

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052419\
 Data File : BF114576.D
 Acq On : 24 May 2019 18:19
 Operator : JU/SJ
 Sample : K2993-18
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-3

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-BF051019.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	5.045	500	503	511	rVB	31558	46852	1.13%	0.119%
2	5.451	568	572	596	rBV	3470693	3782508	91.52%	9.630%
3	6.463	740	744	762	rBV	3648035	4075407	98.60%	10.376%
4	6.592	762	766	779	rVB	4072313	3837856	92.86%	9.771%
5	6.810	800	803	812	rBV	1037765	900186	21.78%	2.292%
6	6.969	826	830	844	rBV	3356411	2909166	70.39%	7.407%
7	7.375	895	899	911	rBV	2532488	2464920	59.64%	6.276%
8	8.092	1017	1021	1037	rBV	1280579	1167977	28.26%	2.974%
9	9.169	1199	1204	1207	rBV	4535113	4016655	97.18%	10.226%
10	9.563	1267	1271	1277	rBV	299500	264323	6.40%	0.673%
11	9.845	1316	1319	1328	rVB	1339206	1273148	30.80%	3.241%
12	10.245	1382	1387	1390	rBV	95003	81705	1.98%	0.208%
13	10.639	1450	1454	1464	rBV	2504520	2595758	62.80%	6.609%
14	11.333	1569	1572	1580	rBV	1576050	1411294	34.15%	3.593%
