

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021419\
 Data File : BF112564.D
 Acq On : 14 Feb 2019 13:37
 Operator : JU/SJ
 Sample : K1458-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6

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

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

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	500	503	515	rBV	53028	79795	3.61%	0.366%
2	5.463	571	574	596	rBV	1452388	1683870	76.17%	7.718%
3	6.481	743	747	763	rBV	1696393	1812291	81.98%	8.306%
4	6.604	765	768	786	rVB	2172202	1973030	89.25%	9.043%
5	6.828	803	806	815	rBV	619866	539340	24.40%	2.472%
6	6.987	829	833	848	rBV	1664248	1501692	67.93%	6.883%
7	7.392	898	902	915	rBV	1227895	1148974	51.97%	5.266%
8	8.110	1021	1024	1037	rBV	736716	693512	31.37%	3.179%
9	9.186	1202	1207	1216	rBV	2339469	2210658	100.00%	10.132%
10	9.581	1269	1274	1279	rBV	139484	144353	6.53%	0.662%
11	9.869	1319	1323	1331	rVB	792804	793248	35.88%	3.636%
12	10.663	1454	1458	1470	rBV	1337691	1370676	62.00%	6.282%
13	11.357	1572	1576	1588	rBV	811797	764935	34.60%	3.506%
14	11.875	1660	1664	1672	rBV	392733	445285	20.14%	2.041%
15	12.580	1779	1784	1787	rBV6	33297	59279	2.68%	0.272%
16	12.657	1794	1797	1802	rBV	267533	300465	13.59%	1.377%
17	12.933	1840	1844	1848	rBV	1945342	1772031	80.16%	8.122%
18	13.498	1937	1940	1946	rVB5	40937	52543	2.38%	0.241%
19	13.745	1979	1982	1987	rBV6	21333	32066	1.45%	0.147%
20	13.821	1992	1995	2004	rVV	357393	436713	19.75%	2.002%
21	13.892	2004	2007	2010	rVB	113321	98656	4.46%	0.452%
22	13.957	2016	2018	2022	rVB	31212	28708	1.30%	0.132%
23	14.004	2022	2026	2033	rBV	731691	682491	30.87%	3.128%
24	14.139	2046	2049	2053	rBV	86496	106447	4.82%	0.488%
