dimethoxy-4-h...	11.95	3.0 ng		248459	4	11.27	1679980	20.0
4-Chloro-3-methox...	11.97	3.4 ng		287426	4	11.27	1679980	20.0
Octadecanoic acid	12.59	6.9 ng		490621	5	13.90	1419130	20.0
Heptadecyl hepta...	13.75	12.3 ng		870255	5	13.90	1419130	20.0
Triacontane	14.07	6.0 ng		428669	5	13.90	1419130	20.0
2-methyloctacosane	14.37	10.0 ng		710094	5	13.90	1419130	20.0
Heneicosane	14.67	16.8 ng		1089870	6	15.33	1300610	20.0
Eicosane	14.99	17.4 ng		1132340	6	15.33	1300610	20.0
Tetracosane	15.76	12.2 ng		791902	6	15.33	1300610	20.0
Octacosane	16.23	6.4 ng		418080	6	15.33	1300610	20.0