15	11.863	1658	1662	1670	rBV	419777	490559	11.87%	1.249%
16	12.645	1791	1795	1804	rBV	131117	181782	4.40%	0.463%
17	12.915	1837	1841	1845	rBV	4036531	4133093	100.00%	10.523%
18	13.392	1917	1922	1927	rBV	102778	119528	2.89%	0.304%
19	13.804	1989	1992	2001	rBV	272486	438367	10.61%	1.116%
20	13.980	2018	2022	2032	rBV	1398890	1275737	30.87%	3.248%
21	14.127	2043	2047	2049	rBV	50161	57948	1.40%	0.148%
22	14.433	2095	2099	2108	rVB	102322	156281	3.78%	0.398%
23	14.733	2144	2150	2153	rBV2	207529	240494	5.82%	0.612%
24	14.804	2160	2162	2167	rVB	42555	45533	1.10%	0.116%
25	15.062	2202	2206	2212	rBV	339711	399441	9.66%	1.017%
26	15.445	2264	2271	2284	rBV2	921223	1608620	38.92%	4.096%
27	15.856	2336	2341	2347	rBV	305712	454151	10.99%	1.156%
28	16.351	2420	2425	2447	rVB2	198452	759390	18.37%	1.933%
29	16.921	2519	2522	2531	rVB3	43977	88500	2.14%	0.225%

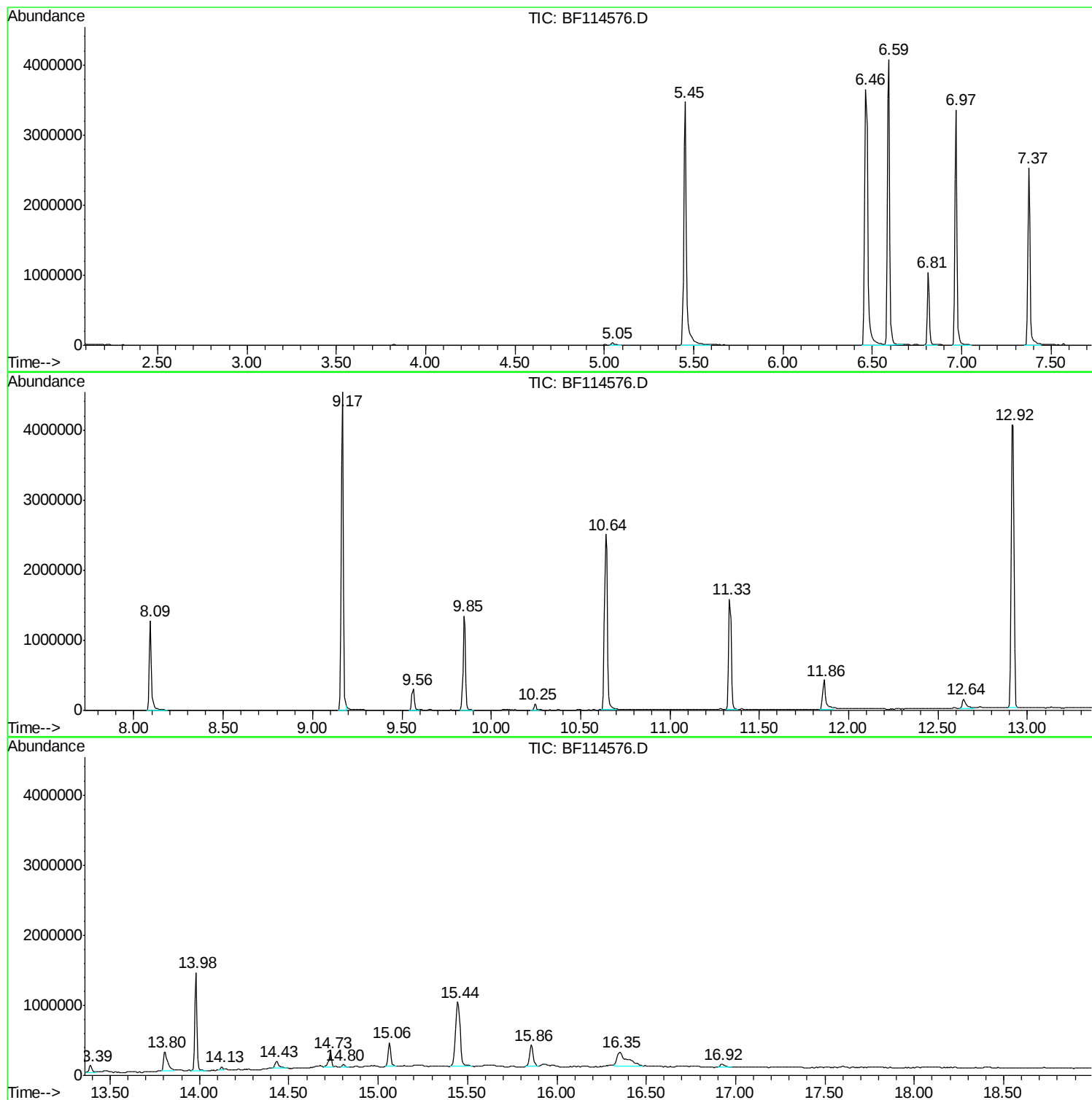
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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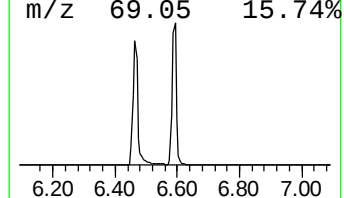
