

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
 Data File : BF112949.D
 Acq On : 8 Mar 2019 17:28
 Operator : JU/SJ
 Sample : K1761-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N4871

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-BF022719.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	5.334	548	552	566	rBV	1906851	1993184	35.60%	4.546%
2	6.357	723	726	741	rBV	1362153	1303291	23.28%	2.972%
3	6.498	745	750	753	rBV	4178803	3856430	68.88%	8.795%
4	6.563	758	761	766	rVB	52442	56326	1.01%	0.128%
5	6.728	785	789	793	rBV	1376806	1119577	20.00%	2.553%
6	6.887	812	816	819	rBV	4130677	3549201	63.40%	8.094%
7	7.292	879	885	888	rBV	2849010	3041099	54.32%	6.936%
8	8.010	1003	1007	1014	rBV	1472661	1411915	25.22%	3.220%
9	9.086	1186	1190	1204	rBV	5611967	5598384	100.00%	12.768%
10	9.210	1208	1211	1215	rVB	85805	84754	1.51%	0.193%
11	9.757	1300	1304	1313	rBV	1669744	1660745	29.66%	3.788%
12	10.545	1433	1438	1453	rBV	3804219	3973277	70.97%	9.062%
13	11.110	1530	1534	1538	rBV5	38922	57120	1.02%	0.130%
14	11.233	1551	1555	1561	rBV	1726504	1750176	31.26%	3.991%
15	11.280	1561	1563	1570	rVB3	148446	166943	2.98%	0.381%
16	11.469	1592	1595	1598	rBV3	54582	63197	1.13%	0.144%
17	11.774	1643	1647	1660	rBV2	891310	997742	17.82%	2.275%
18	12.186	1714	1717	1722	rVB	127804	115031	2.05%	0.262%
19	12.292	1730	1735	1740	rBV3	94941	125997	2.25%	0.287%
20	12.439	1756	1760	1762	rBV3	49284	61552	1.10%	0.140%
21	12.486	1765	1768	1776	rVB3	56323	90719	1.62%	0.207%
