

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041819\
 Data File : BF113824.D
 Acq On : 18 Apr 2019 18:35
 Operator : JU/SJ
 Sample : K2422-11
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP3-S

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-BF041819.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	2.210	17	21	26	rVB	42352	53444	1.45%	0.150%
2	5.516	577	583	586	rBV	3620148	3460261	93.91%	9.731%
3	6.516	747	753	756	rBV	3513640	3431236	93.12%	9.649%
4	6.663	773	778	781	rBV	3916288	3564321	96.73%	10.023%
5	6.722	785	788	794	rVB2	83740	78671	2.14%	0.221%
6	6.892	814	817	821	rBV	1270779	1047991	28.44%	2.947%
7	7.051	840	844	847	rBV	3363478	2855945	77.51%	8.031%
8	7.451	906	912	915	rBV	2281328	2110889	57.29%	5.936%
9	8.175	1031	1035	1038	rBV	1518461	1238034	33.60%	3.481%
10	9.251	1213	1218	1221	rBV	4113935	3684752	100.00%	10.362%
11	9.633	1280	1283	1287	rVB	469208	406326	11.03%	1.143%
12	9.927	1329	1333	1337	rVB	1454708	1224496	33.23%	3.443%
13	10.710	1462	1466	1469	rBV	2356689	1979704	53.73%	5.567%
14	11.410	1581	1585	1588	rBV	1342326	1132187	30.73%	3.184%
15	11.933	1668	1674	1679	rBV	312061	309561	8.40%	0.871%
16	12.615	1787	1790	1793	rBV	40722	40514	1.10%	0.114%
17	12.715	1804	1807	1815	rBV	123816	143456	3.89%	0.403%
18	12.992	1849	1854	1857	rBV	4172013	3583795	97.26%	10.078%
19	13.886	2002	2006	2009	rBV	561653	520458	14.12%	1.464%
20	13.915	2009	2011	2016	rVB3	91374	86922	2.36%	0.244%
21	14.039	2027	2032	2035	rBV	1713820	1547582	42.00%	4.352%
22	14.215	2058	2062	2066	rBV	78733	77749	2.11%	0.219%
23	14.515	2110	2113	2118	rBV	130906	114992	3.12%	0.323%
24	14.827	2162	2166	2174	rVB	166094	201578	5.47%	0.567%
25	15.174	2221	2225	2233	rVB	148623	200874	5.45%	0.565%
26	15.509	2276	2282	2286	rBV	1377738	1716975	46.60%	4.828%
27	15.556	2286	2290	2299	rVB2	161189	250873	6.81%	0.705%