25	14.445	2098	2101	2108	rBV2	180460	310374	14.04%	1.423%
26	14.751	2149	2153	2156	rVB	199241	208418	9.43%	0.955%
27	14.892	2175	2177	2180	rVB2	51320	40026	1.81%	0.183%
28	15.080	2205	2209	2213	rBV	362864	390423	17.66%	1.789%
29	15.116	2213	2215	2220	rVB3	70493	82667	3.74%	0.379%
30	15.457	2269	2273	2274	rBV	317840	377807	17.09%	1.732%
31	15.480	2274	2277	2282	rVB	486493	624646	28.26%	2.863%
32	15.880	2341	2345	2351	rVB	312450	475421	21.51%	2.179%
33	15.951	2353	2357	2363	rVV6	54152	104754	4.74%	0.480%
34	16.380	2425	2430	2436	rBV	170030	297791	13.47%	1.365%

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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 >
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35	16.957	2525	2528	2537	rVB	95923	174808	7.91%	0.801%
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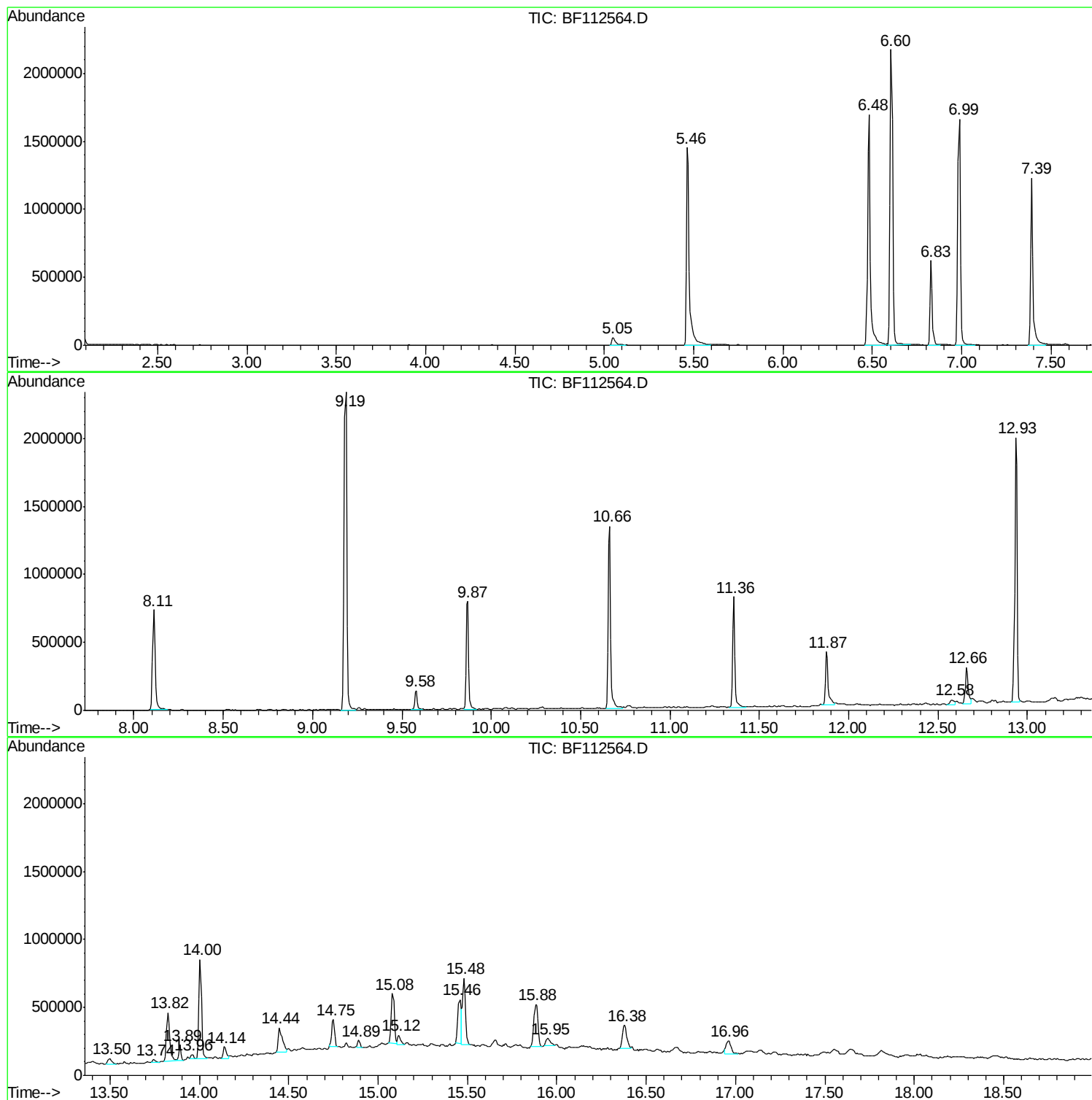
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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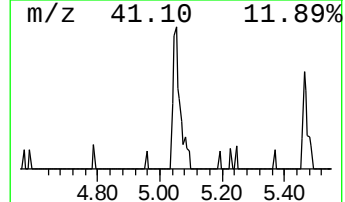
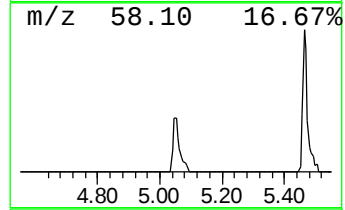
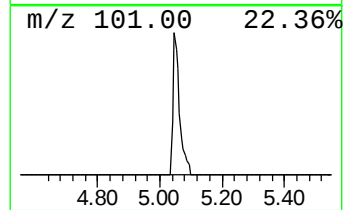
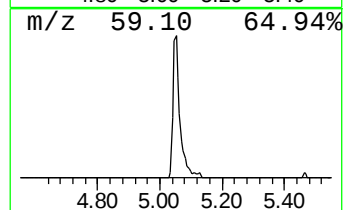
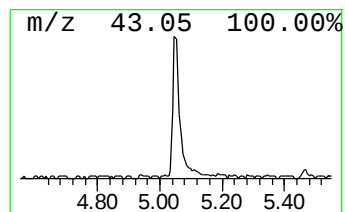
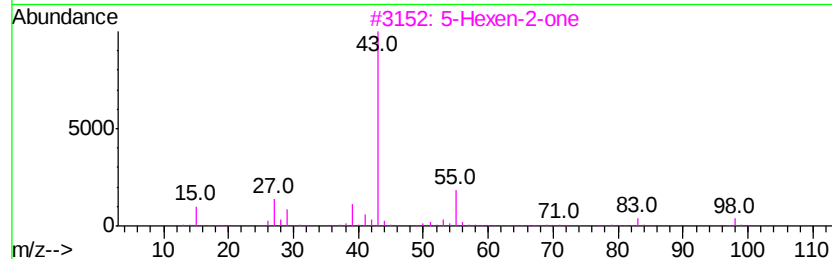
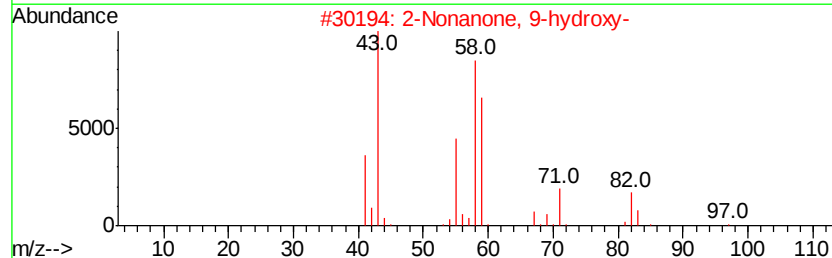
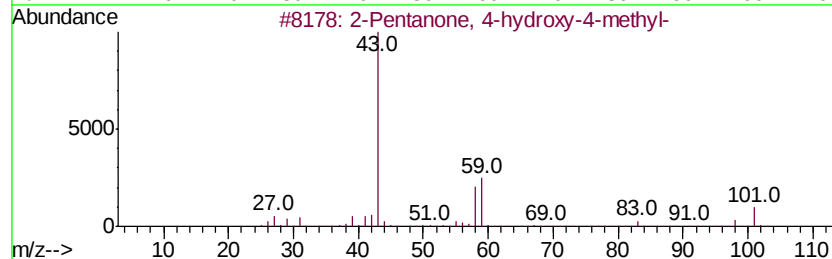
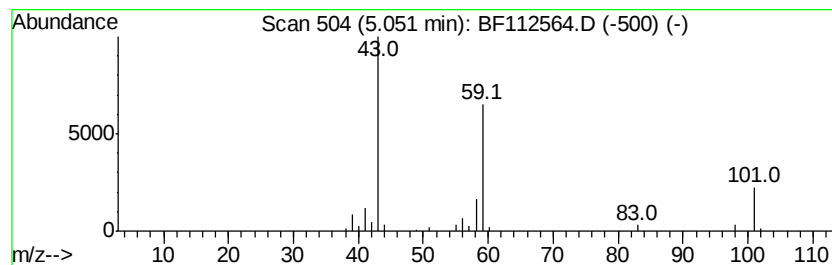
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.96 ng	79795	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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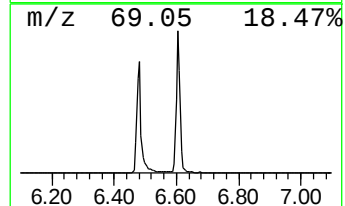
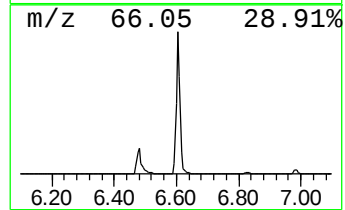
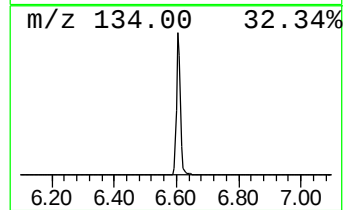
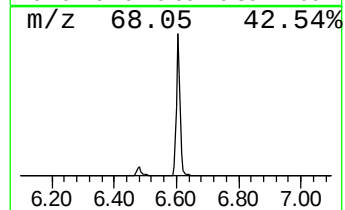
