

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107727.D
 Acq On : 27 Jul 2018 5:03
 Operator : JU/SJ
 Sample : J4146-01
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SES-CS-PH4-COA-01

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-BF072018.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	5.189	482	485	495	rBV	51221	74302	1.15%	0.186%
2	5.595	551	554	578	rBV	439125	1209140	18.71%	3.033%
3	6.595	721	724	744	rBV	265506	854616	13.22%	2.144%
4	6.731	744	747	773	rVV	2083024	2954296	45.72%	7.411%
5	6.960	783	786	808	rVB	601654	1067335	16.52%	2.677%
6	7.113	808	812	837	rBV	3343259	4278353	66.21%	10.732%
7	7.525	878	882	906	rBV	2200875	3569588	55.24%	8.954%
8	8.242	1000	1004	1033	rBV	1010015	1487448	23.02%	3.731%
9	9.313	1179	1186	1201	rBV	4778905	6462161	100.00%	16.210%
10	9.707	1248	1253	1258	rBV	228447	338554	5.24%	0.849%
11	9.901	1280	1286	1289	rVV5	79566	120098	1.86%	0.301%
12	10.001	1299	1303	1311	rBV	1294726	1382150	21.39%	3.467%
13	10.401	1369	1371	1374	rVB3	98870	98700	1.53%	0.248%