22	12.557	1776	1780	1790	rBV	719675	851520	15.21%	1.942%
23	12.821	1820	1825	1828	rBV	5247151	5522441	98.64%	12.595%
24	13.721	1974	1978	1989	rBV3	344671	466174	8.33%	1.063%
25	13.857	1997	2001	2012	rBV	1334343	1479892	26.43%	3.375%
26	14.039	2029	2032	2040	rVB	210473	207638	3.71%	0.474%
27	14.345	2081	2084	2094	rVB	360479	341891	6.11%	0.780%
28	14.639	2130	2134	2139	rVB	474597	444288	7.94%	1.013%
29	14.957	2183	2188	2197	rBV	454535	522655	9.34%	1.192%
30	15.262	2235	2240	2244	rBV	897704	1202146	21.47%	2.742%
31	15.310	2244	2248	2256	rVB	413807	544620	9.73%	1.242%
32	15.715	2311	2317	2322	rBV	262105	393189	7.02%	0.897%
33	15.762	2322	2325	2334	rVB8	29158	65990	1.18%	0.150%
34	16.180	2390	2396	2407	rVB	144207	264286	4.72%	0.603%

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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 >
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35	16.727	2485	2489	2497	rVB2	52091	97191	1.74%	0.222%
36	17.174	2558	2565	2575	rBV5	138750	367223	6.56%	0.837%

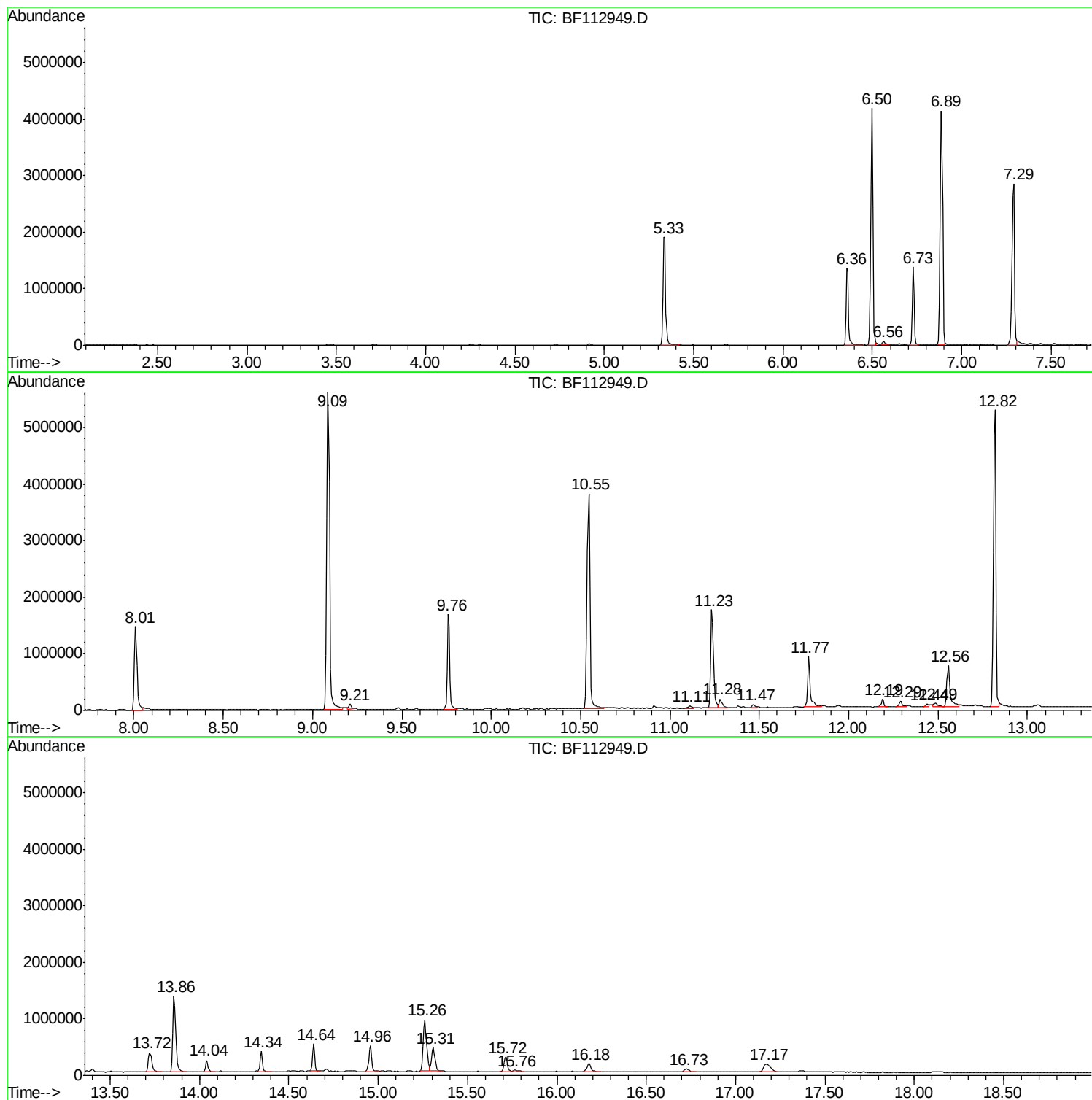
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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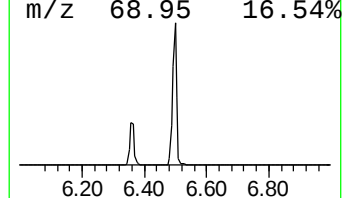
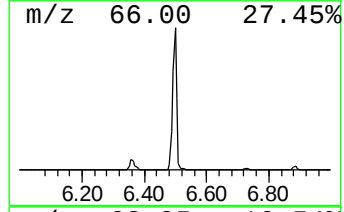
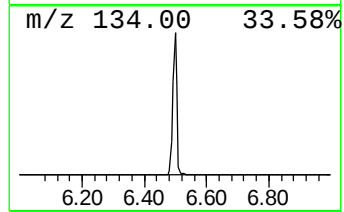
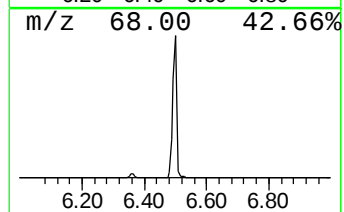
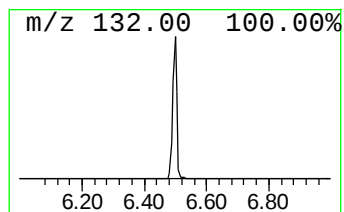
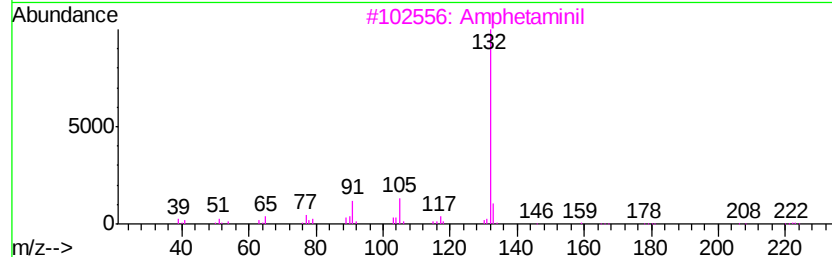