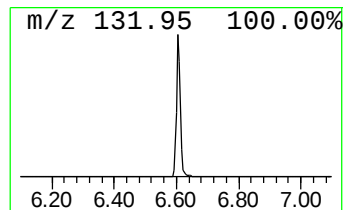
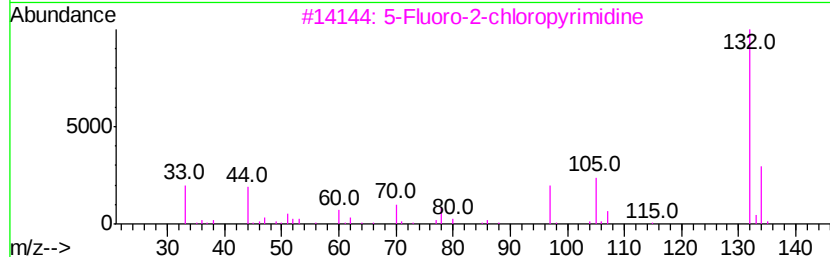
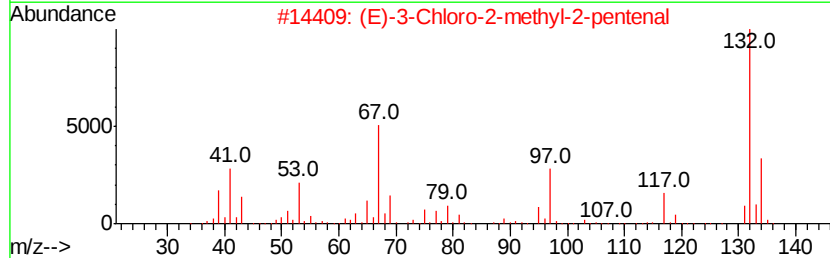
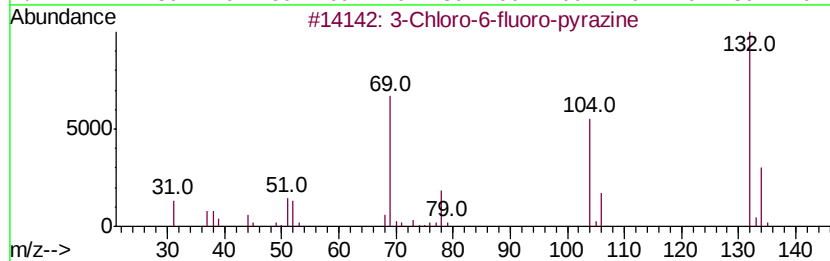
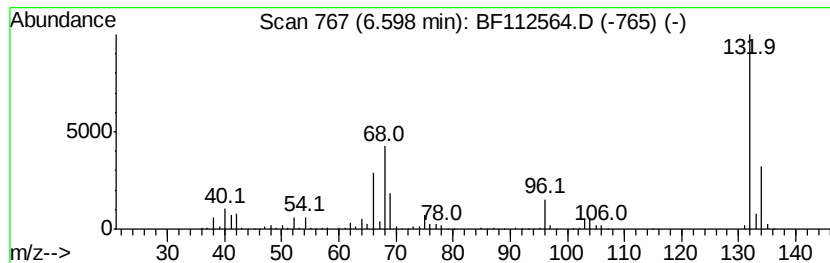
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	73.16 ng	1973030	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16	
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
4	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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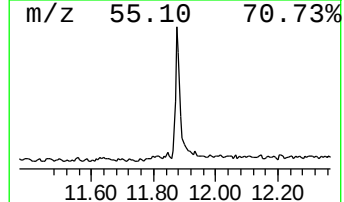
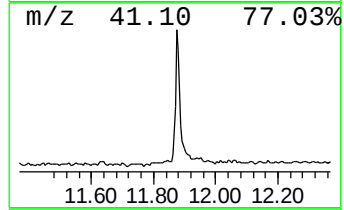
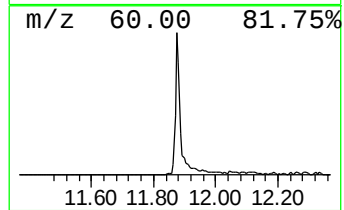
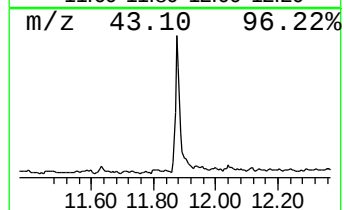
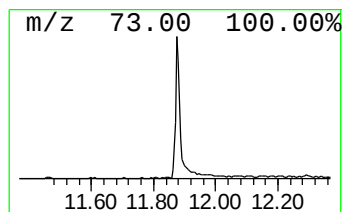
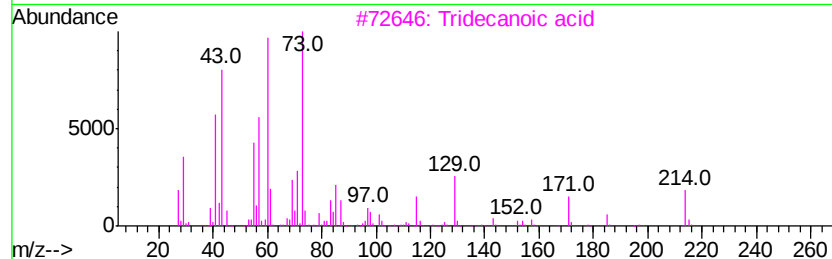
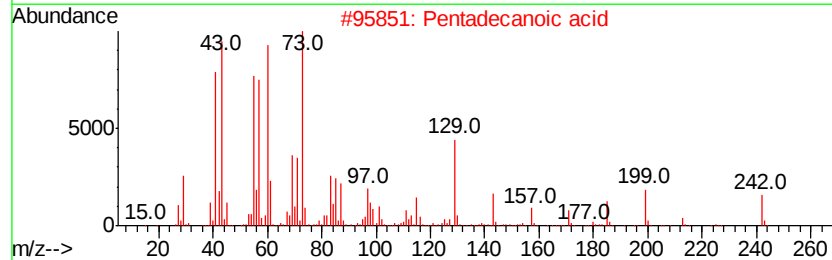
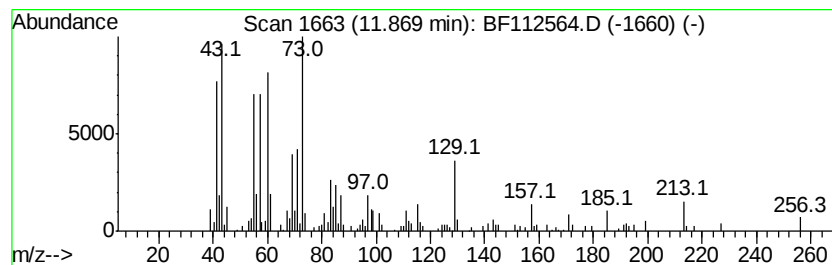
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	11.64 ng	445285	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



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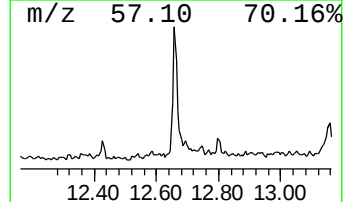
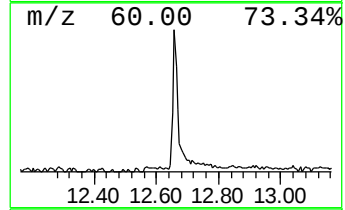
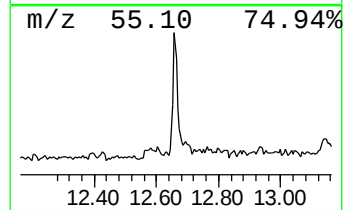
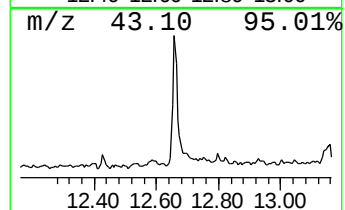
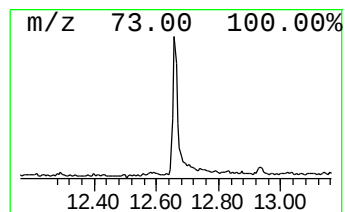
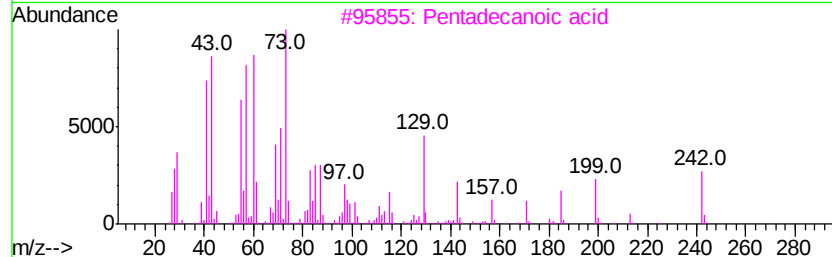
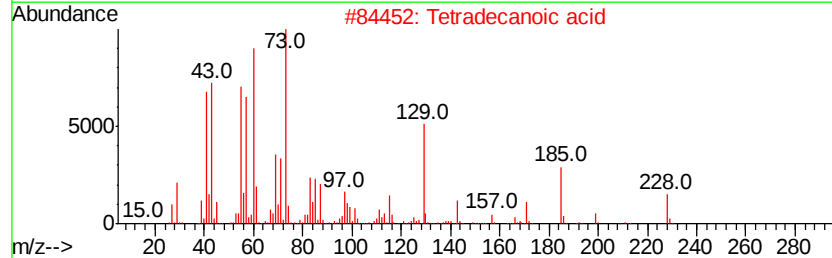
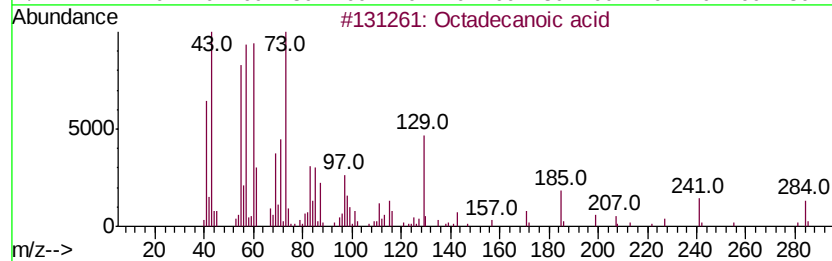
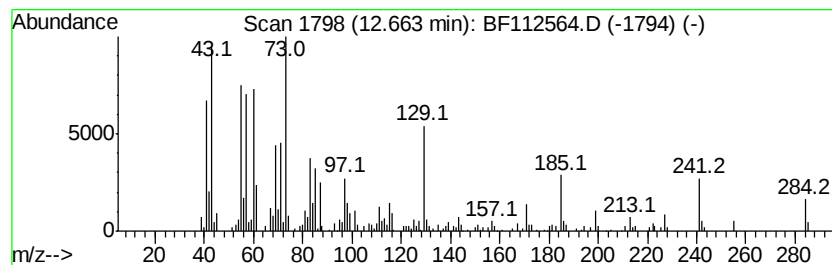
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	7.86 ng	300465	Phenanthrene-d10	11.36

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	72



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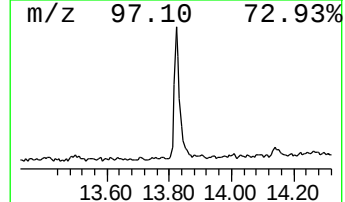
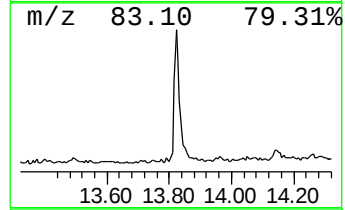
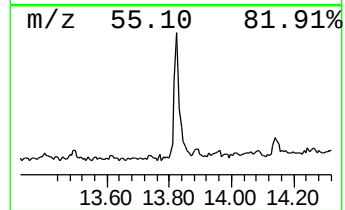