14	10.442	1375	1378	1380	rBV	92175	96945	1.50%	0.243%
15	10.630	1405	1410	1412	rBV	297934	397229	6.15%	0.996%
16	10.795	1434	1438	1445	rBV	1874008	2379066	36.82%	5.968%
17	10.895	1451	1455	1458	rBV	752355	793729	12.28%	1.991%
18	11.360	1531	1534	1537	rBV	538133	516959	8.00%	1.297%
19	11.495	1554	1557	1569	rVB	1052968	1431550	22.15%	3.591%
20	12.001	1641	1643	1648	rVB4	160832	153501	2.38%	0.385%
21	12.248	1683	1685	1688	rVB	207152	173993	2.69%	0.436%
22	13.077	1822	1826	1842	rVB	3640599	4031028	62.38%	10.112%
23	13.954	1972	1975	1982	rVB	94385	106371	1.65%	0.267%
24	14.142	2003	2007	2020	rBV	984318	1140162	17.64%	2.860%
25	14.271	2026	2029	2032	rVB	109690	98418	1.52%	0.247%
26	14.577	2077	2081	2087	rBV	261701	255146	3.95%	0.640%
27	14.895	2131	2135	2139	rBV	436412	449359	6.95%	1.127%
28	15.248	2190	2195	2202	rVB	571744	634896	9.82%	1.593%
29	15.648	2258	2263	2265	rBV	639205	903052	13.97%	2.265%
30	15.671	2265	2267	2282	rVB	688918	954686	14.77%	2.395%
31	16.106	2335	2341	2348	rBV	463500	705577	10.92%	1.770%