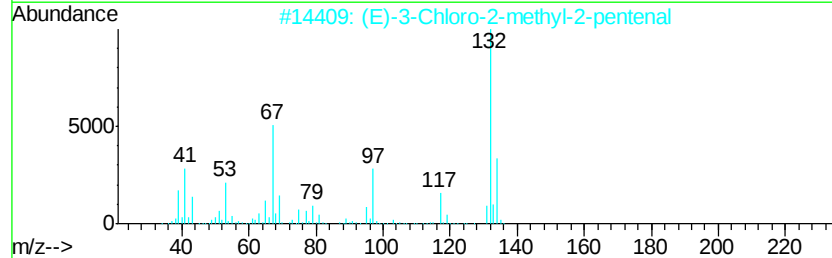
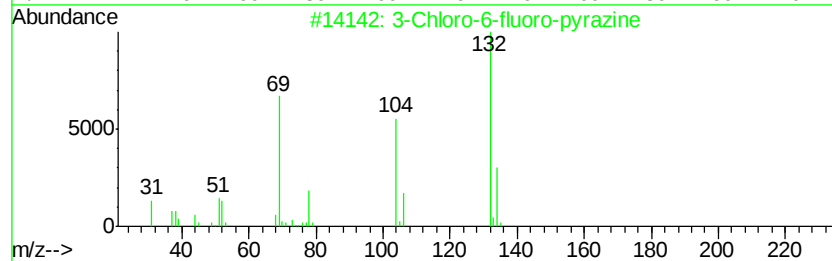
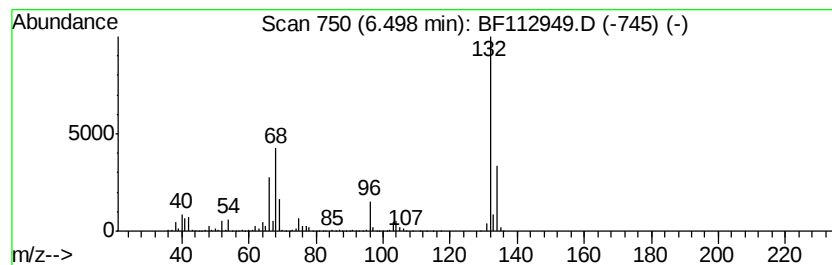
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	68.89 ng	3856430	1,4-Dichlorobenzene-d4	6.73

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		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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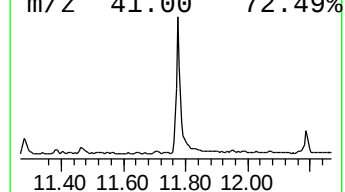
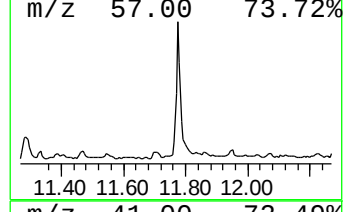
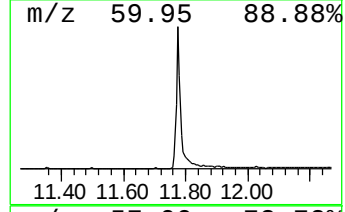
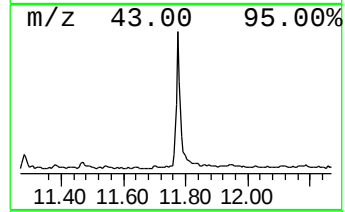
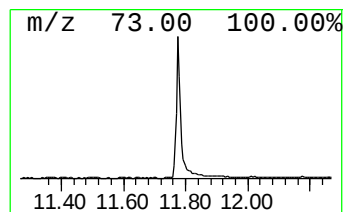
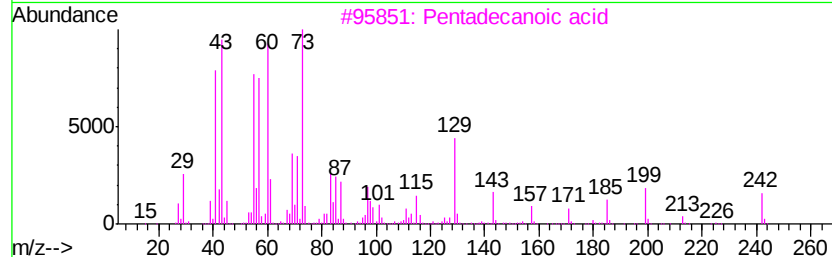
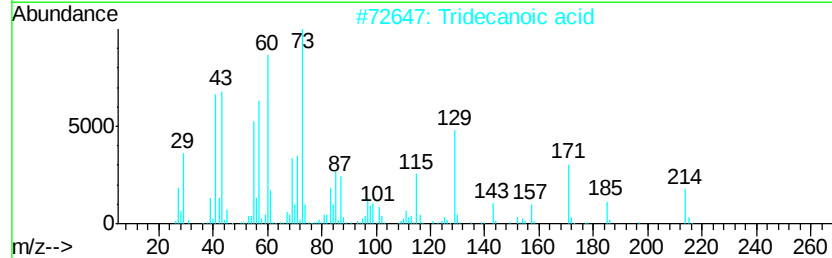
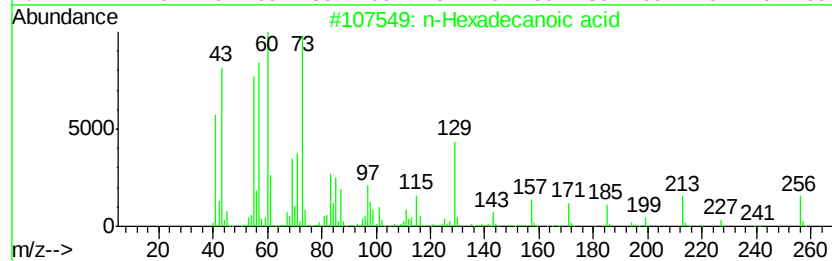
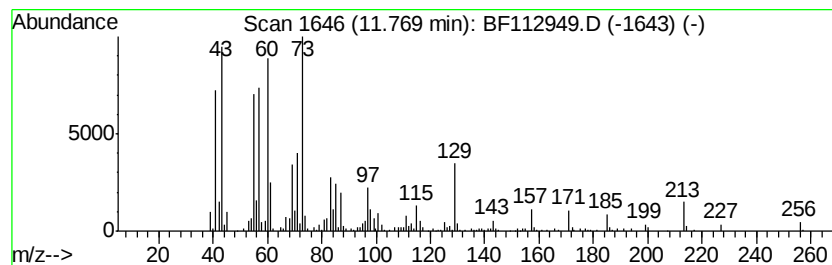
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	11.40 ng	997742	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20



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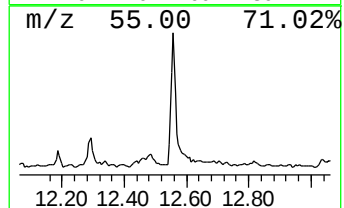
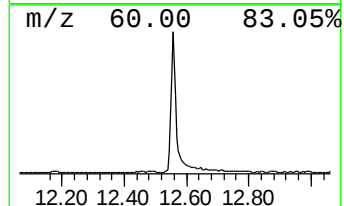
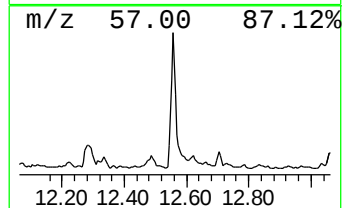
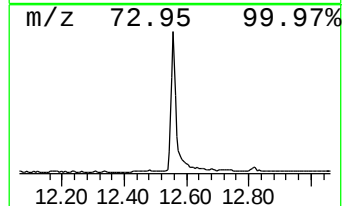
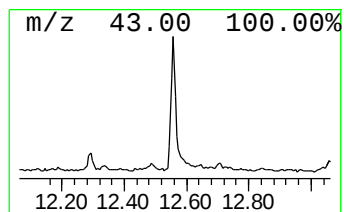
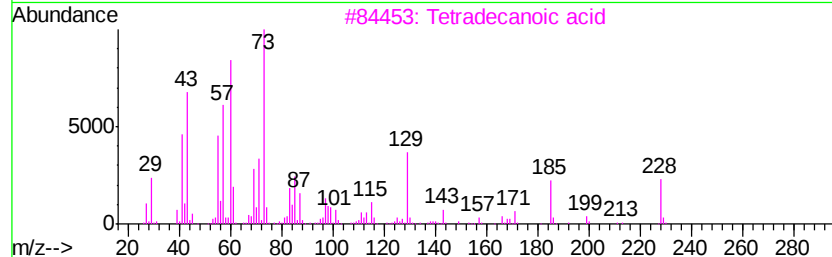
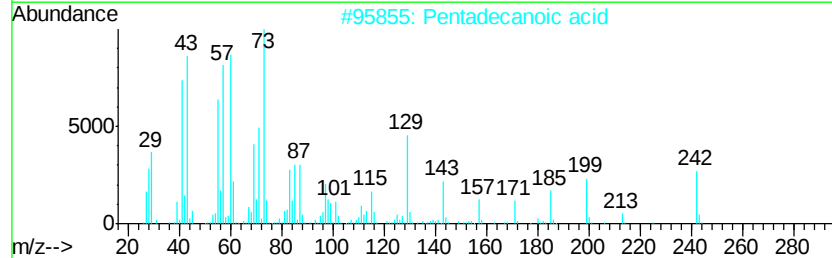
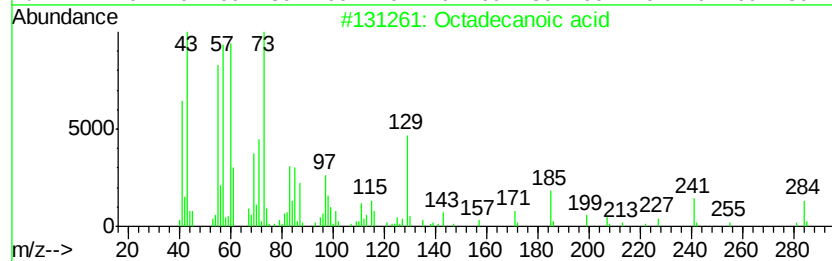
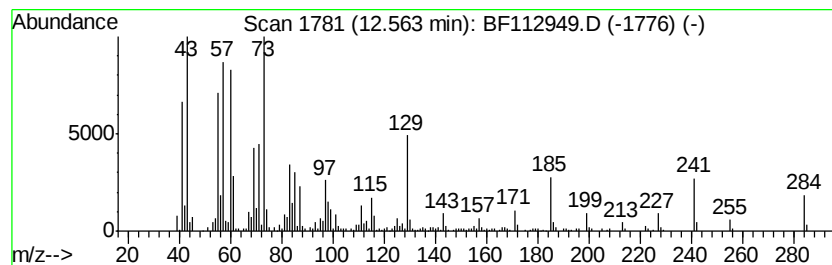
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	11.51 ng	851520	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5		Tridecanoic acid	214	C13H26O2	000638-53-9	74