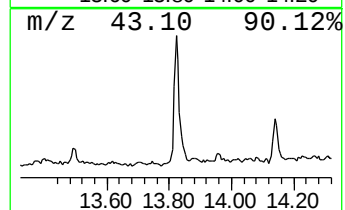
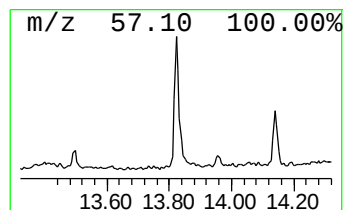
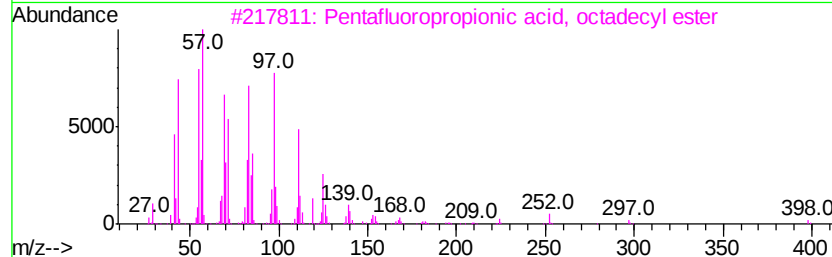
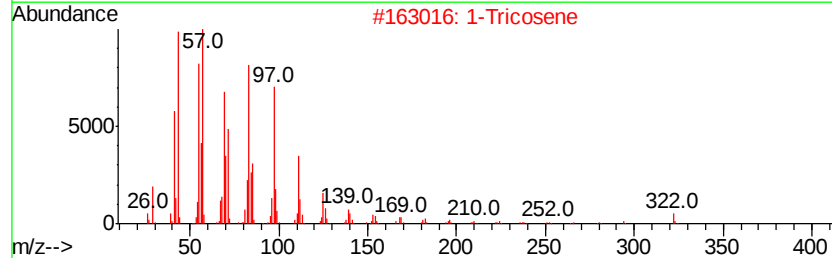
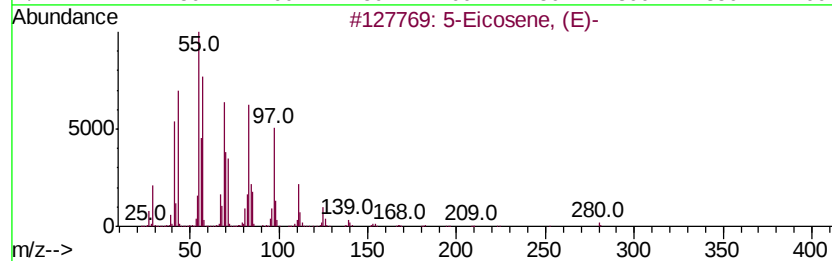
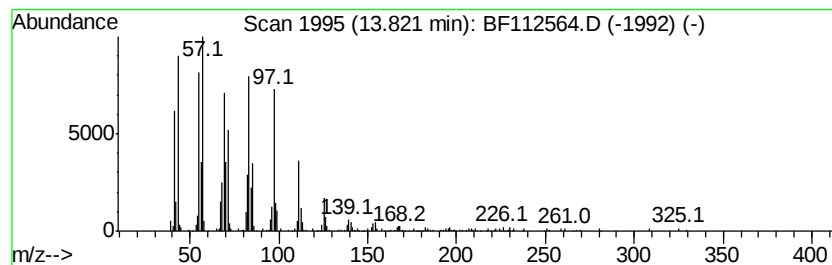
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Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	12.80 ng	436713	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2		1-Tricosene	322	C23H46	018835-32-0	94
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	94
4		1-Docosene	308	C22H44	001599-67-3	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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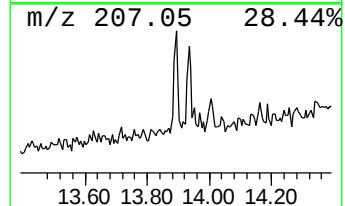
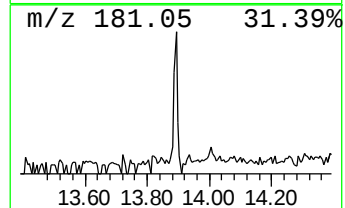
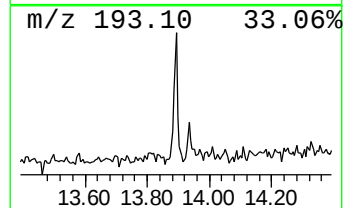
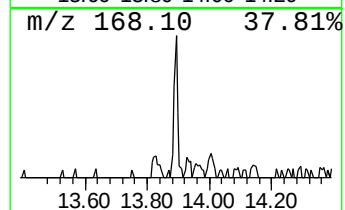
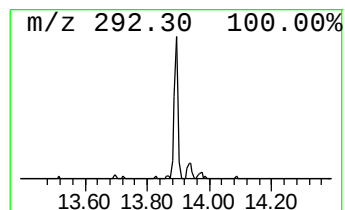
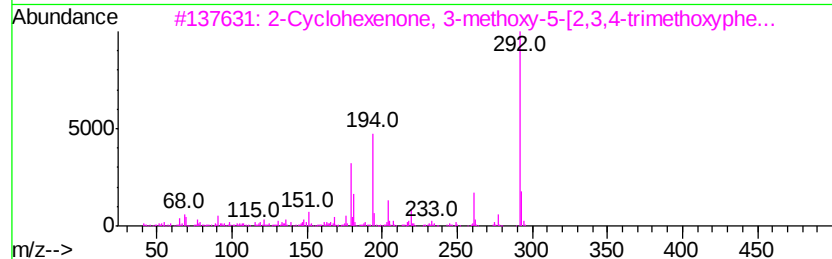
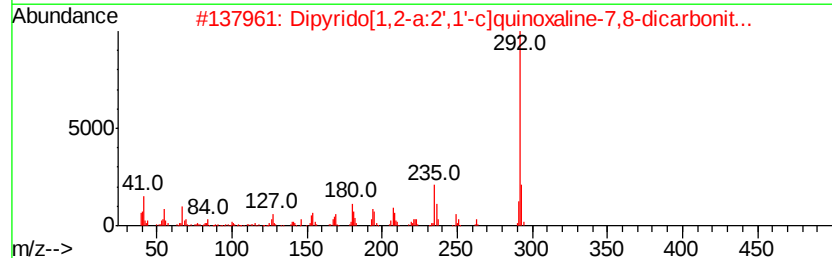
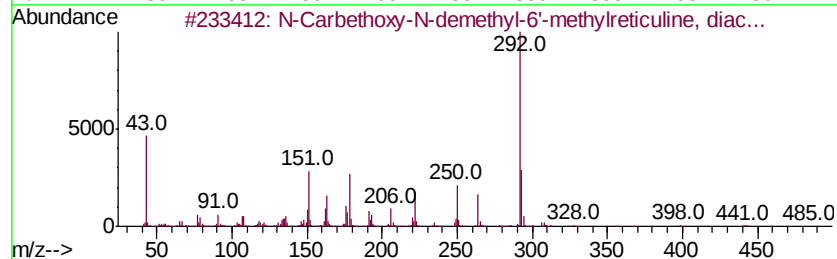
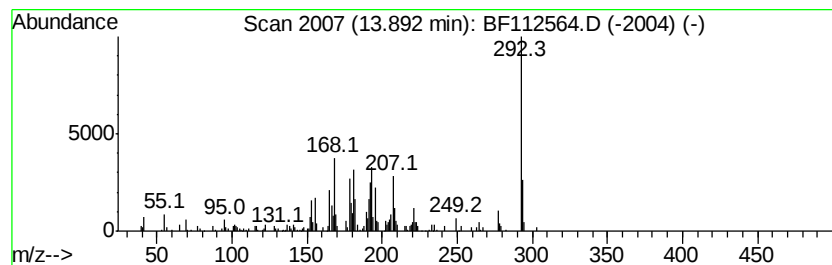
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.89 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.89 ng	98656	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-Carboethoxy-N-demethyl-6'-methy...	485	C26H31N08	1000127-80-3	38
2		Dipyrido[1,2-a:2',1'-c]quinoxali...	292	C18H20N4	1000303-96-3	38
3		2-Cyclohexenone, 3-methoxy-5-[2,...	292	C16H20O5	119101-25-6	32
4		1,4-Naphthoquinone, 2-acetyl-3,5...	292	C14H12O7	014090-52-9	32
5		1,3-Cyclohexanedione, 2,2'-methy...	292	C17H24O4	002181-22-8	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
Data File : BF112564.D
Acq On : 14 Feb 2019 13:37
Operator : JU/SJ
Sample : K1458-09