28	16.003	2361	2366	2369	rBV	97910	139855	3.80%	0.393%
29	16.045	2369	2373	2378	rVB2	95851	147788	4.01%	0.416%
30	16.515	2446	2453	2458	rBV2	98770	209276	5.68%	0.589%

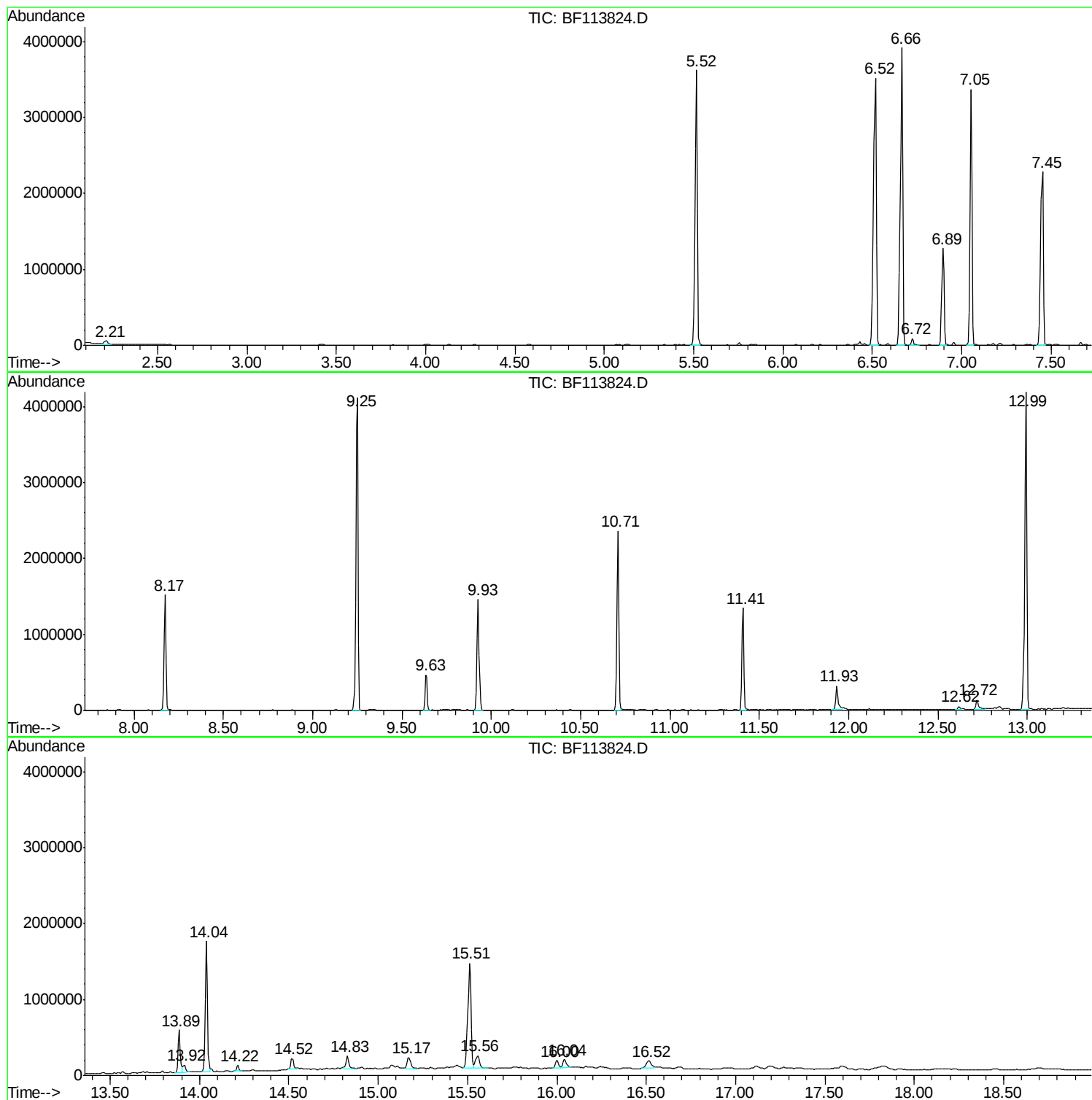
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Instrument :
BNA_F
ClientSampled :
TP3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF041819.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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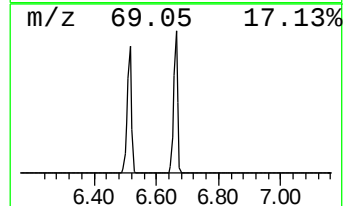
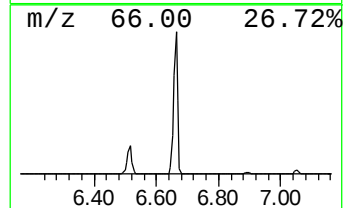
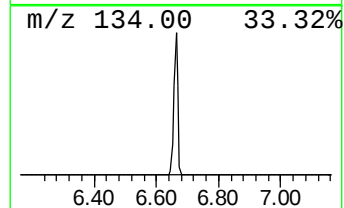
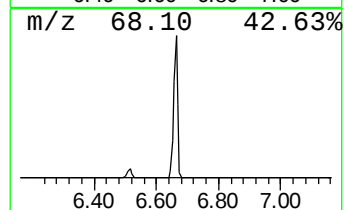
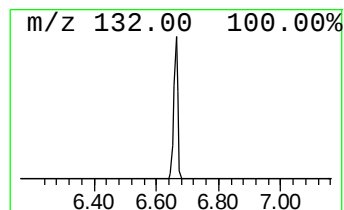
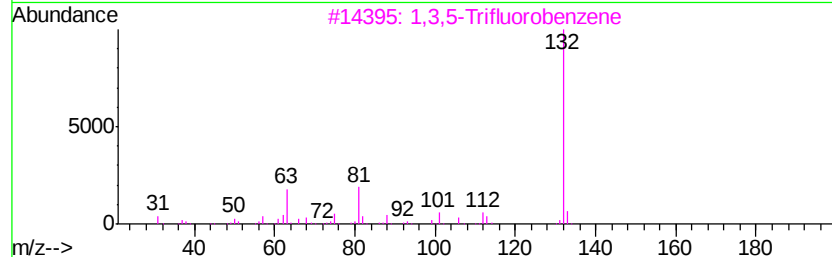
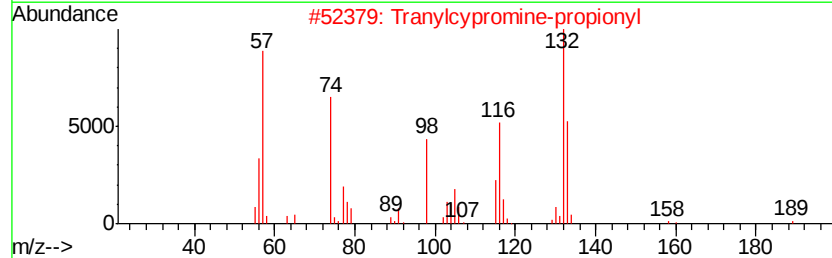
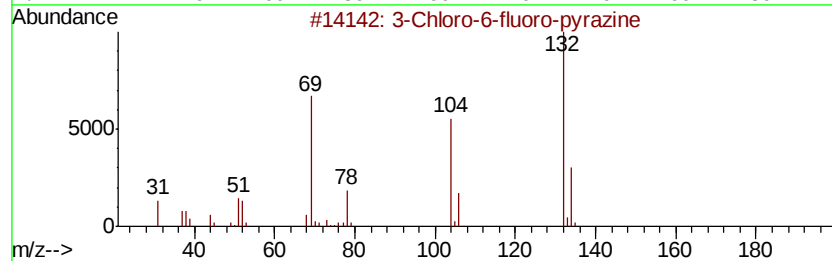
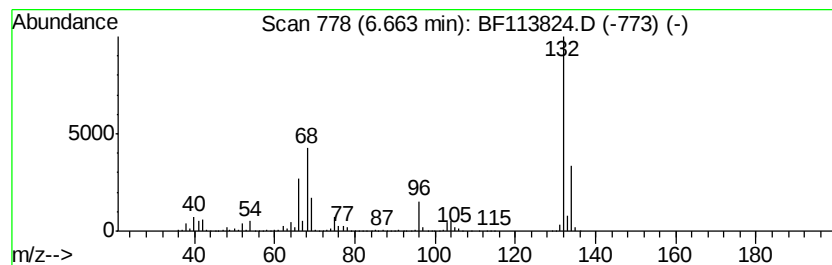
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.02 ng	3564320	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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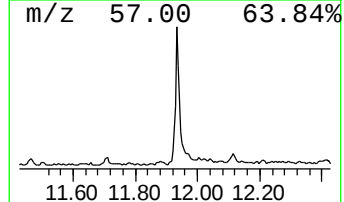