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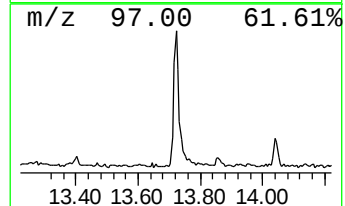
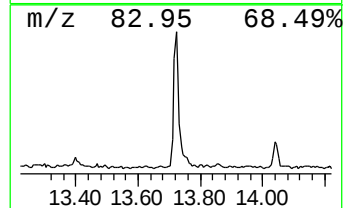
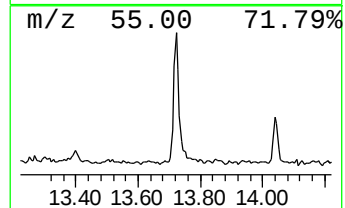
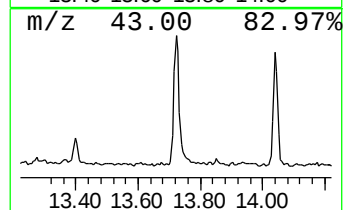
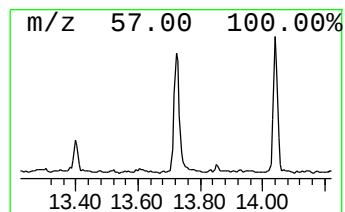
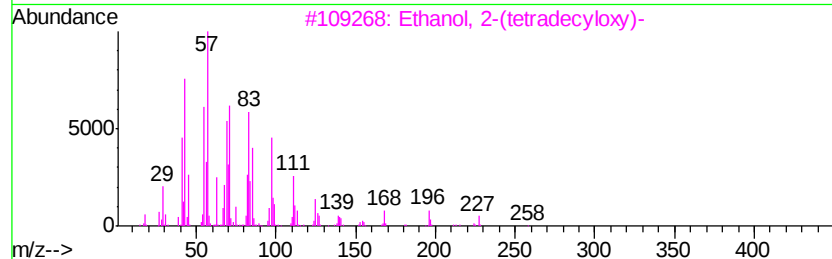
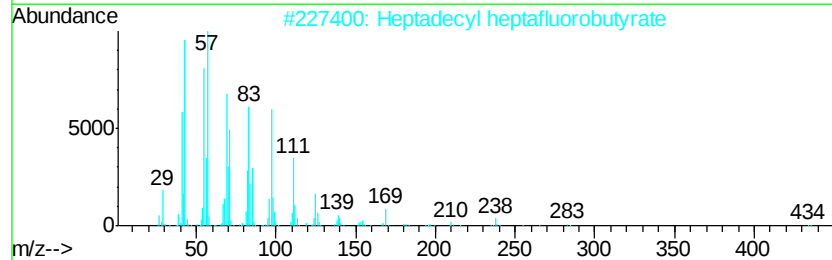
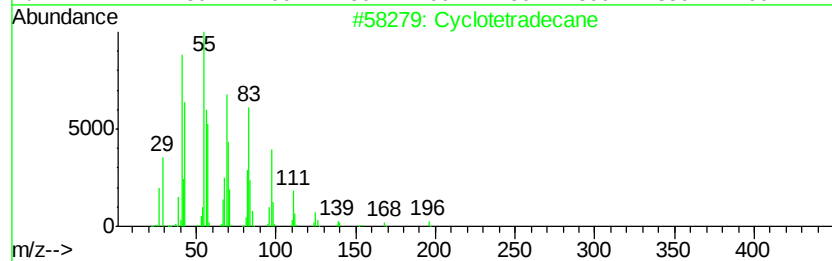
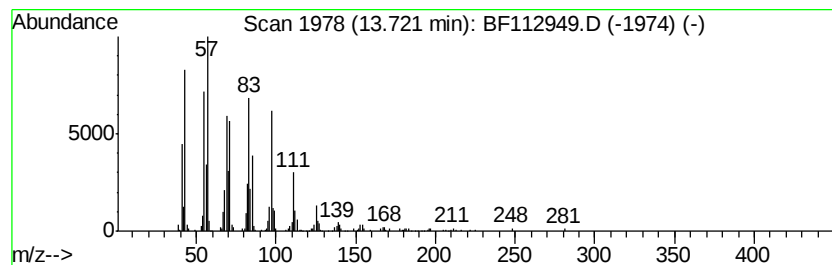
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclotetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	6.30 ng	466174	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetradecane	196	C14H28	000295-17-0	95
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90



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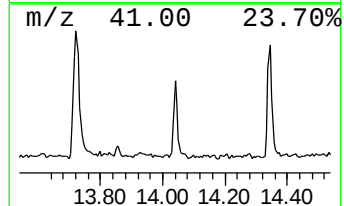
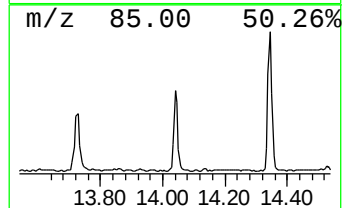
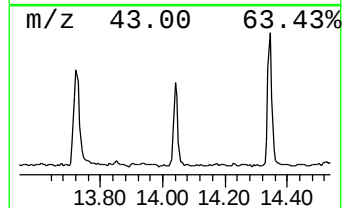
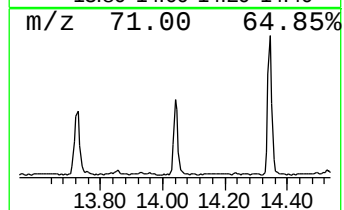
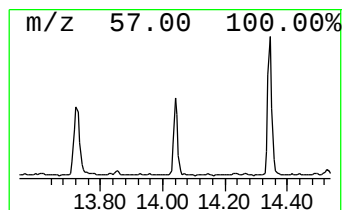
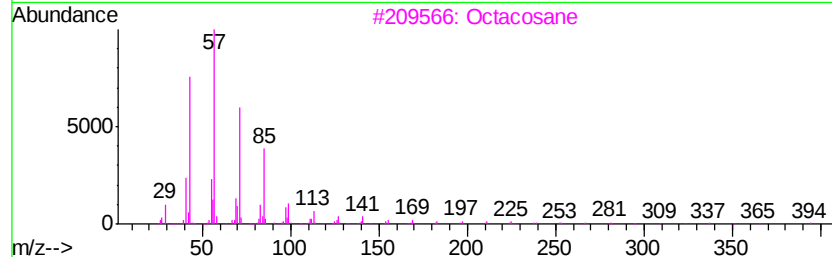
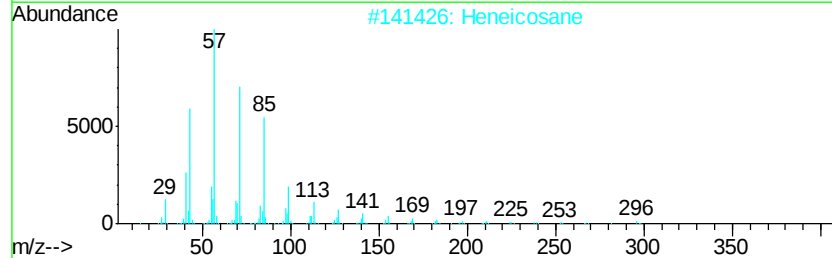
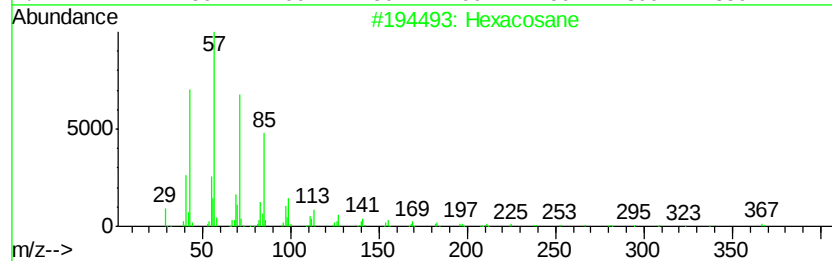
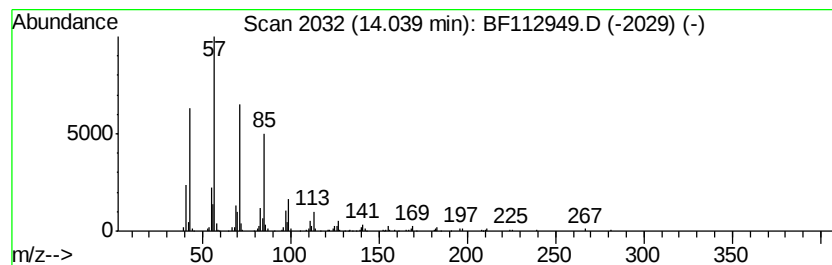
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Peak Number 6 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.81 ng	207638	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Tetracosane	338	C24H50	000646-31-1	90
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112949.D
Acq On : 8 Mar 2019 17:28
Operator : JU/SJ