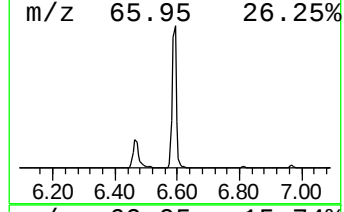
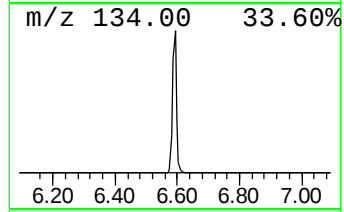
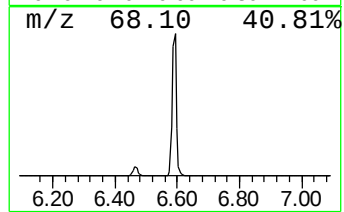
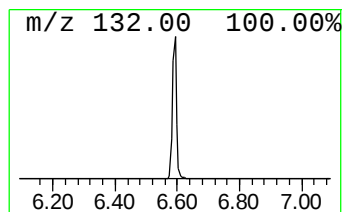
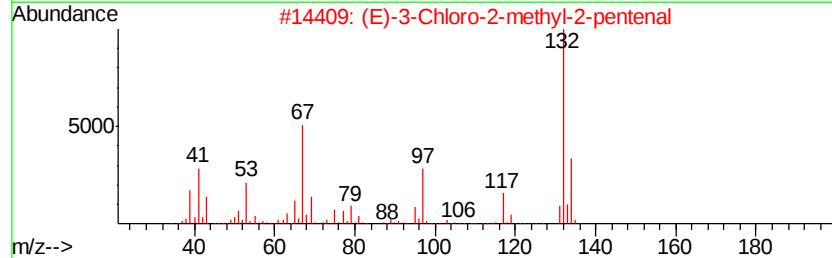
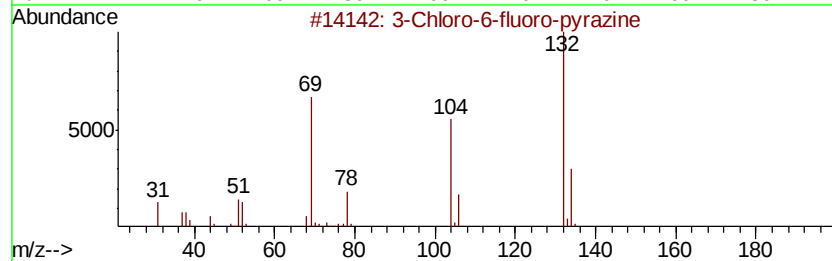
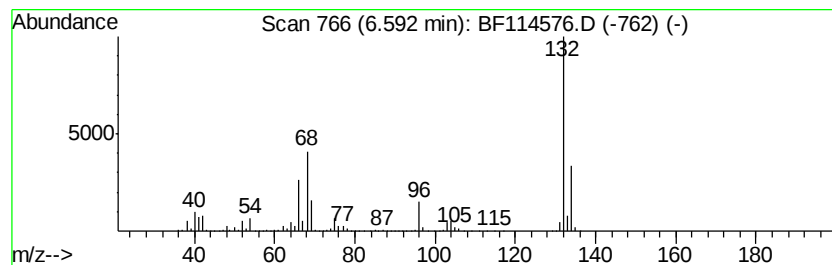
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	85.27 ng	3837860	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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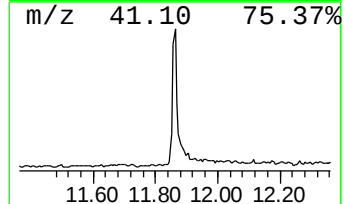
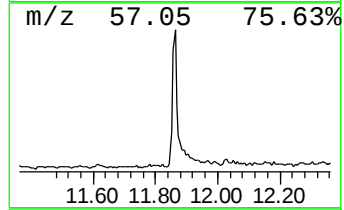
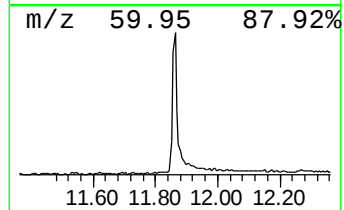
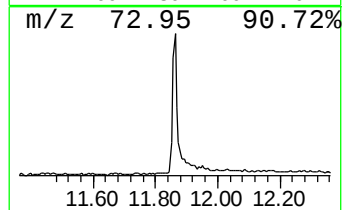
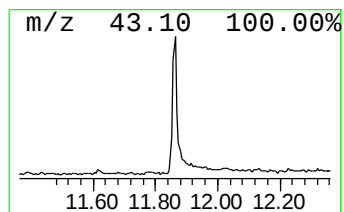
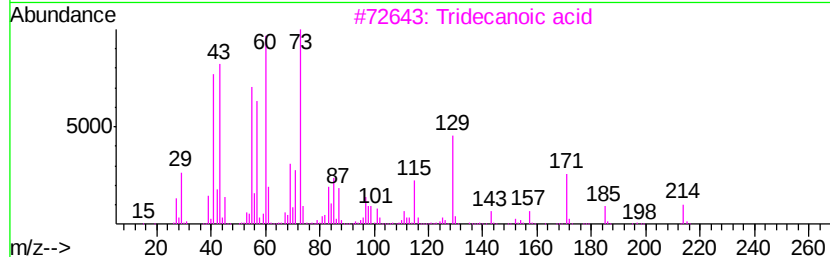
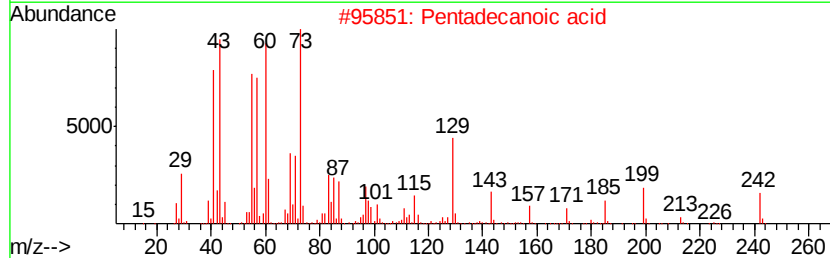
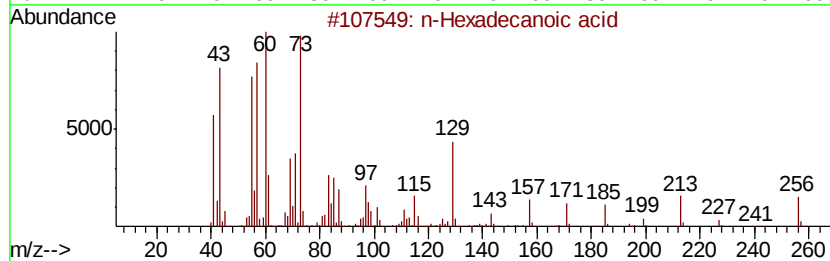
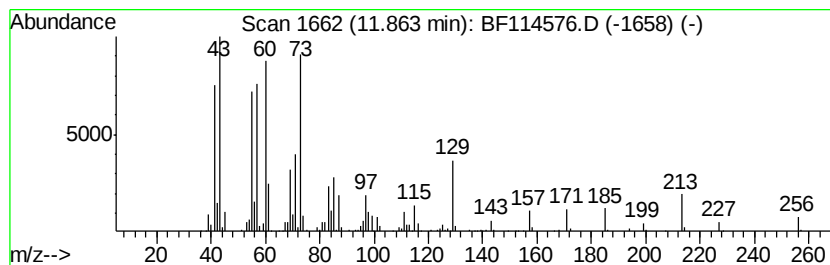
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	6.95 ng	490559	Phenanthrene-d10	11.33	
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	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	74