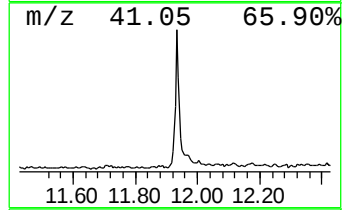
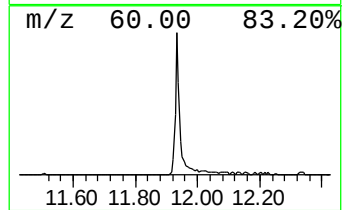
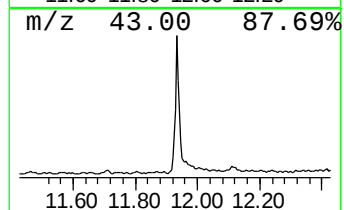
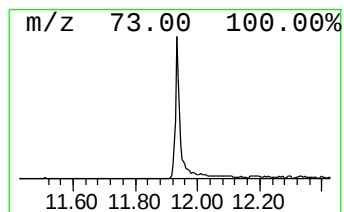
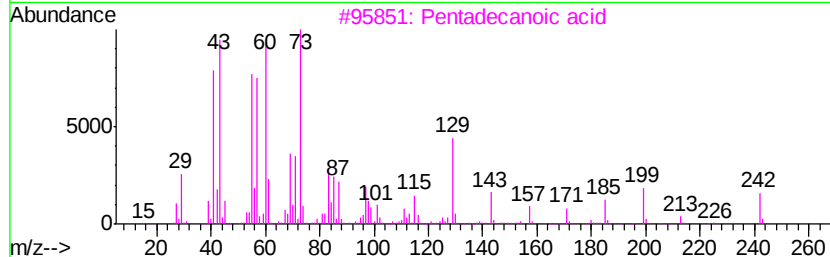
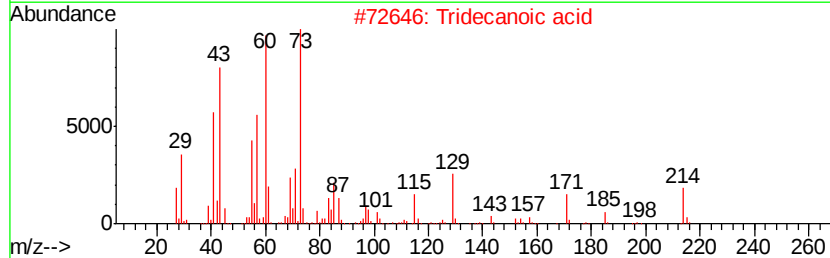
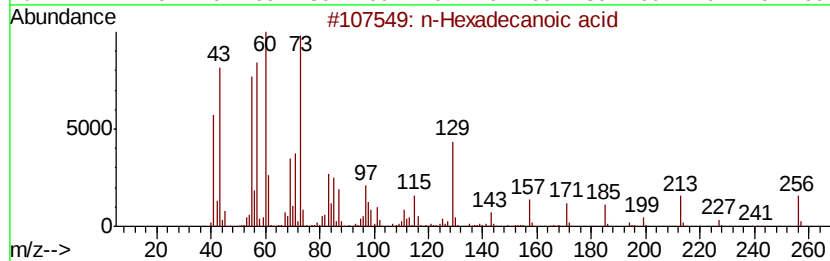
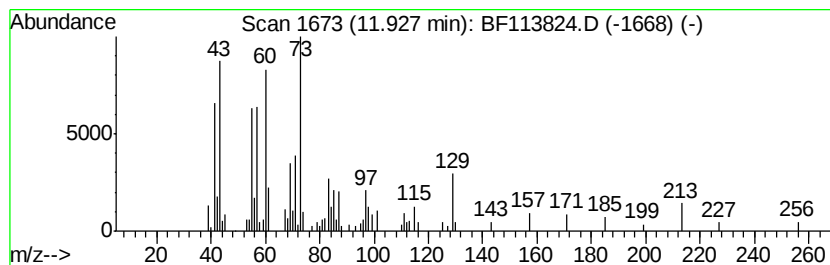
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	5.47 ng	309561	Phenanthrene-d10	11.41

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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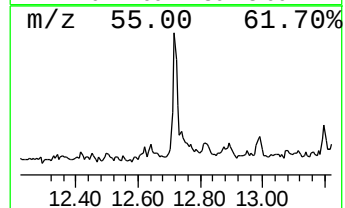
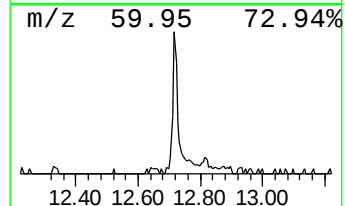
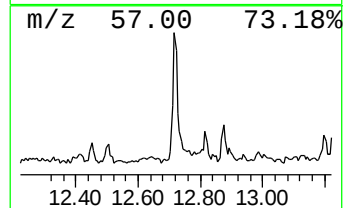
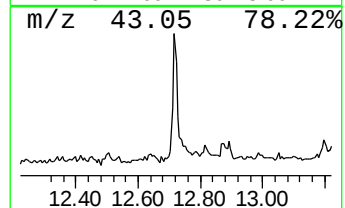
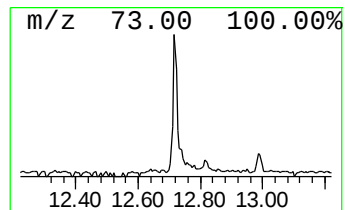
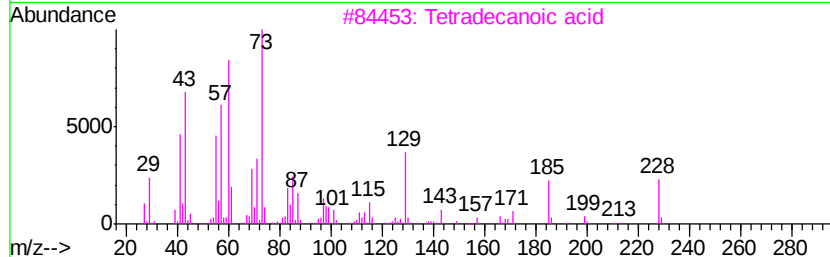
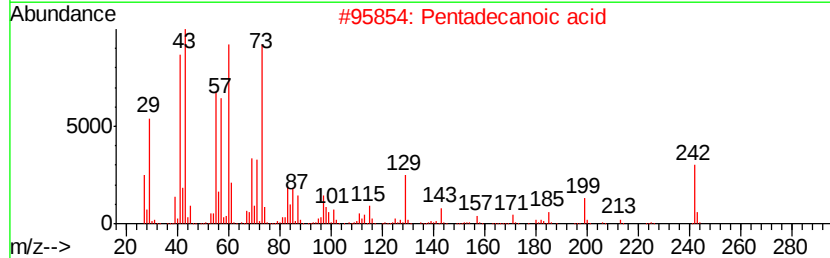