Sample : K1761-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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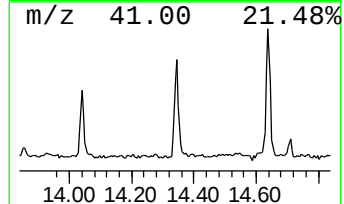
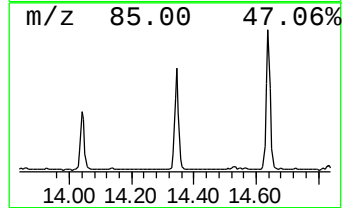
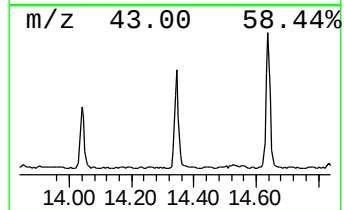
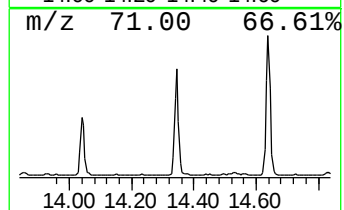
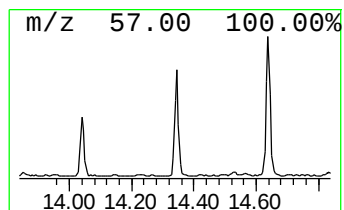
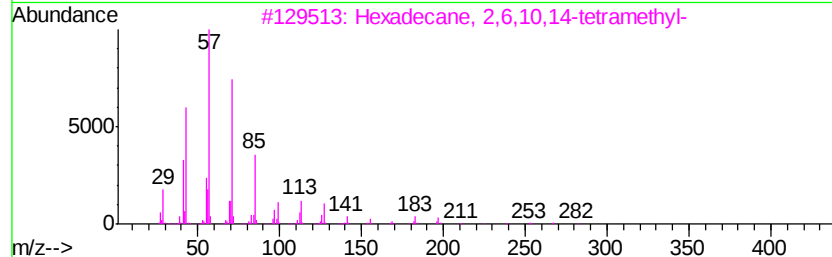
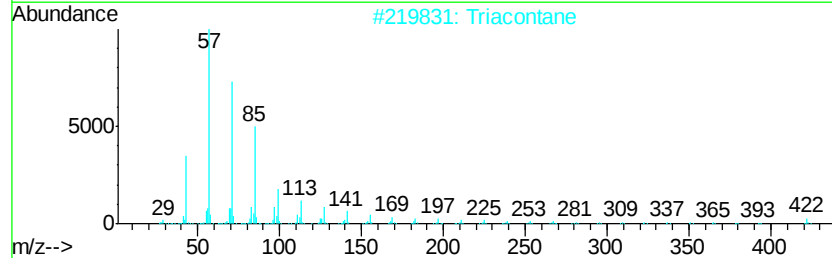
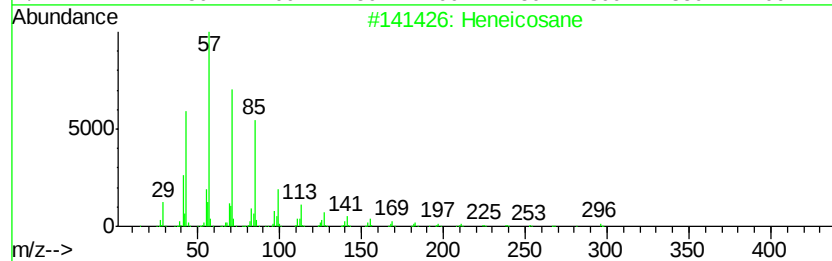
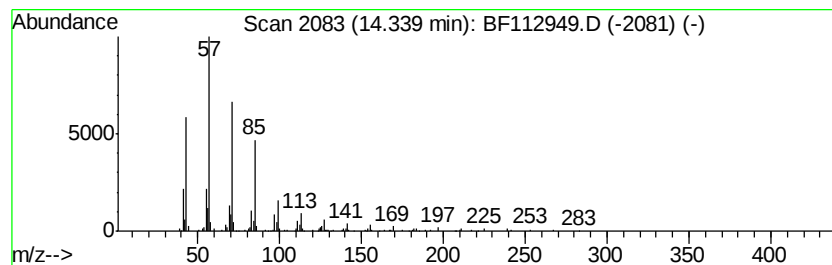
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.62 ng	341891	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Triacotane		422	C30H62	000638-68-6	91
3	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	91
4	Heptadecane		240	C17H36	000629-78-7	91
5	Tetracosane		338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
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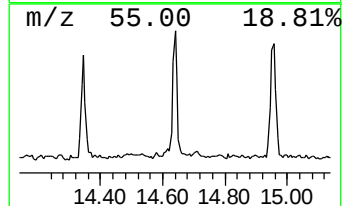
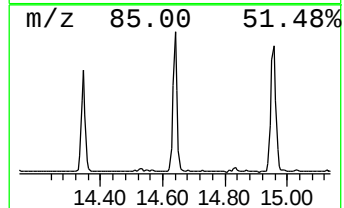
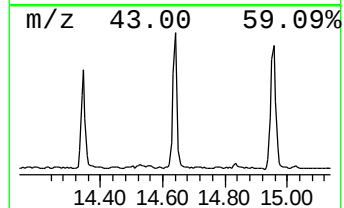
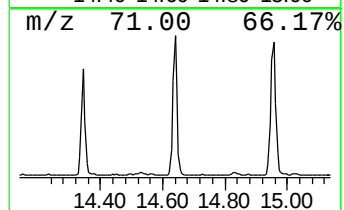
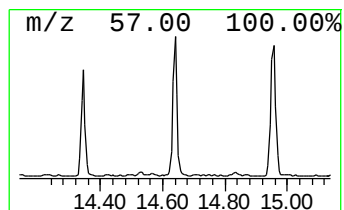
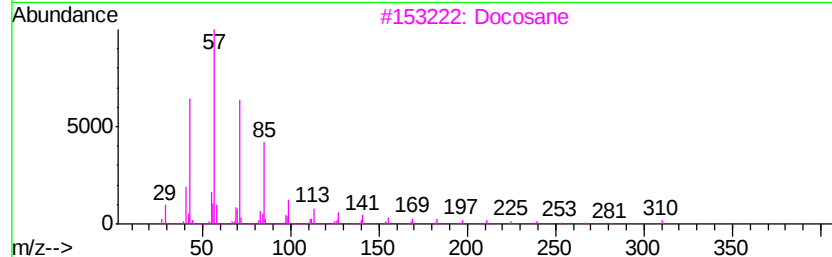
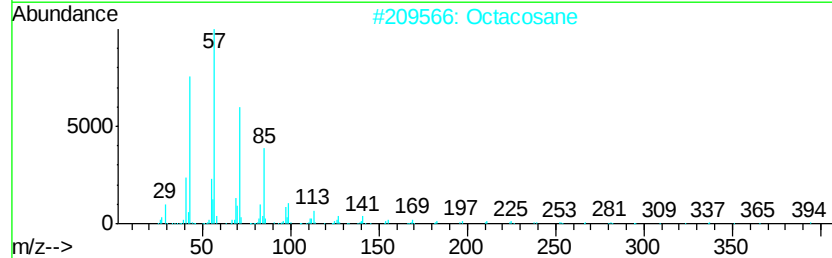
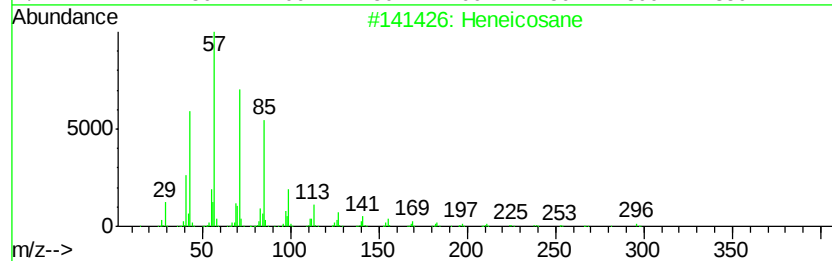
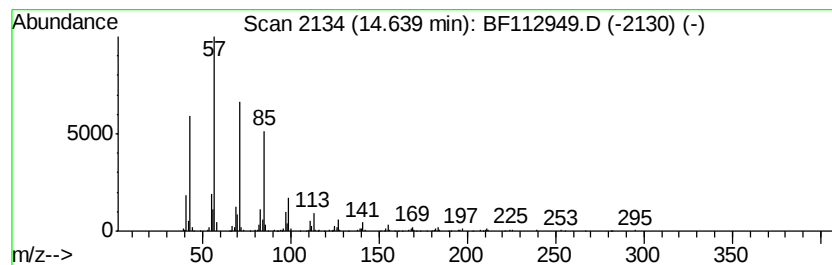
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.64 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	7.39 ng	444288	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Docosane	310	C22H46	000629-97-0	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112949.D