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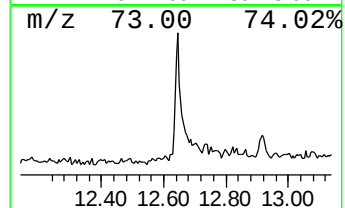
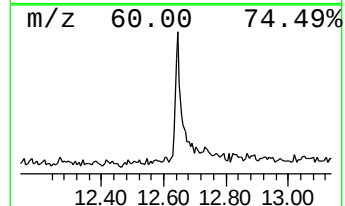
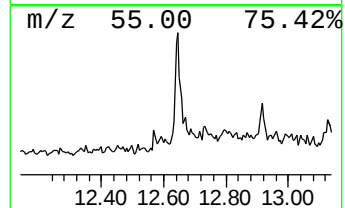
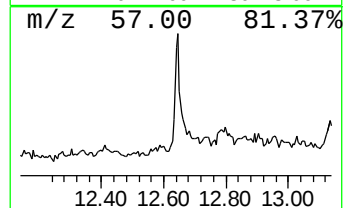
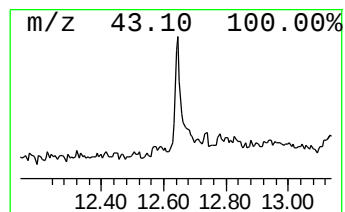
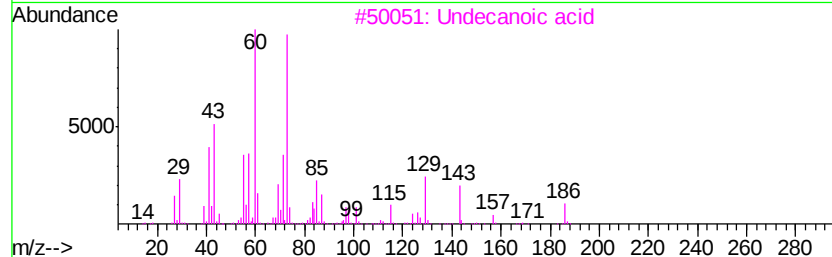
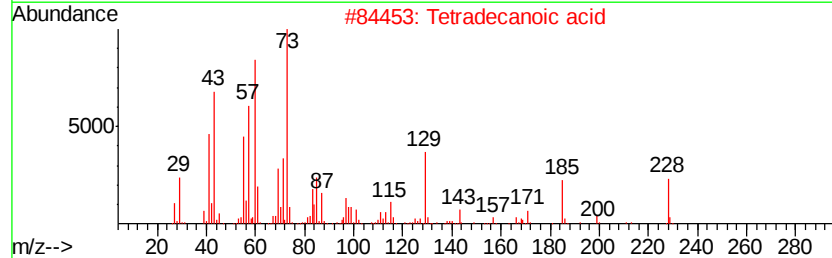
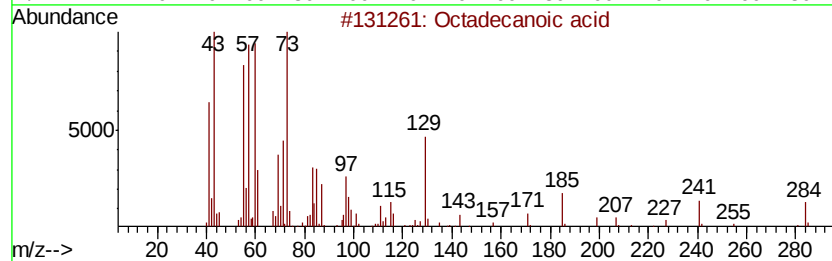
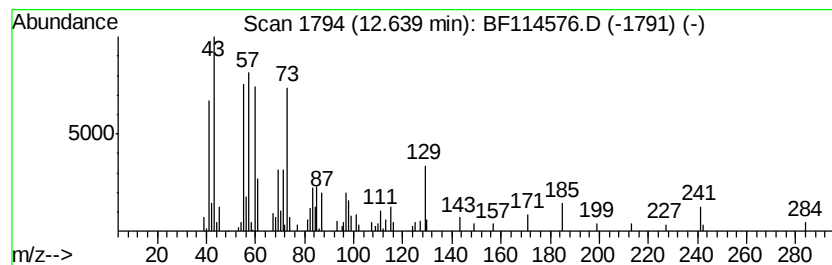
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.58 ng	181782	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Undecanoic acid	186	C11H22O2	000112-37-8	58
4		Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	18



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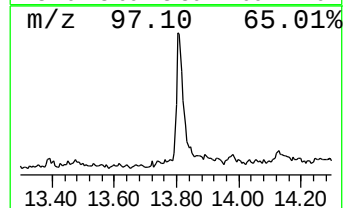
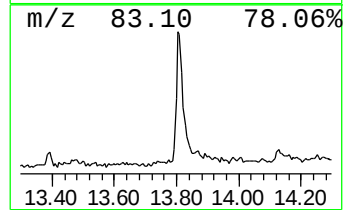
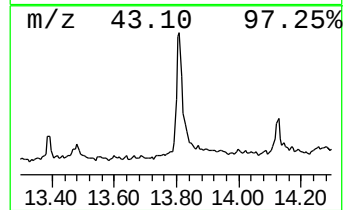
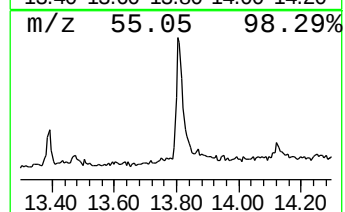
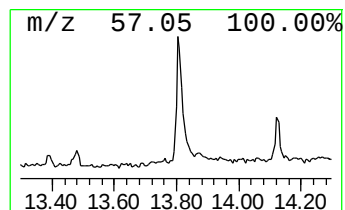
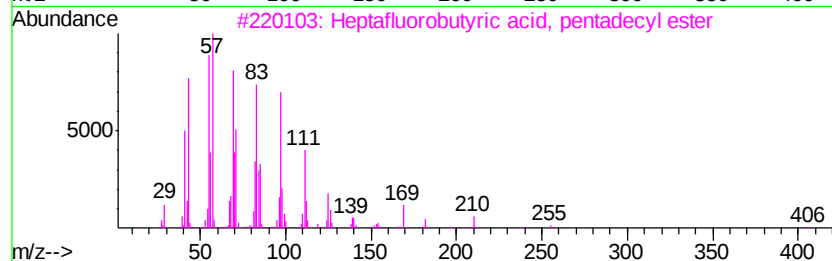
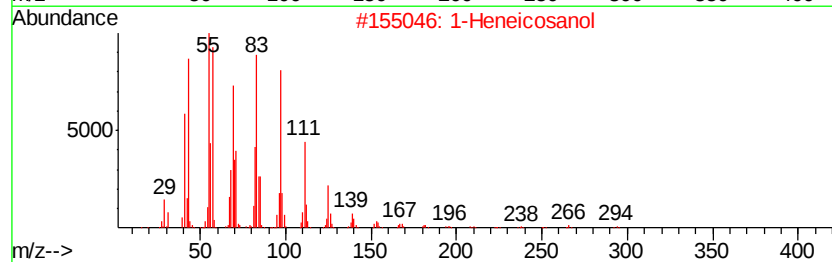
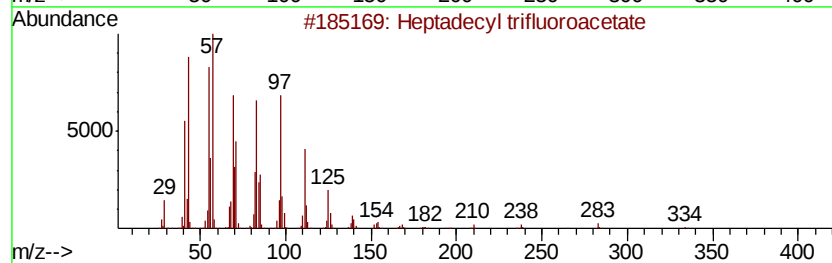
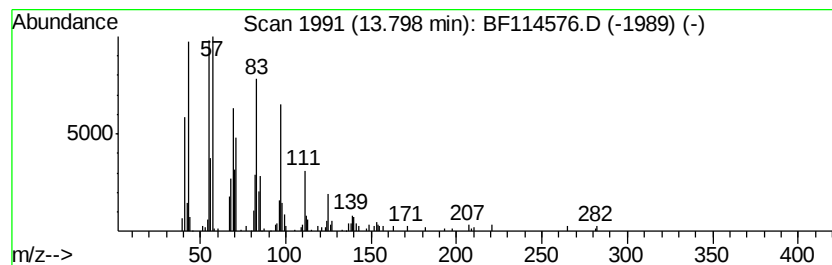