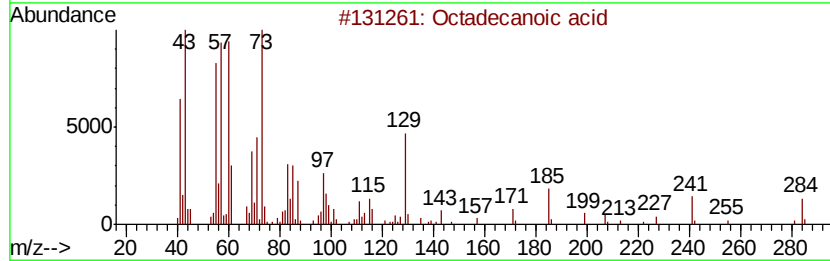
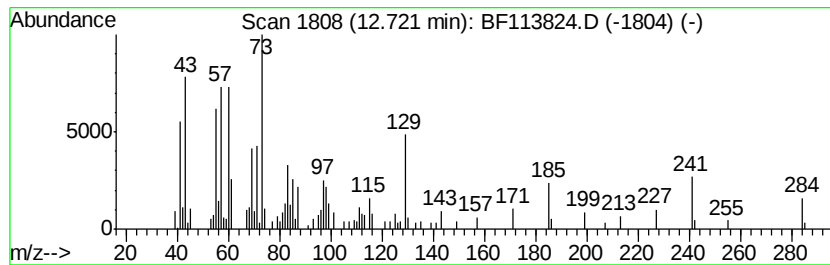
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.53 ng	143456	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5		Undecanoic acid	186	C11H22O2	000112-37-8	49



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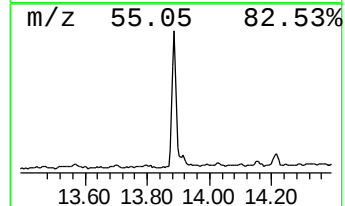
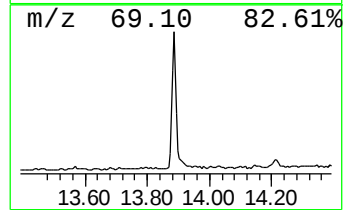
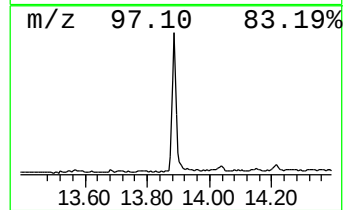
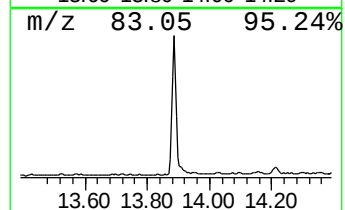
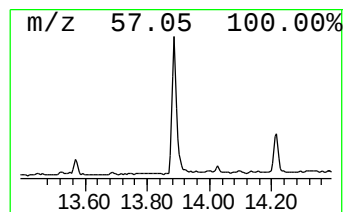
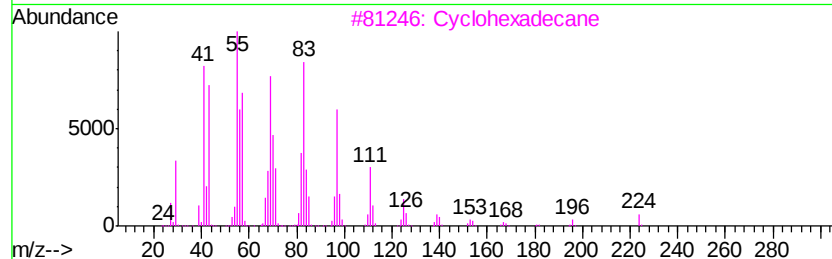
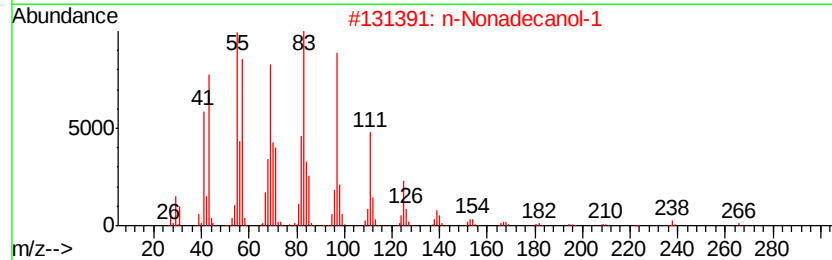
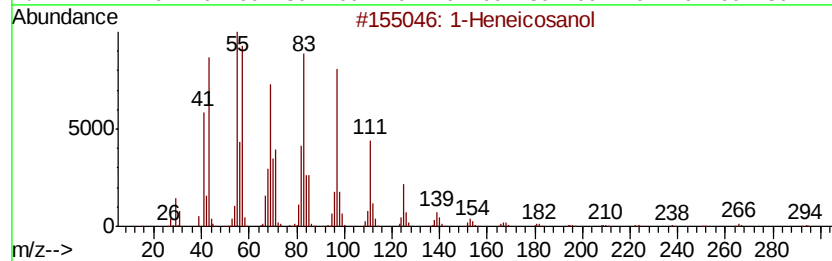
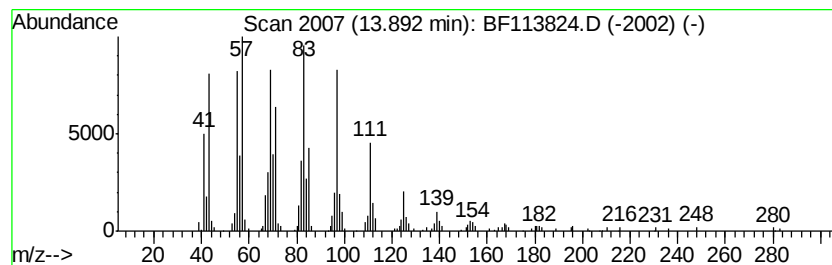
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.89	6.73 ng	520458	Chrysene-d12		14.04
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Cvclohexadecane	224	C16H32	000295-65-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	93