Misc :
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Instrument :
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ClientSampleId :
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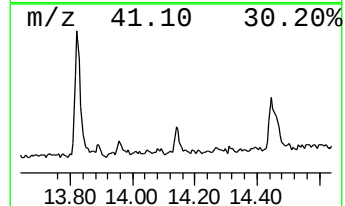
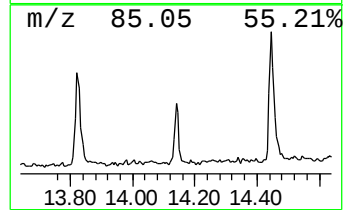
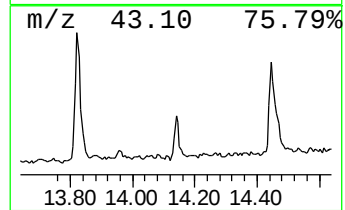
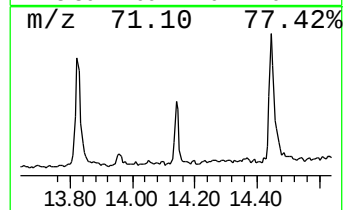
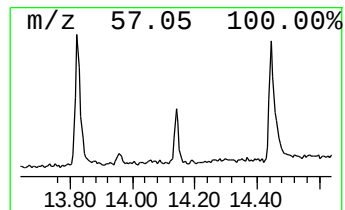
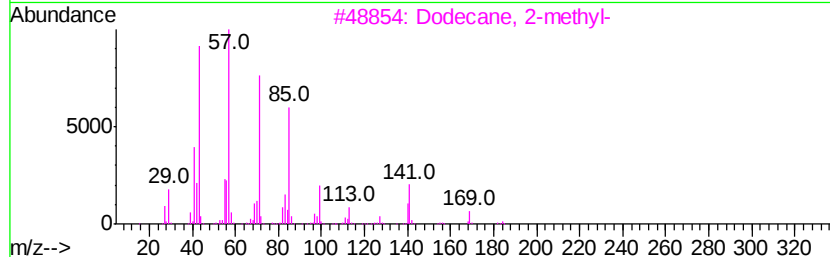
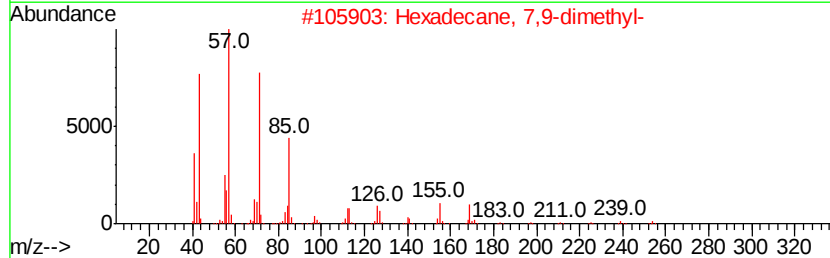
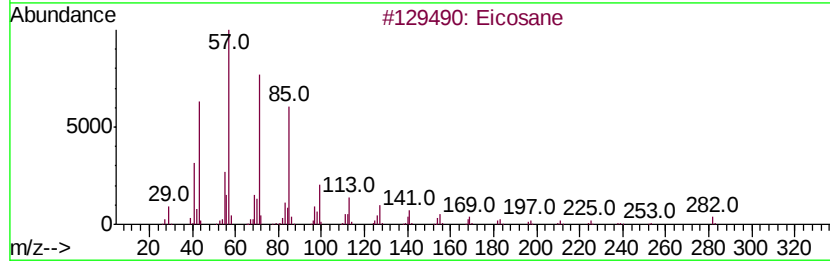
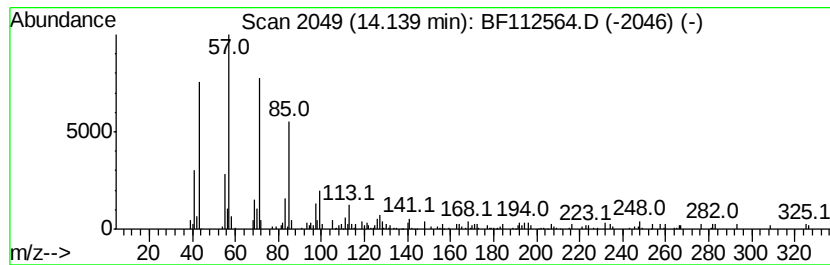
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	3.12 ng	106447	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	93
2	Hexadecane, 7,9-dimethyl-		254	C18H38	021164-95-4	90
3	Dodecane, 2-methyl-		184	C13H28	001560-97-0	90
4	Heneicosane		296	C21H44	000629-94-7	87
5	Heptacosane		380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
Data File : BF112564.D
Acq On : 14 Feb 2019 13:37
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Sample : K1458-09
Misc :
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Instrument :
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ClientSampleId :
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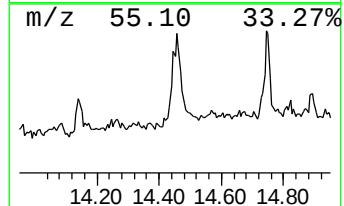
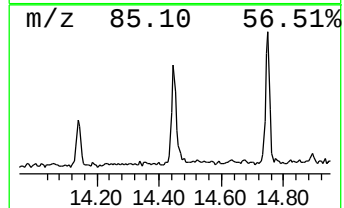
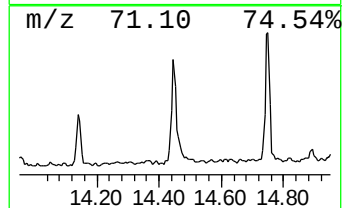
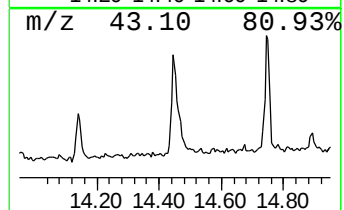
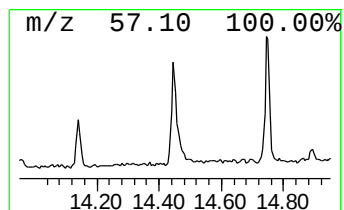
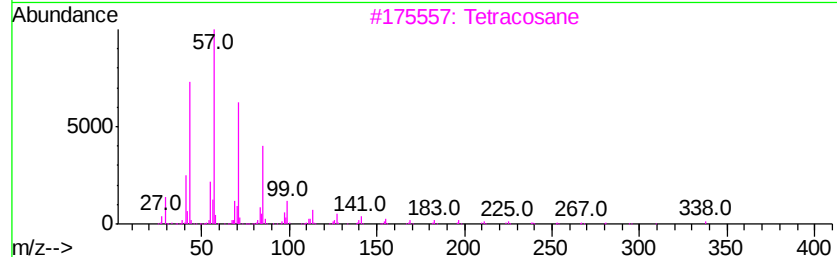
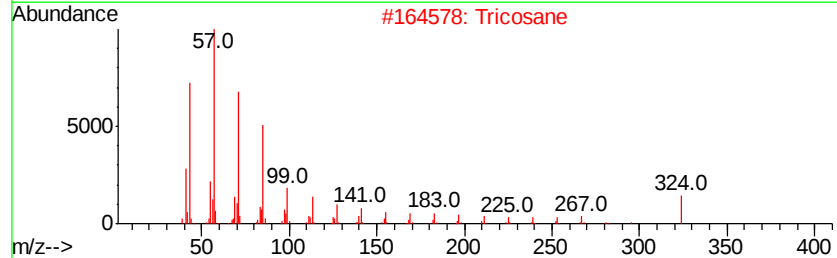
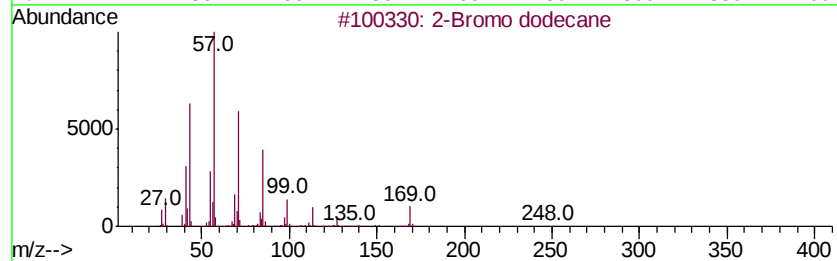
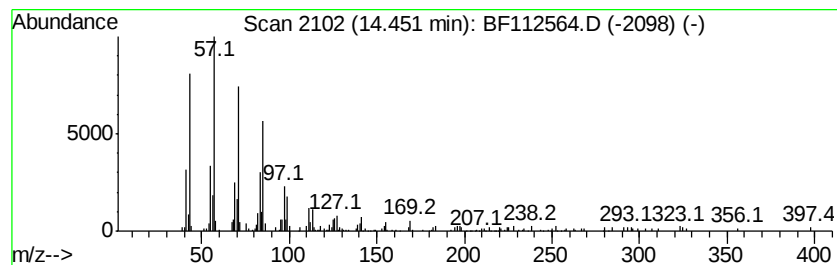