Acq On : 8 Mar 2019 17:28
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Sample : K1761-01
Misc :
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Instrument :
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ClientSampleId :
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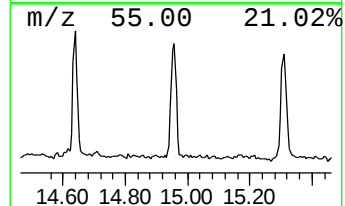
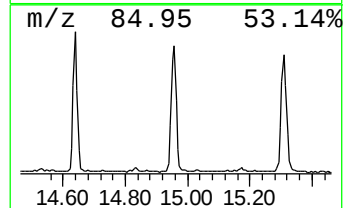
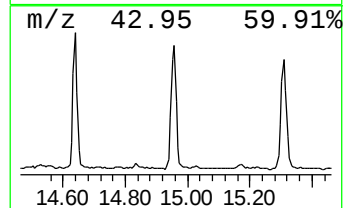
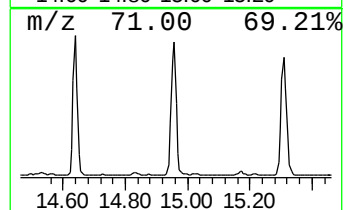
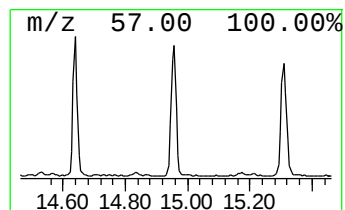
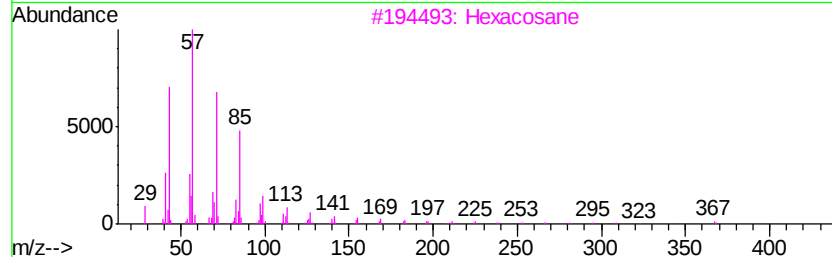
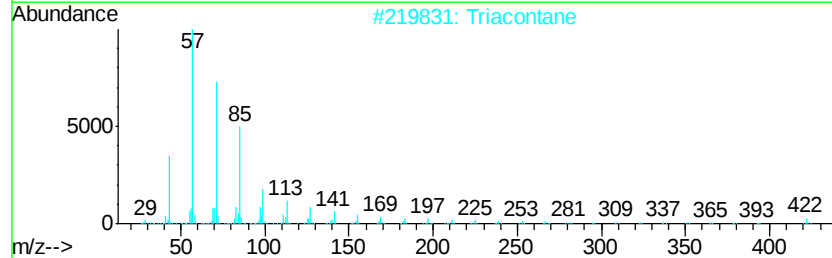
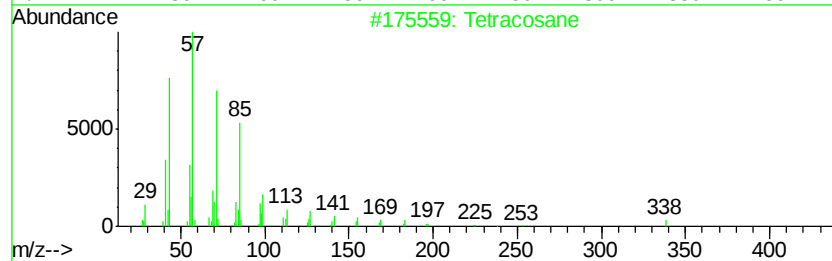
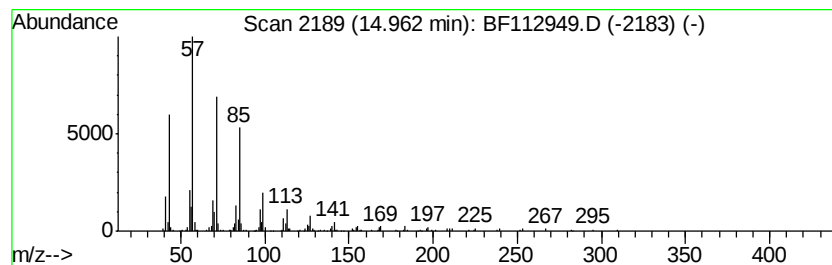
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	8.70 ng	522655	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112949.D
Acq On : 8 Mar 2019 17:28
Operator : JU/SJ
Sample : K1761-01
Misc :
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Instrument :
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ClientSampleId :
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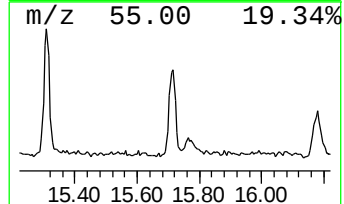
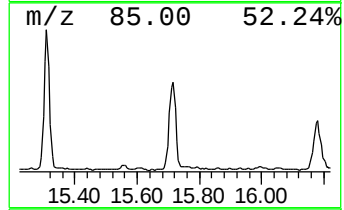
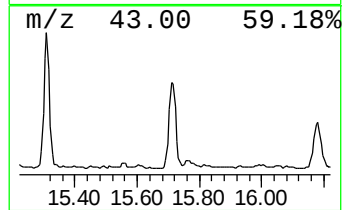
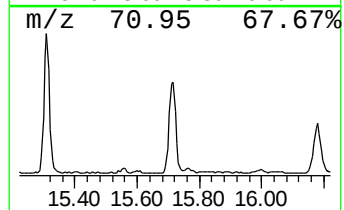
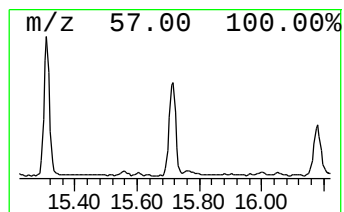
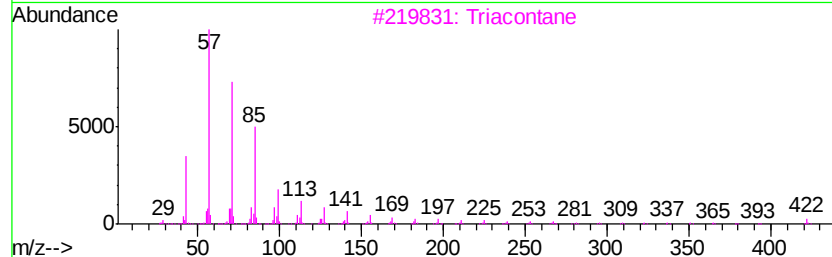
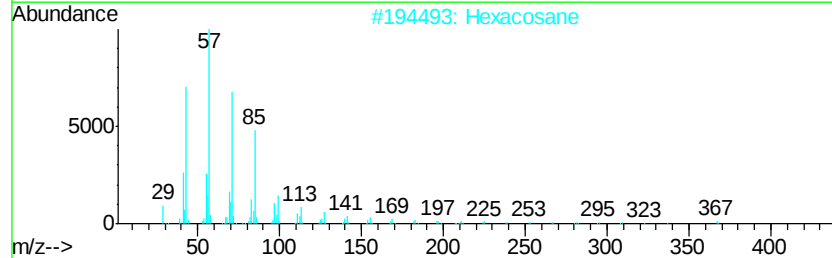
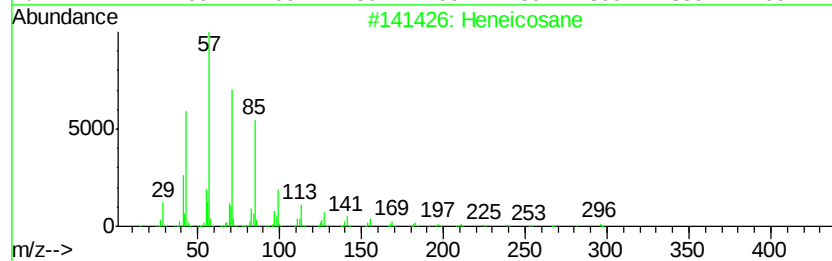