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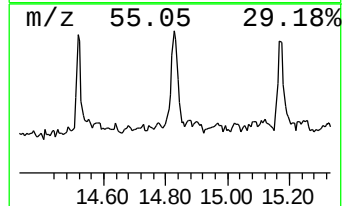
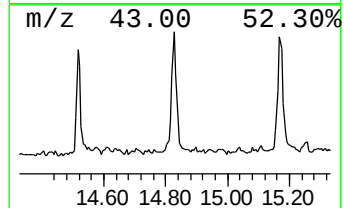
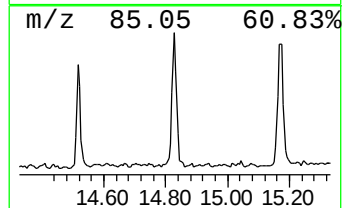
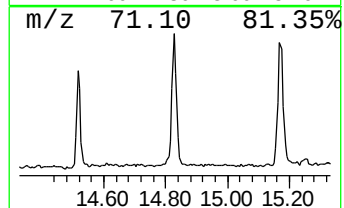
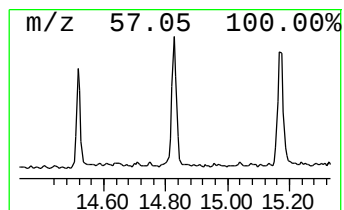
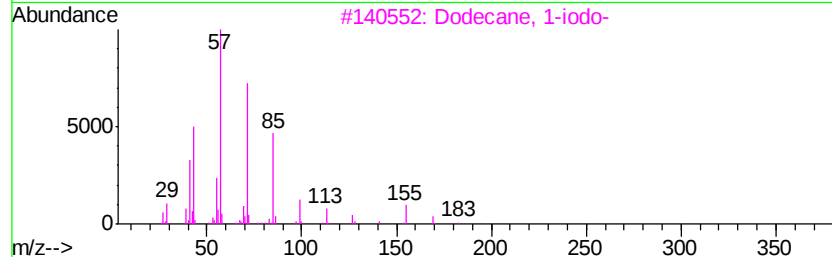
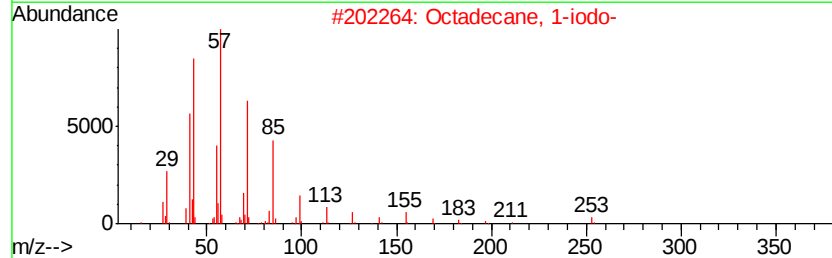
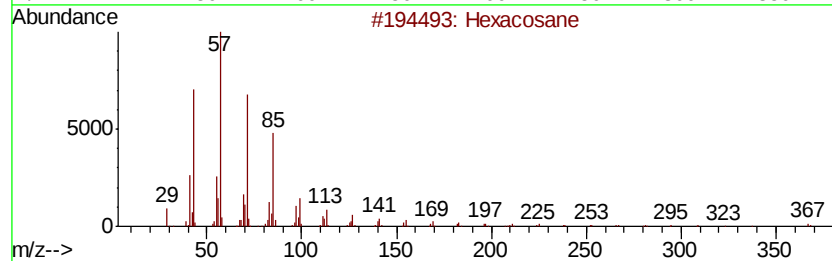
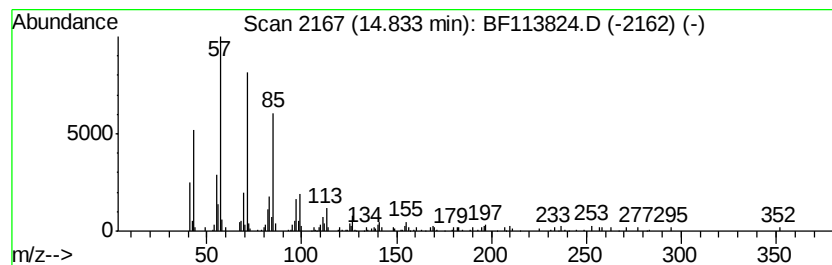
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.35 ng	201578	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	87
2	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	86
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	80
4	Octadecane		254	C18H38	000593-45-3	80
5	Octacosane		394	C28H58	000630-02-4	80



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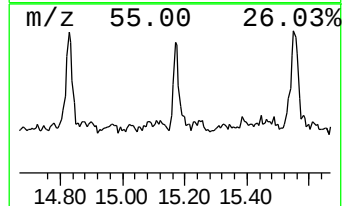
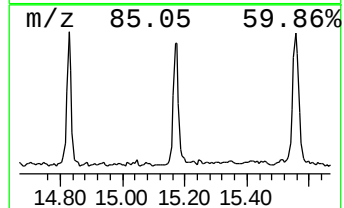
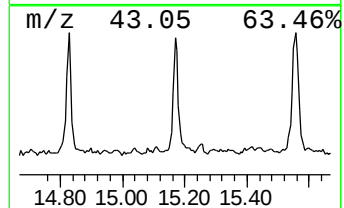
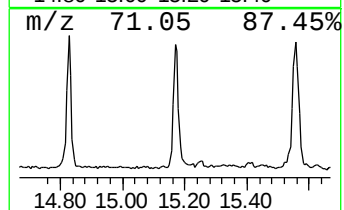