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	6.87 ng	438367	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



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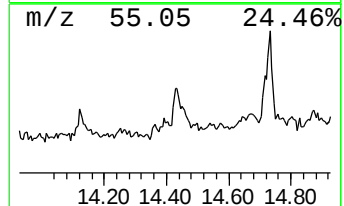
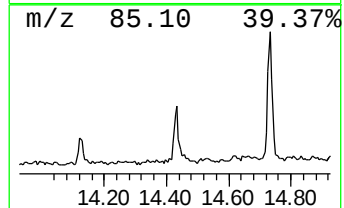
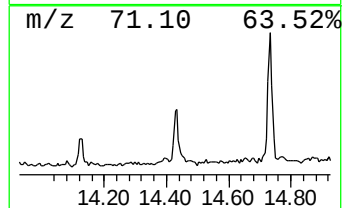
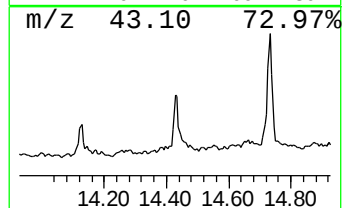
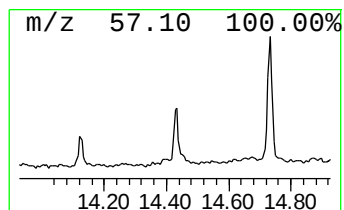
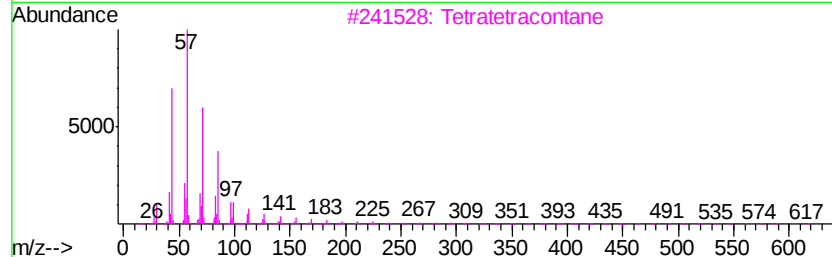
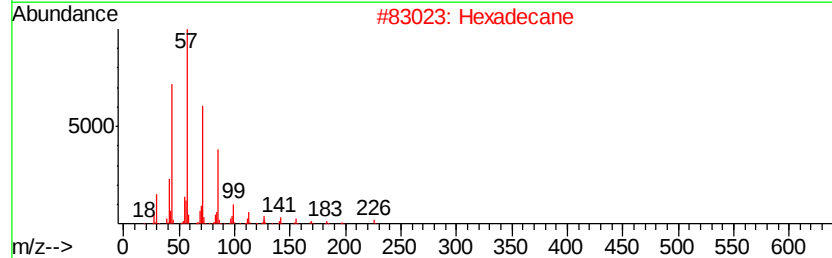
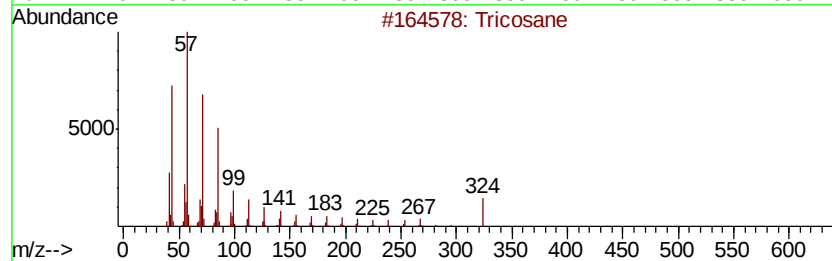
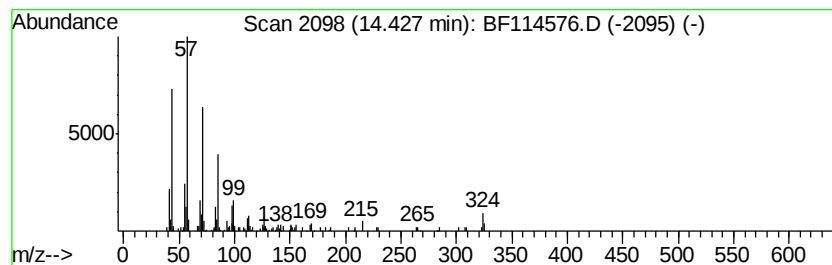
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Tricosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.45 ng	156281	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	94
2		Hexadecane	226	C16H34	000544-76-3	94
3		Tetratetracontane	619	C44H90	007098-22-8	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



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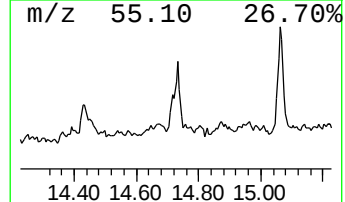
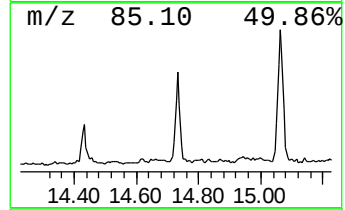
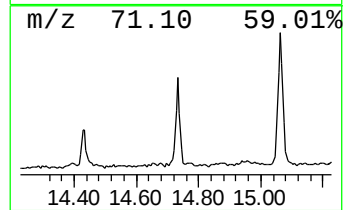
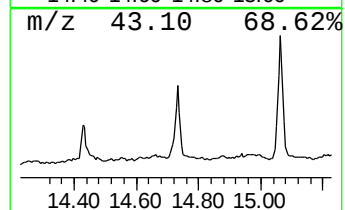