32	16.642	2426	2432	2438	rBV	255166	437128	6.76%	1.097%
33	17.265	2532	2538	2546	rVB2	94837	204231	3.16%	0.512%
34	18.012	2660	2665	2674	rVB2	43352	105426	1.63%	0.264%

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

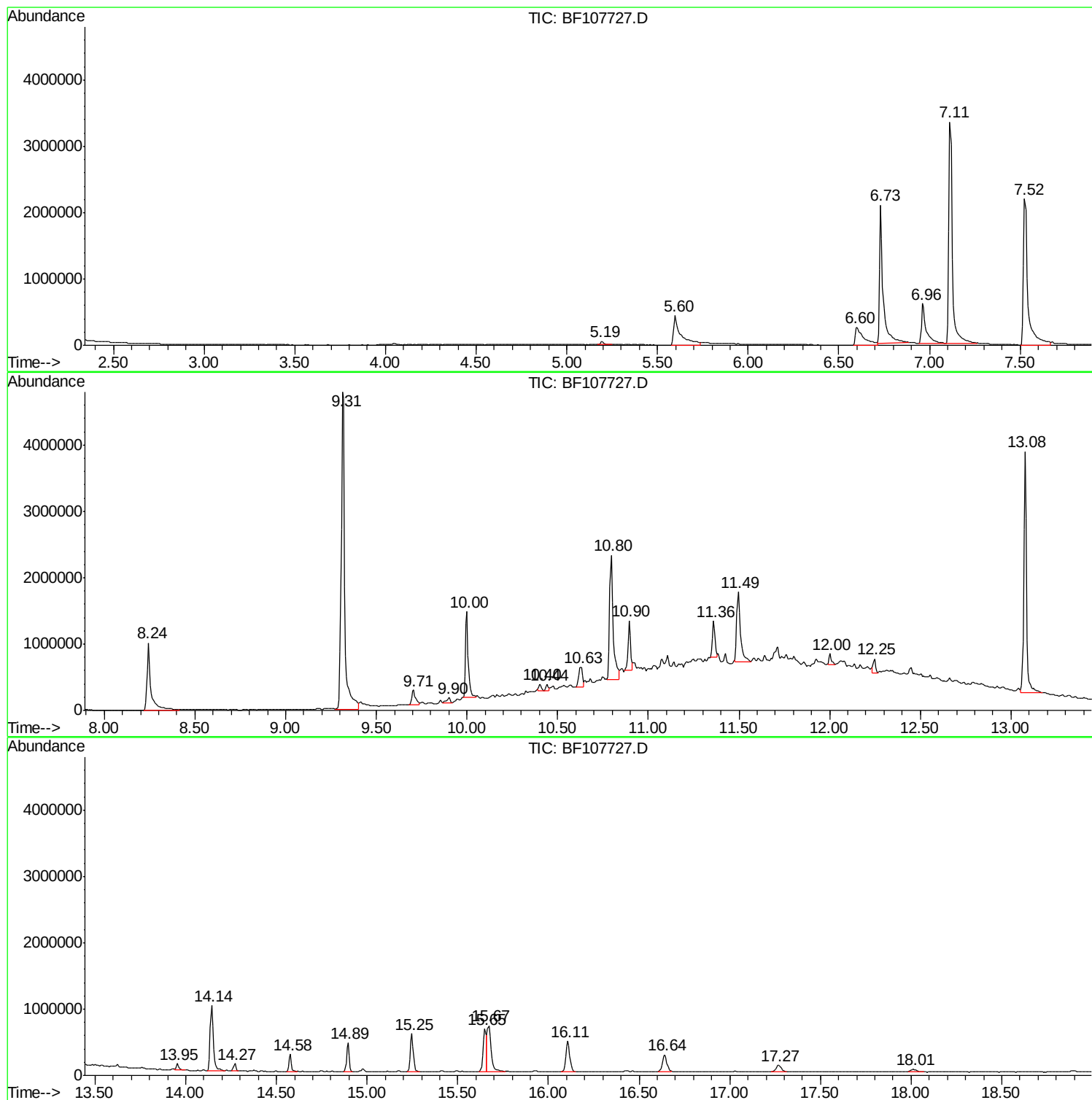
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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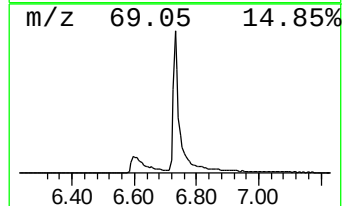
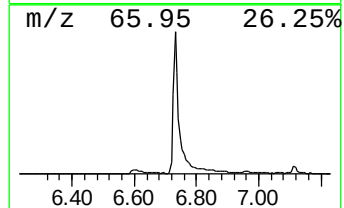
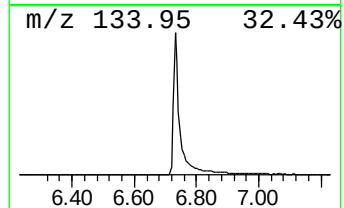
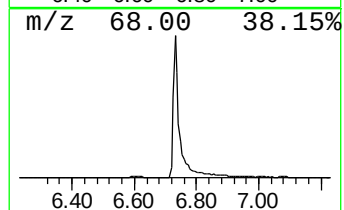
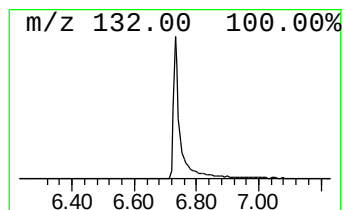
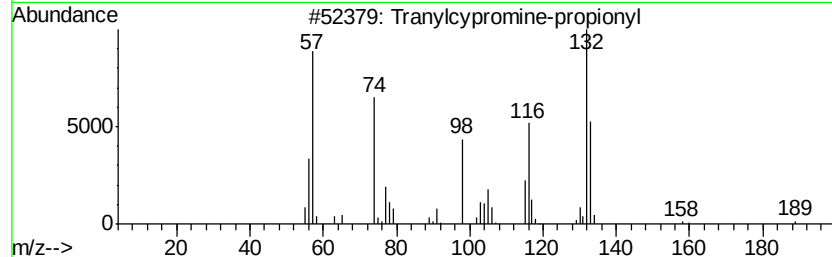
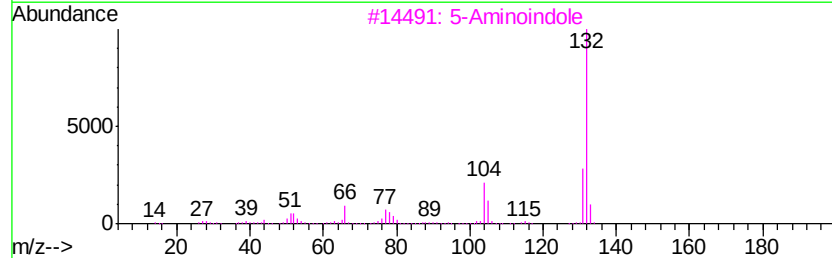
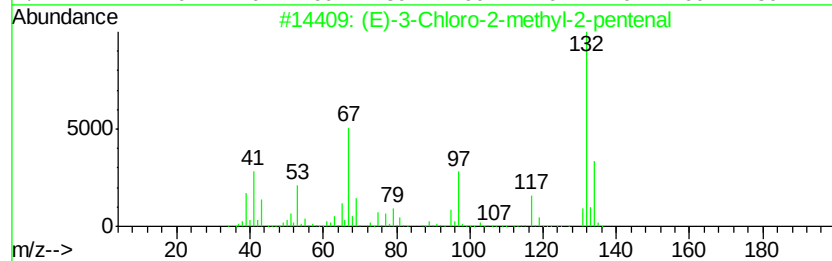
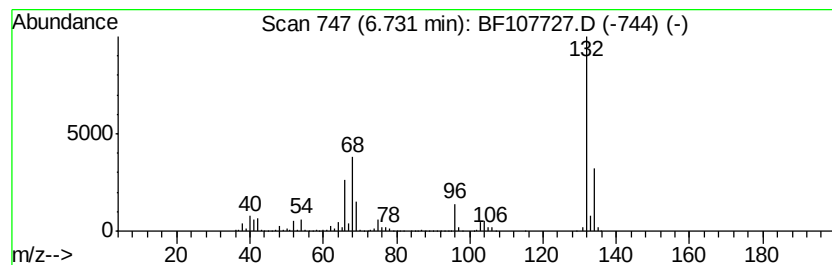
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	55.36 ng	2954300	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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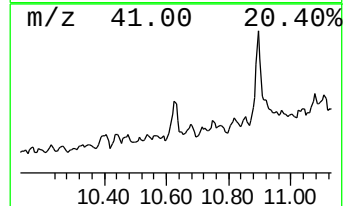
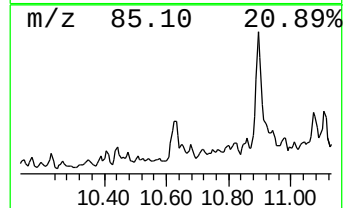
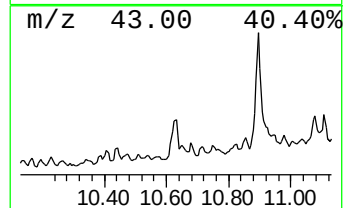