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Bromo dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	9.10 ng	310374	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2		Tricosane	324	C23H48	000638-67-5	91
3		Tetracosane	338	C24H50	000646-31-1	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
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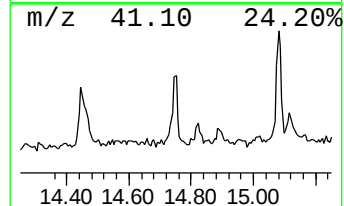
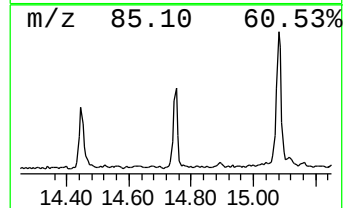
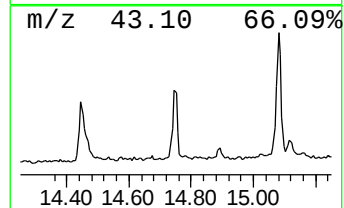
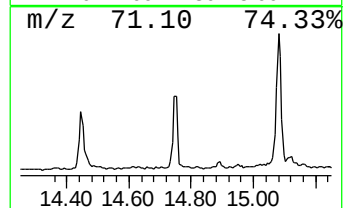
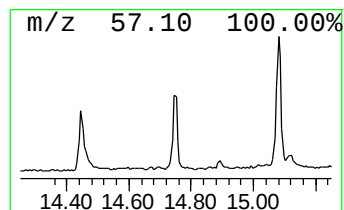
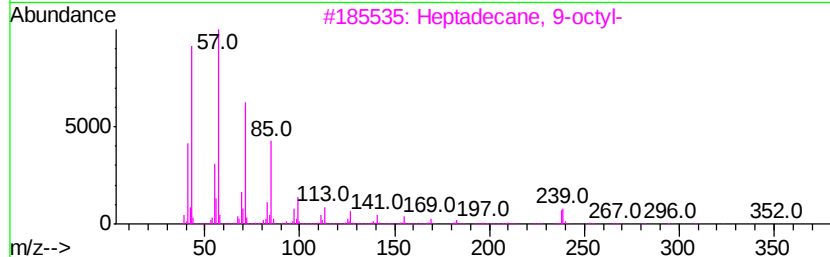
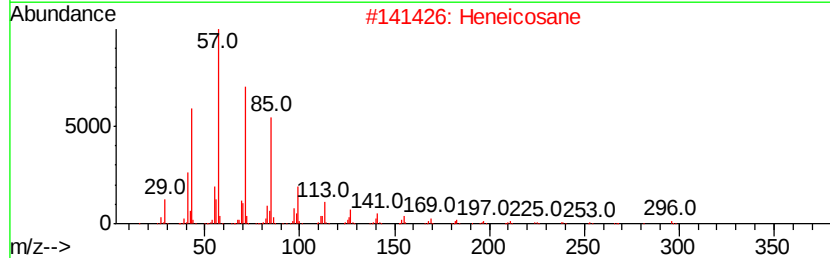
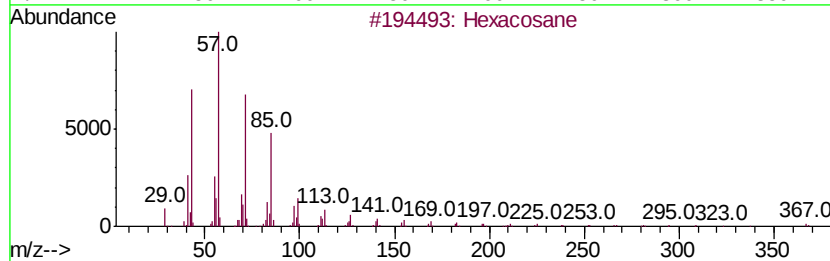
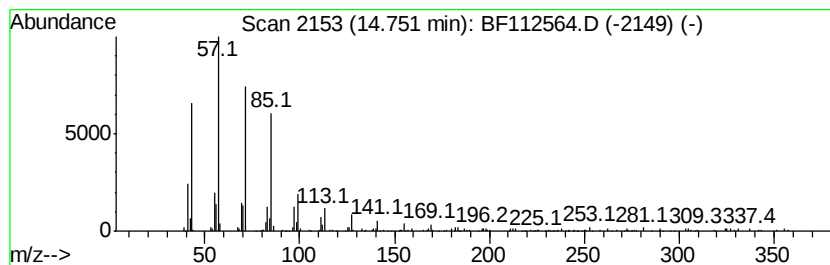
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	6.67 ng	208418	Perylene-d12	15.48

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		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
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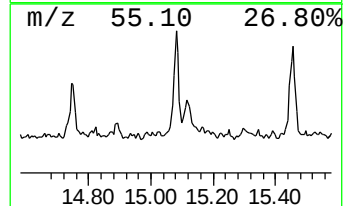
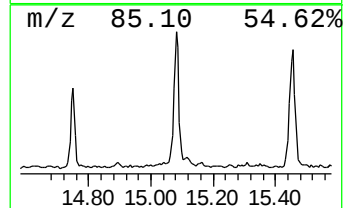
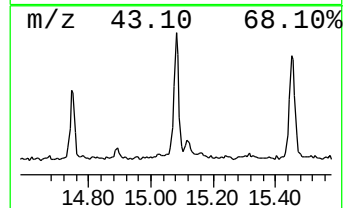
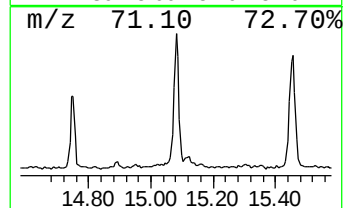
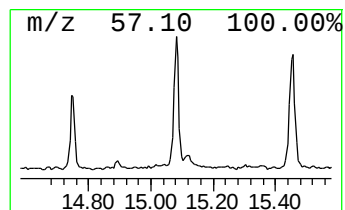
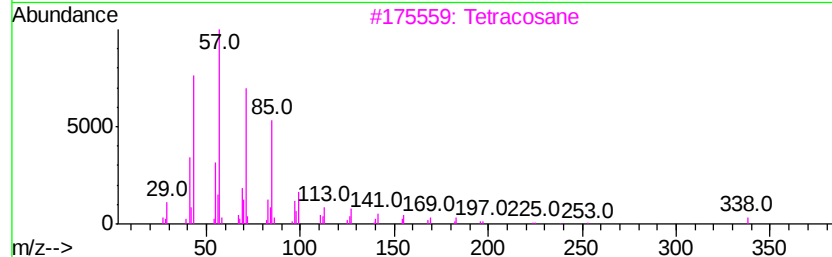
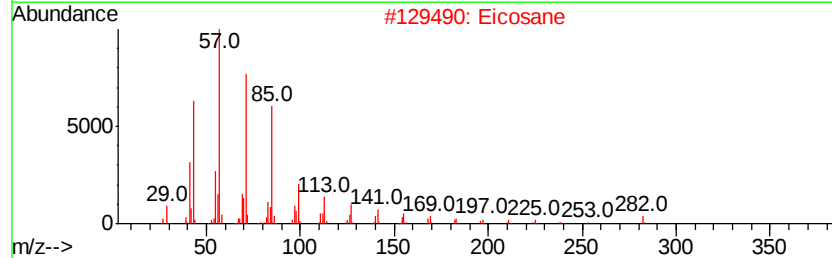
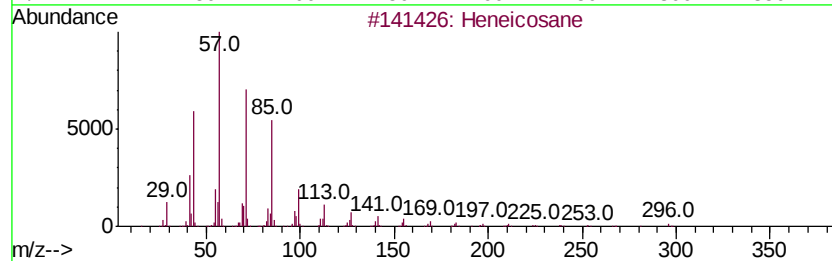
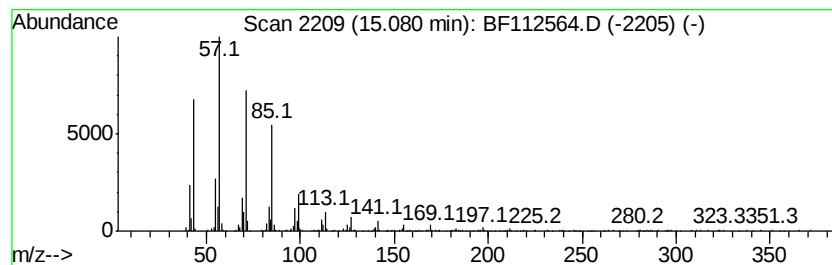
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	12.50 ng	390423	Perylene-d12	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	96
2	Eicosane		282	C20H42	000112-95-8	95
3	Tetracosane		338	C24H50	000646-31-1	91
4	Hexacosane		366	C26H54	000630-01-3	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
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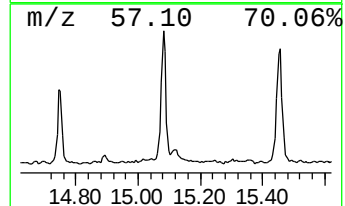
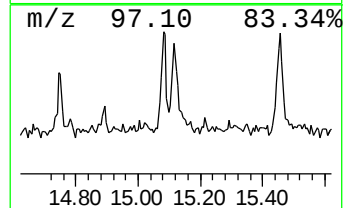