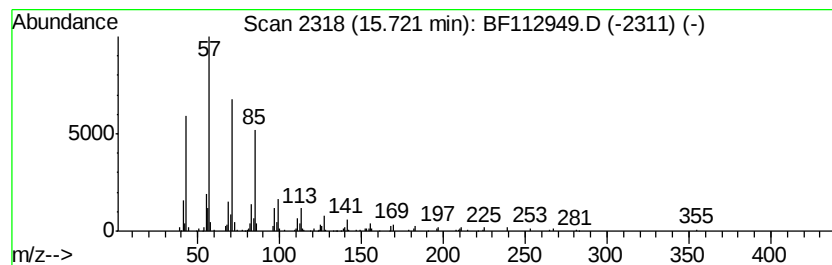
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.72 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	6.54 ng	393189	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			triacontane	422	C30H62	000638-68-6	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112949.D
Acq On : 8 Mar 2019 17:28
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Sample : K1761-01
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ClientSampleId :
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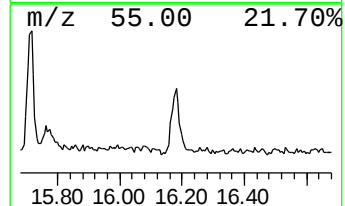
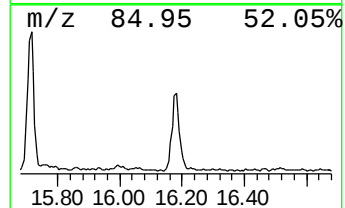
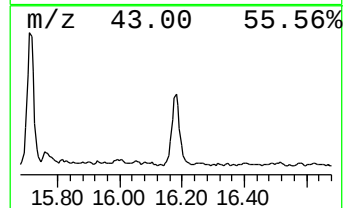
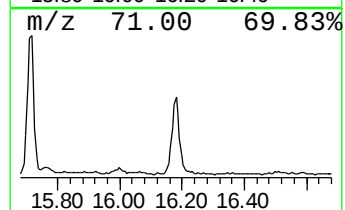
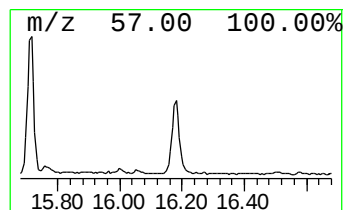
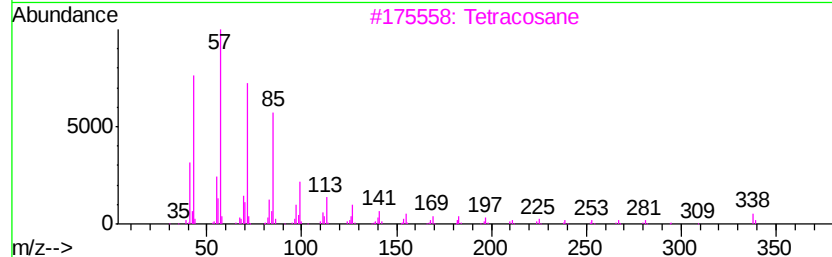
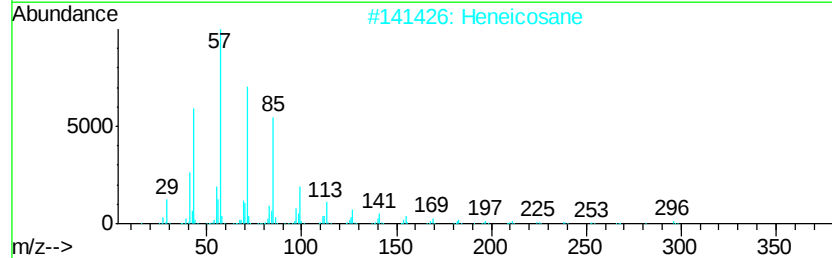
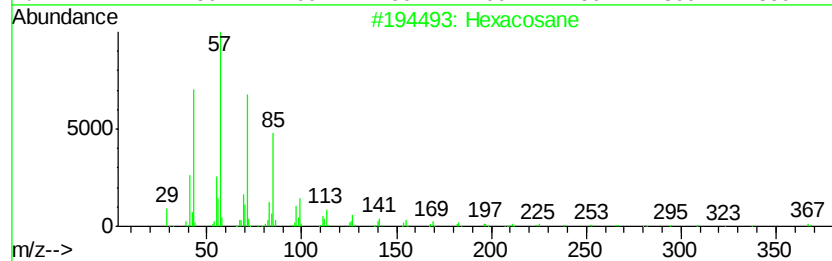
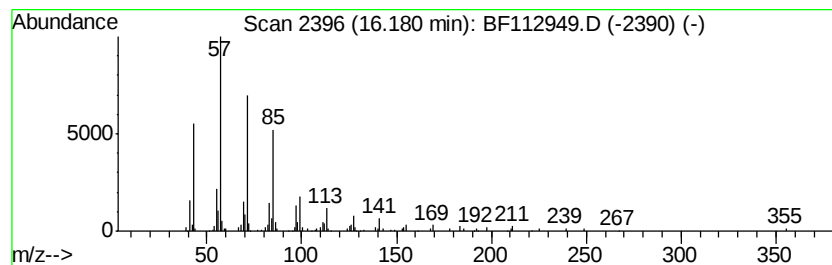
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.18 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	4.40 ng	264286	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Nonadecane	268	C19H40	000629-92-5	87
5			Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112949.D
Acq On : 8 Mar 2019 17:28
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Sample : K1761-01
Misc :
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ClientSampleId :
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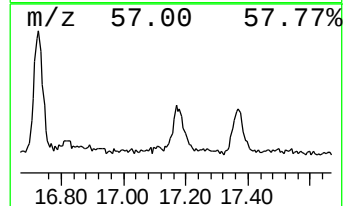