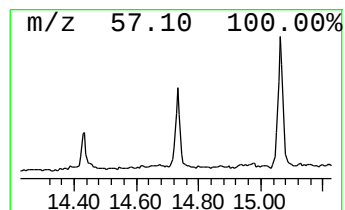
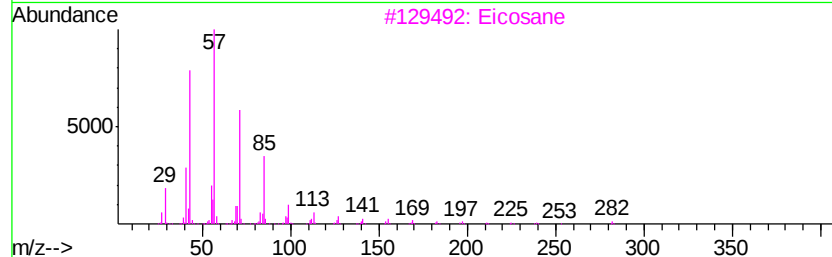
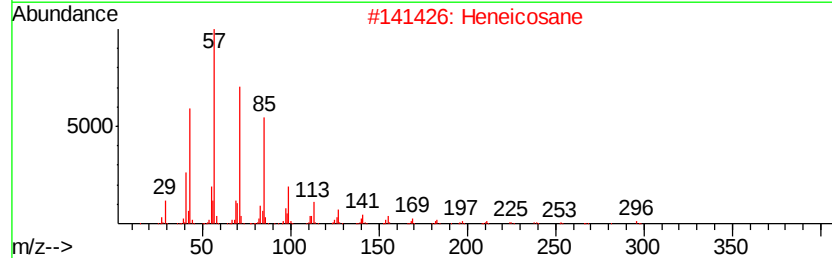
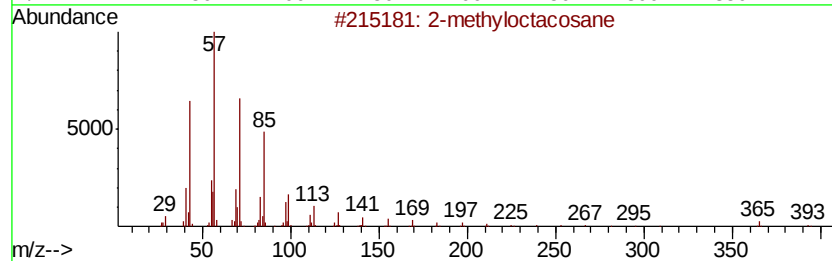
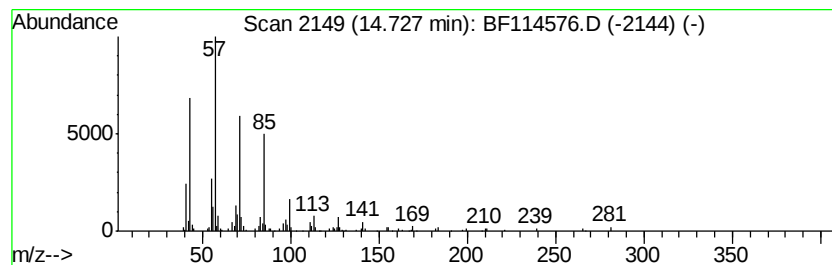
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.99 ng	240494	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Eicosane	282	C20H42	000112-95-8	87
4		Nonadecane	268	C19H40	000629-92-5	86
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114576.D
Acq On : 24 May 2019 18:19
Operator : JU/SJ
Sample : K2993-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

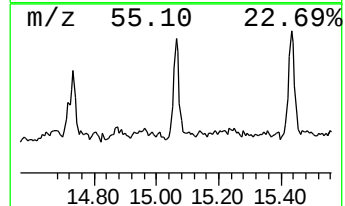
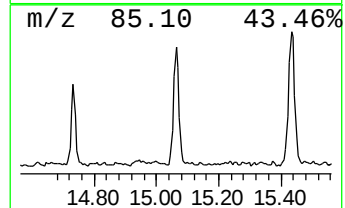
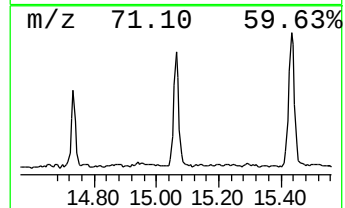
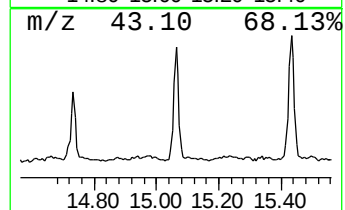
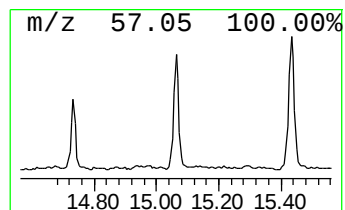
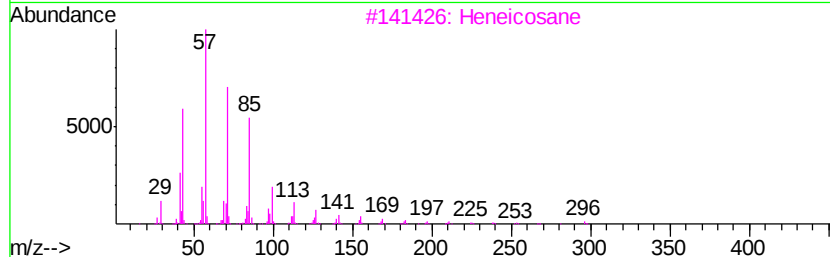
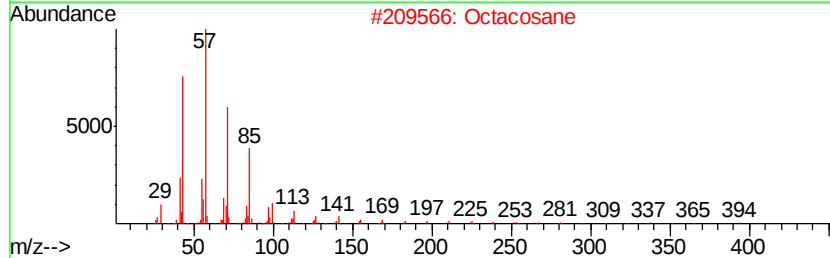
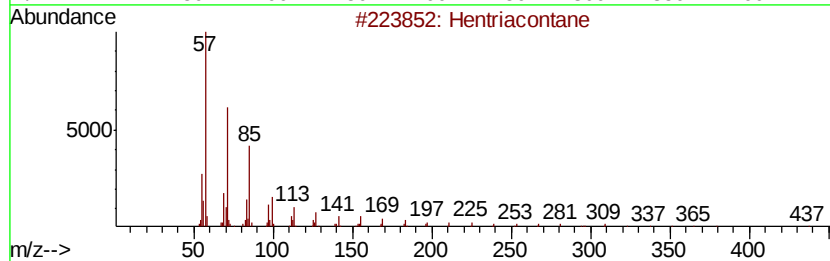
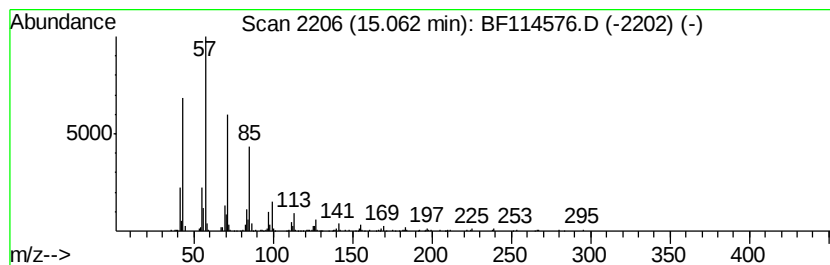
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	4.97 ng	399441	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	Hexacosane		366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114576.D