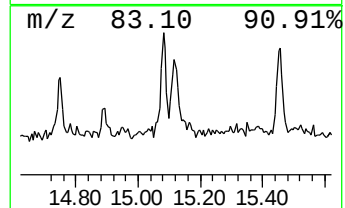
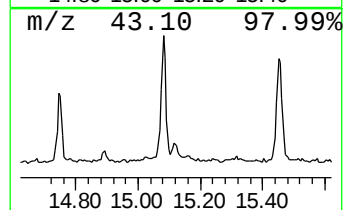
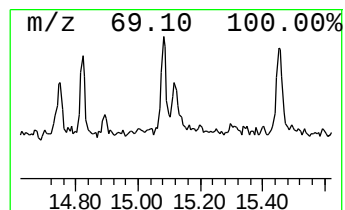
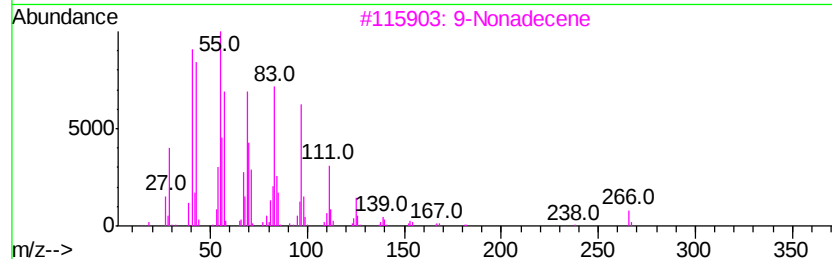
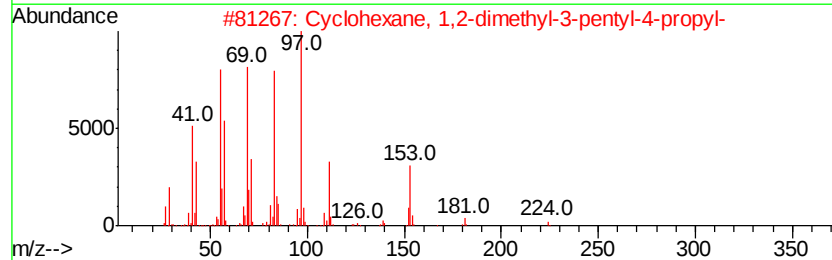
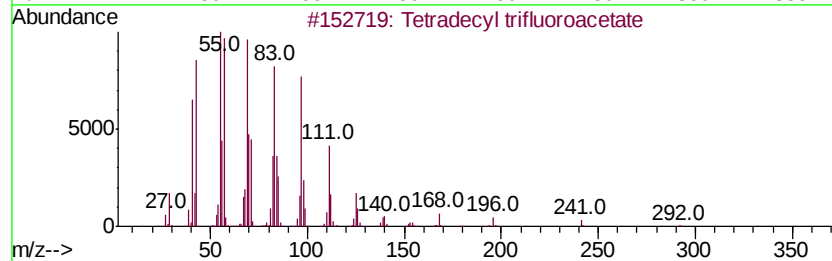
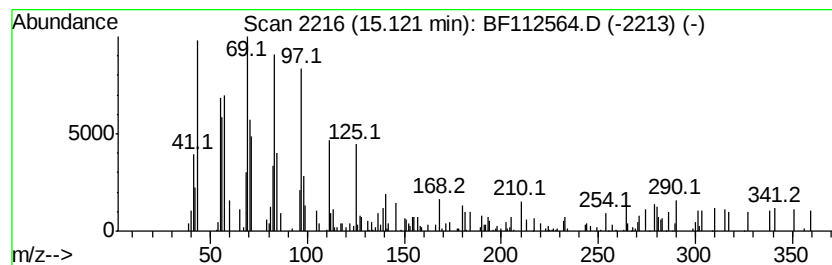
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetradecyl trifluoroacetate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	2.65 ng	82667	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	81
2		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	76
3		9-Nonadecene	266	C19H38	031035-07-1	70
4		1-Docosene	308	C22H44	001599-67-3	62
5		Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
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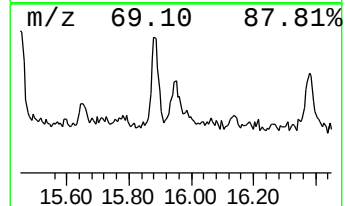
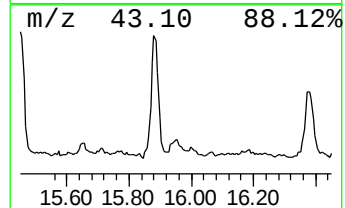
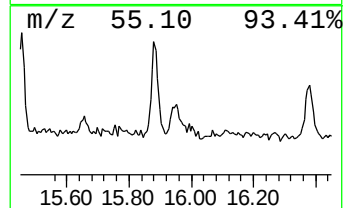
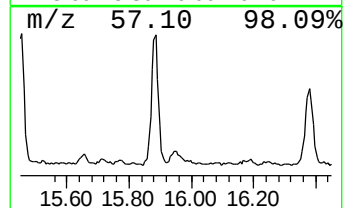
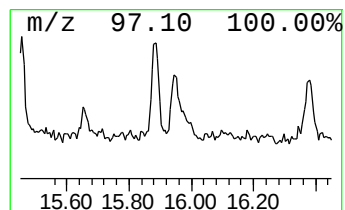
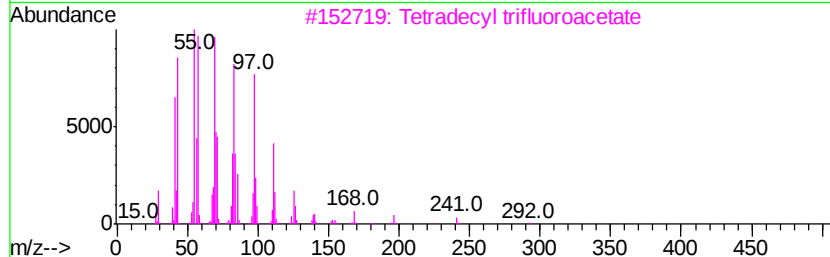
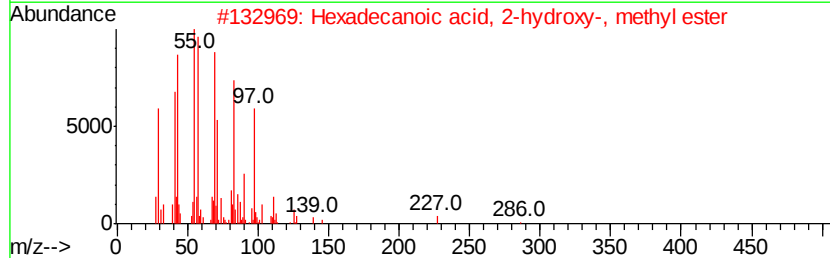
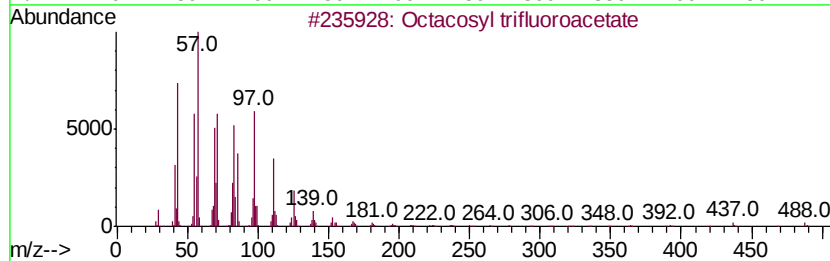
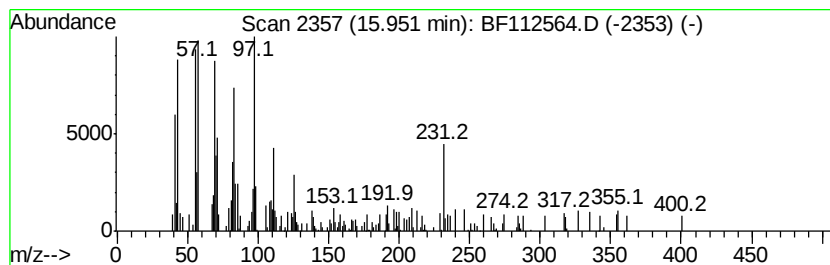
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosyl trifluoroacetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.35 ng	104754	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	55
2		Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	55
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	53
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	53
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
 Data File : BF112564.D
 Acq On : 14 Feb 2019 13:37
 Operator : JU/SJ
 Sample : K1458-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6