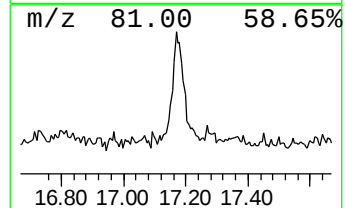
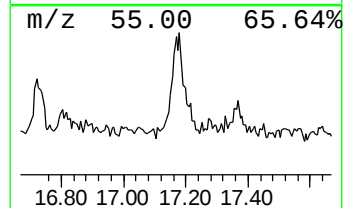
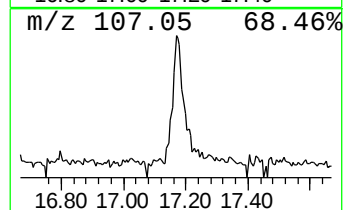
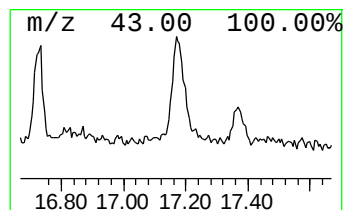
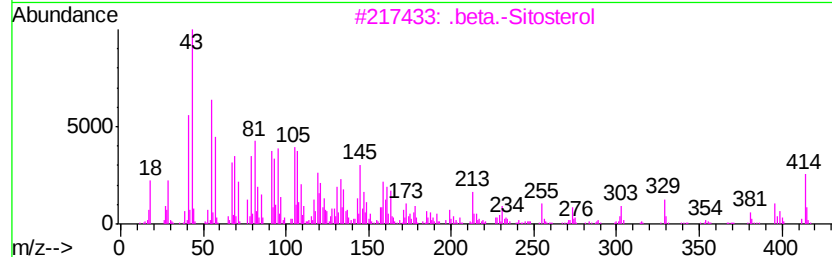
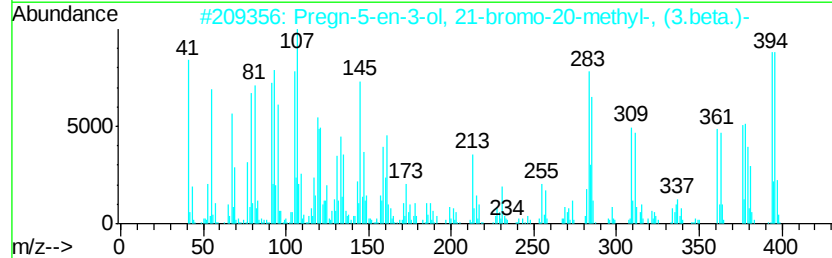
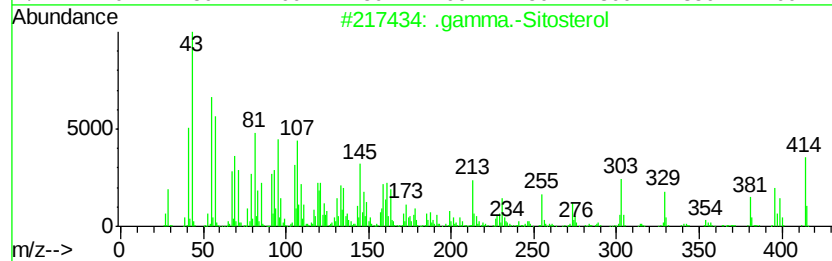
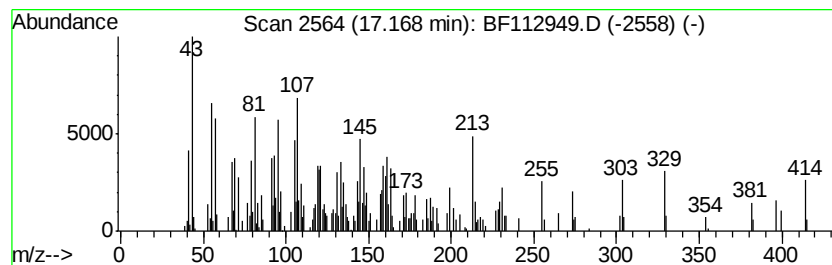
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 .gamma.-Sitosterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.17	6.11 ng	367223	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2			Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	93
3			.beta.-Sitosterol	414	C29H50O	000083-46-5	90
4			Stigmastan-3,5-diene	396	C29H48	1000214-16-4	22
5			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	20



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112949.D
Acq On : 8 Mar 2019 17:28
Operator : JU/SJ
Sample : K1761-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	11.77	11.4	ng	997742	4	11.23	1750180	20.0
Octadecanoic acid	12.56	11.5	ng	851520	5	13.86	1479890	20.0
Cyclotetradecane	13.72	6.3	ng	466174	5	13.86	1479890	20.0
Hexacosane	14.04	2.8	ng	207638	5	13.86	1479890	20.0
Heneicosane	14.34	4.6	ng	341891	5	13.86	1479890	20.0
unknown14.64	14.64	7.4	ng	444288	6	15.26	1202150	20.0
Tetracosane	14.96	8.7	ng	522655	6	15.26	1202150	20.0
unknown15.72	15.72	6.5	ng	393189	6	15.26	1202150	20.0
unknown16.18	16.18	4.4	ng	264286	6	15.26	1202150	20.0
.gamma.-Sitosterol	17.17	6.1	ng	367223	6	15.26	1202150	20.0