Acq On : 24 May 2019 18:19
Operator : JU/SJ
Sample : K2993-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

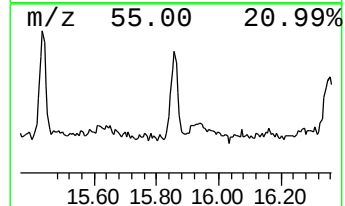
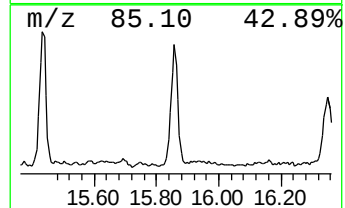
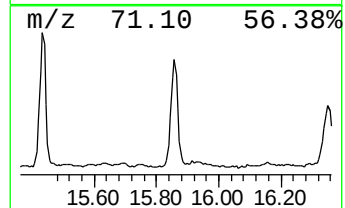
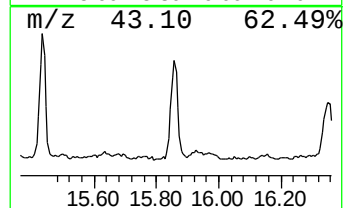
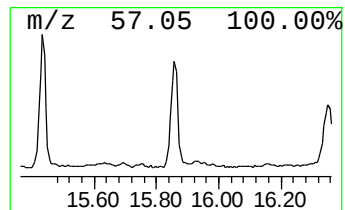
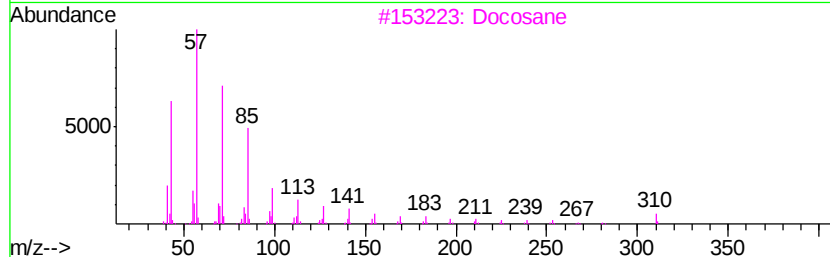
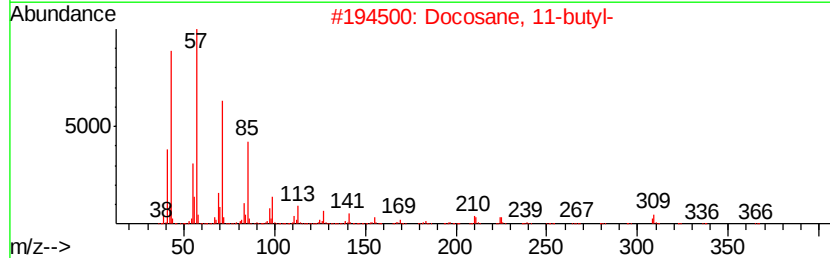
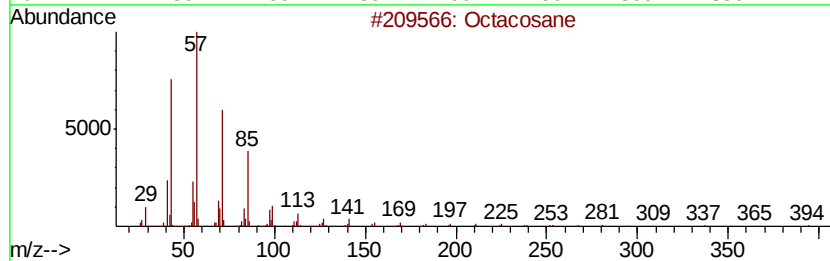
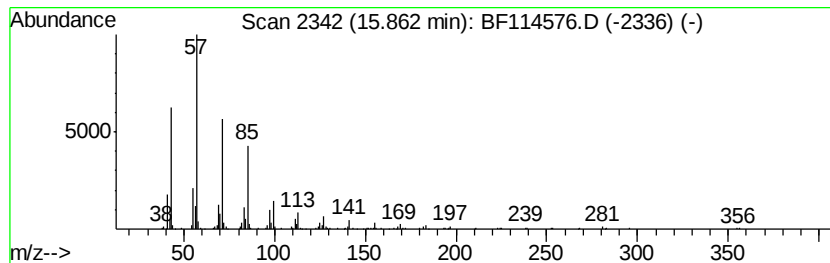
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	5.65 ng	454151	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3		Docosane	310	C22H46	000629-97-0	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114576.D
Acq On : 24 May 2019 18:19
Operator : JU/SJ
Sample : K2993-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

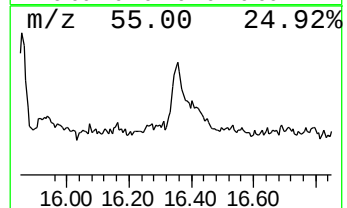
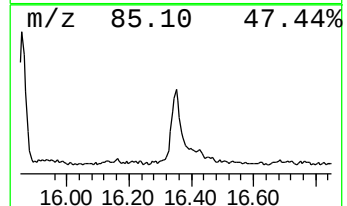
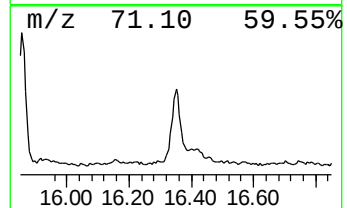
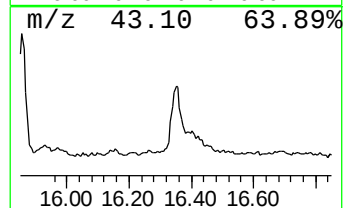
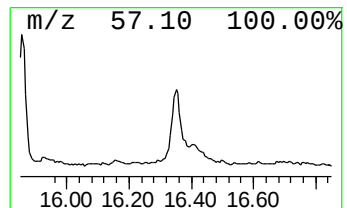