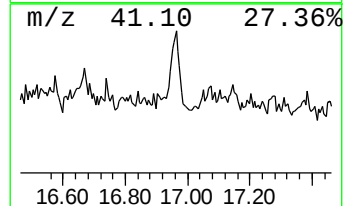
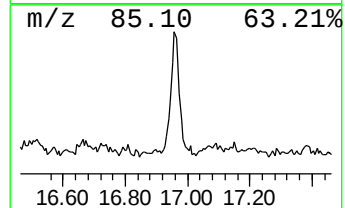
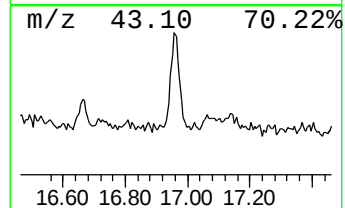
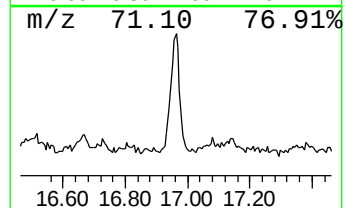
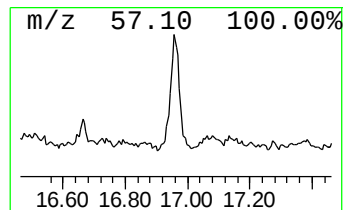
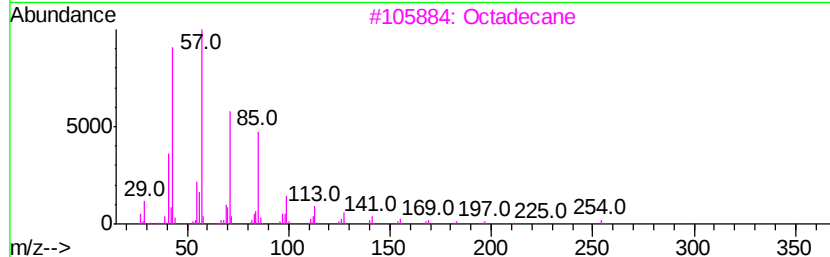
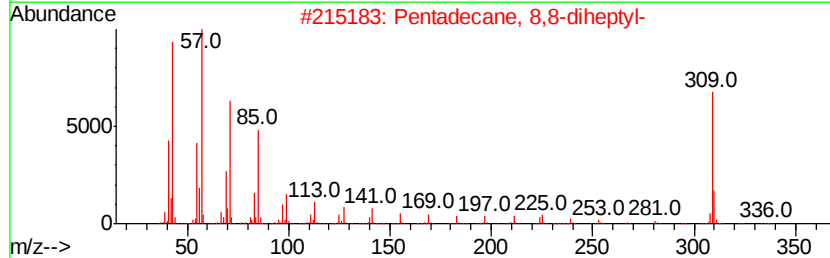
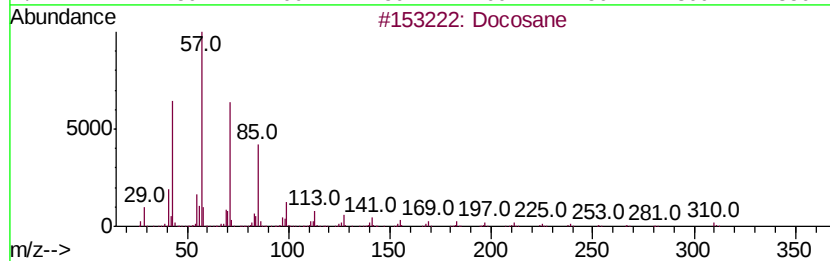
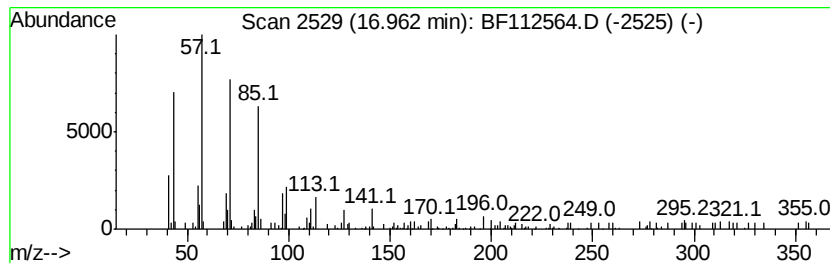
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 16 Docosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	5.60 ng	174808	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	76
2		Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	64
3		Octadecane	254	C18H38	000593-45-3	64
4		Tritetracontane	605	C43H88	007098-21-7	64
5		Hexacosane	366	C26H54	000630-01-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021419\
 Data File : BF112564.D
 Acq On : 14 Feb 2019 13:37
 Operator : JU/SJ
 Sample : K1458-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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...	5.05	3.0	ng	79795	1	6.83	539340	20.0
unknown6.60	6.60	73.2	ng	1973030	1	6.83	539340	20.0
n-Hexadecanoic acid	11.87	11.6	ng	445285	4	11.36	764935	20.0
Octadecanoic acid	12.66	7.9	ng	300465	4	11.36	764935	20.0
5-Eicosene, (E)-	13.82	12.8	ng	436713	5	14.00	682491	20.0
unknown13.89	13.89	2.9	ng	98656	5	14.00	682491	20.0
Eicosane	14.14	3.1	ng	106447	5	14.00	682491	20.0
2-Bromo dodecane	14.45	9.1	ng	310374	5	14.00	682491	20.0
Hexacosane	14.75	6.7	ng	208418	6	15.48	624646	20.0
Heneicosane	15.08	12.5	ng	390423	6	15.48	624646	20.0
Tetradecyl triflu...	15.12	2.6	ng	82667	6	15.48	624646	20.0
Octacosyl trifluo...	15.95	3.4	ng	104754	6	15.48	624646	20.0
Docosane	16.96	5.6	ng	174808	6	15.48	624646	20.0