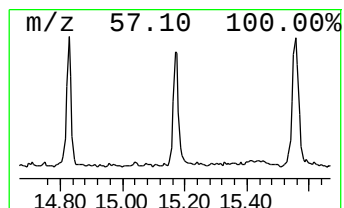
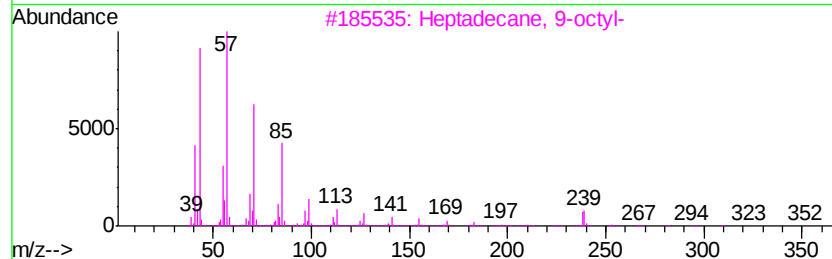
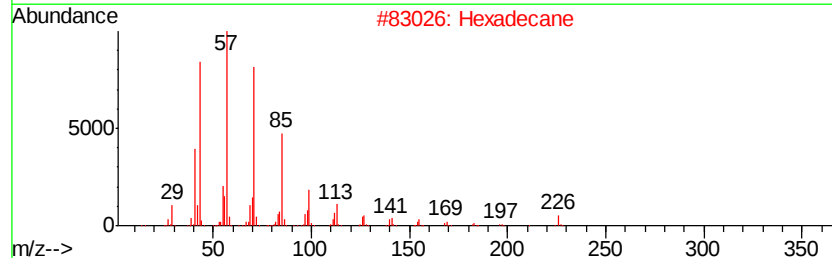
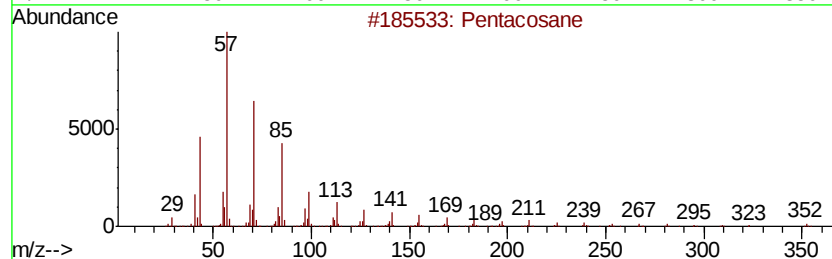
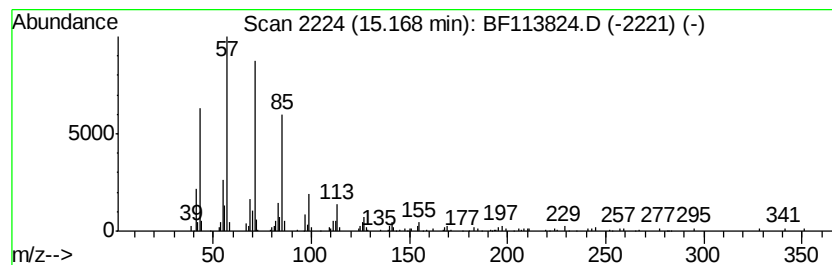
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.34 ng	200874	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	94
2	Hexadecane		226	C16H34	000544-76-3	93
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041819\
Data File : BF113824.D
Acq On : 18 Apr 2019 18:35
Operator : JU/SJ
Sample : K2422-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-S

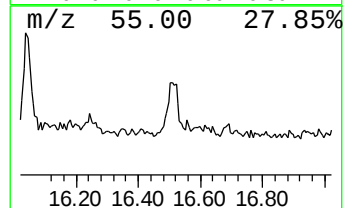
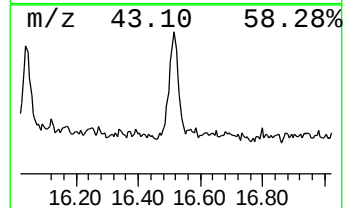
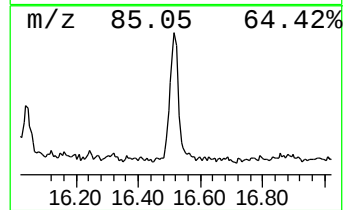
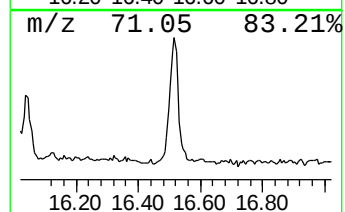
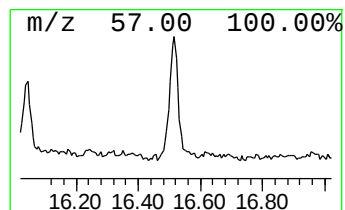
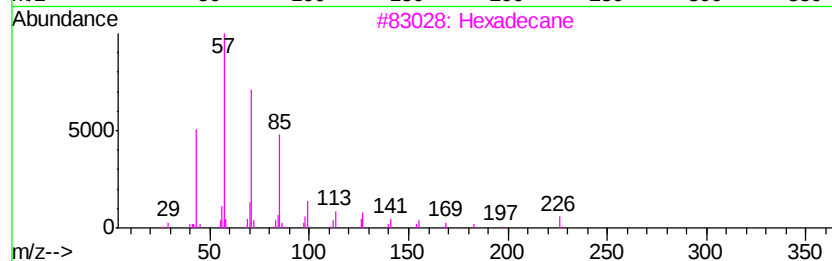
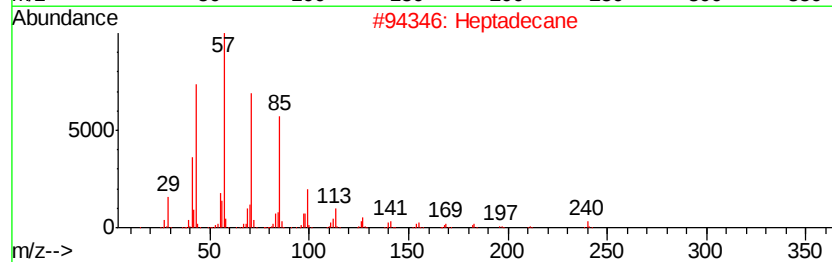
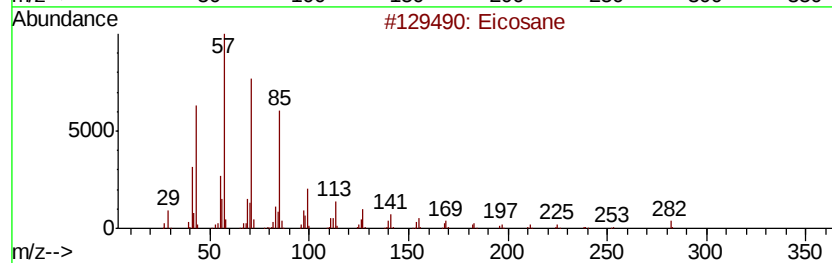
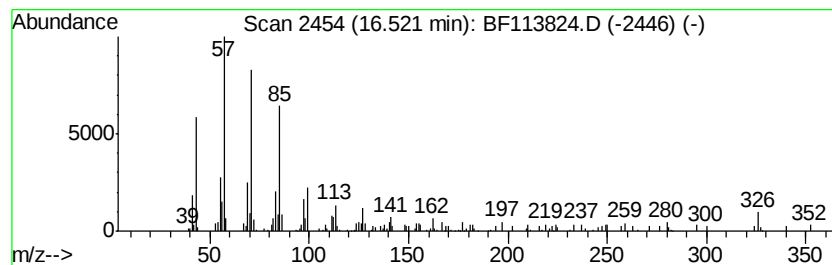
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	2.44 ng	209276	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	96
2	Heptadecane		240	C17H36	000629-78-7	95
3	Hexadecane		226	C16H34	000544-76-3	89
4	Tetratetracontane		619	C44H90	007098-22-8	87
5	Hentriacontane		437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041819\
Data File : BF113824.D
Acq On : 18 Apr 2019 18:35
Operator : JU/SJ
Sample : K2422-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041819.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
unknown6.66	6.66	68.0	ng	3564320	1	6.89	1047990	20.0
n-Hexadecanoic acid	11.93	5.5	ng	309561	4	11.41	1132190	20.0
Octadecanoic acid	12.72	2.5	ng	143456	4	11.41	1132190	20.0
1-Heneicosanol	13.89	6.7	ng	520458	5	14.04	1547580	20.0
Hexacosane	14.83	2.4	ng	201578	6	15.51	1716980	20.0
Pentacosane	15.17	2.3	ng	200874	6	15.51	1716980	20.0
Eicosane	16.52	2.4	ng	209276	6	15.51	1716980	20.0