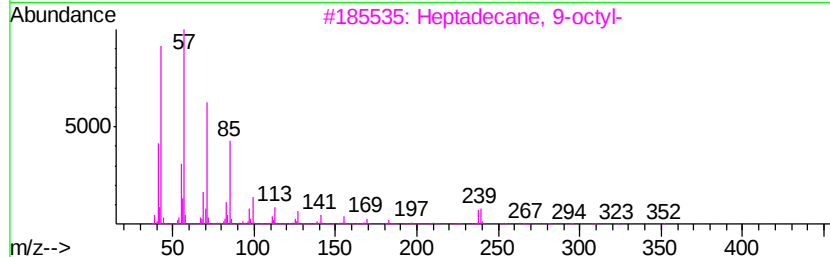
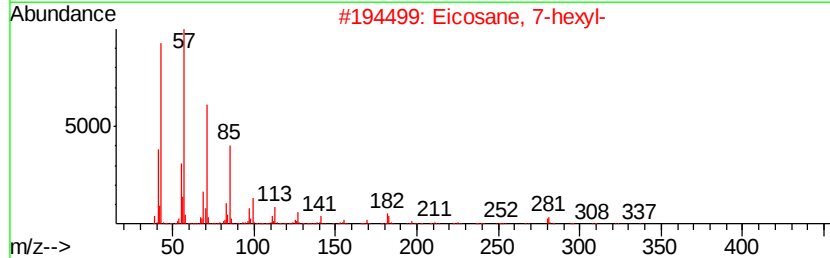
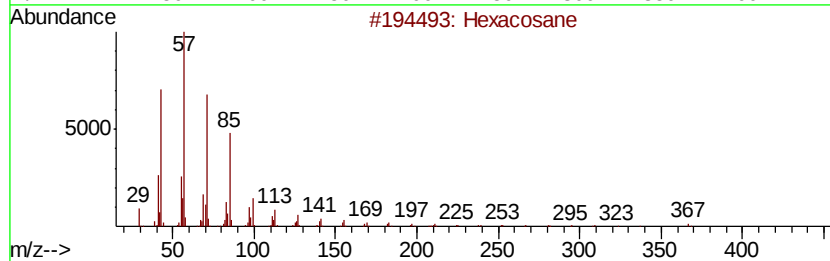
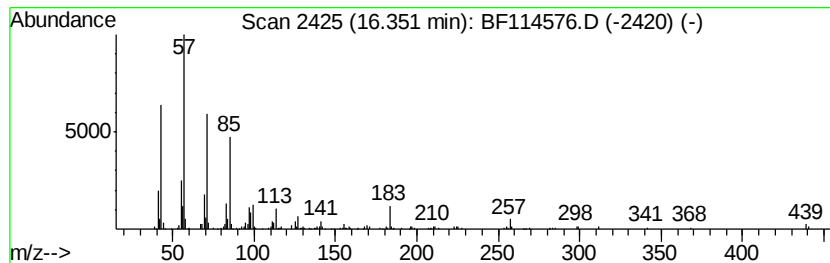
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	9.44 ng	759390	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4		Octadecane	254	C18H38	000593-45-3	83
5		Tetracosane	338	C24H50	000646-31-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052419\
Data File : BF114576.D
Acq On : 24 May 2019 18:19
Operator : JU/SJ
Sample : K2993-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
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n-Hexadecanoic acid	11.86	7.0	ng	490559	4	11.33	1411290	20.0
Octadecanoic acid	12.64	2.6	ng	181782	4	11.33	1411290	20.0
Heptadecyl triflu...	13.80	6.9	ng	438367	5	13.98	1275740	20.0
Tricosane	14.43	2.5	ng	156281	5	13.98	1275740	20.0
2-methyloctacosane	14.73	3.0	ng	240494	6	15.45	1608620	20.0
Hentriacontane	15.06	5.0	ng	399441	6	15.45	1608620	20.0
Octacosane	15.86	5.7	ng	454151	6	15.45	1608620	20.0
Hexacosane	16.35	9.4	ng	759390	6	15.45	1608620	20.0