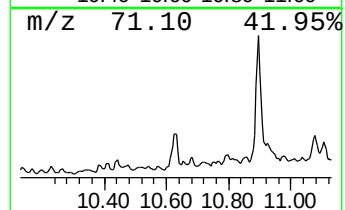
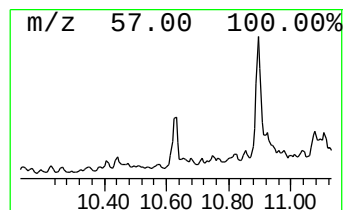
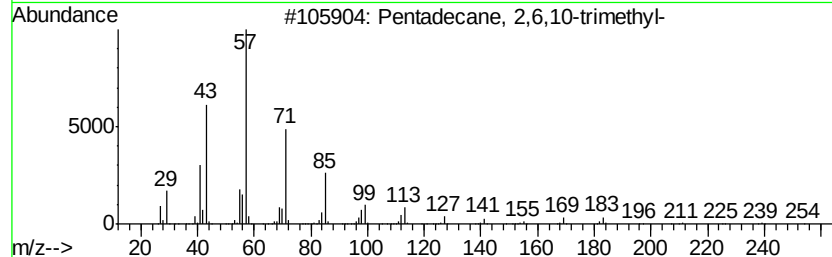
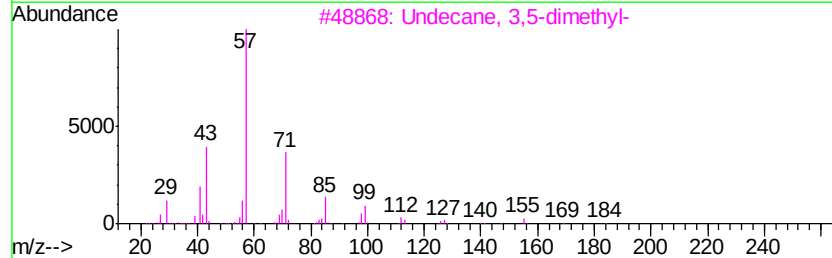
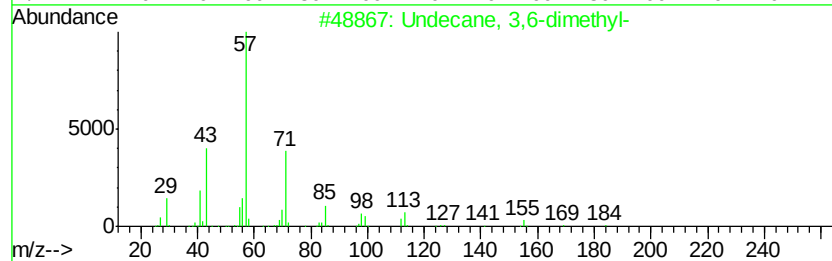
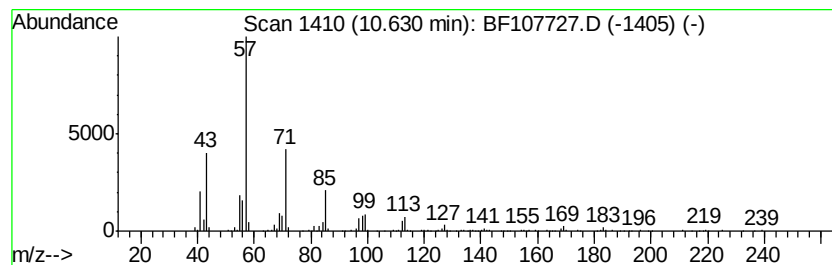
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane, 3,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.63	5.75 ng	397229	Acenaphthene-d10		10.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	81
2	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	74
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
4	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	68
5	Tetradecane, 2-methyl-	212	C15H32	001560-95-8	64



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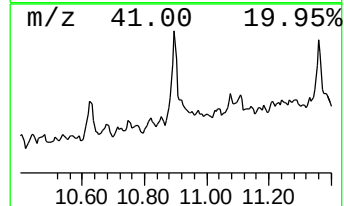
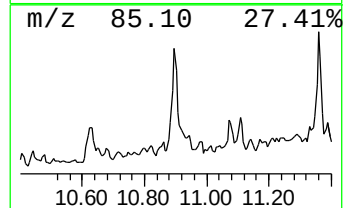
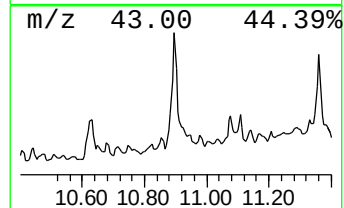
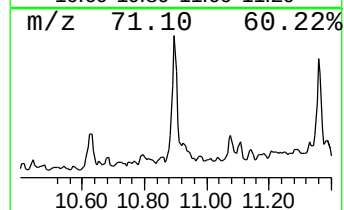
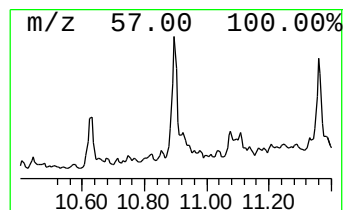
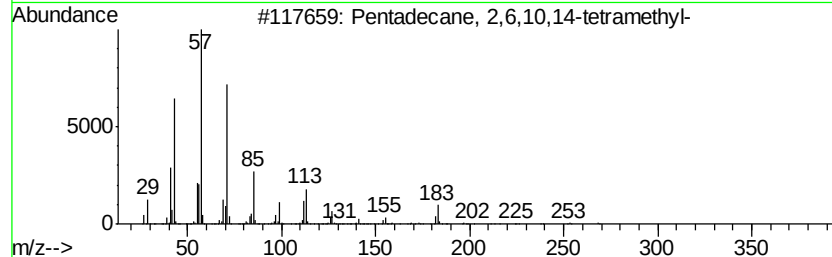
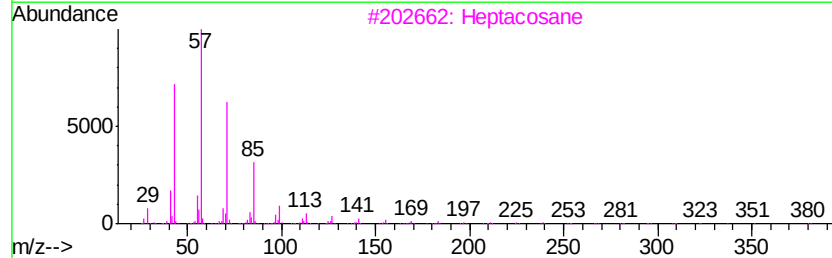
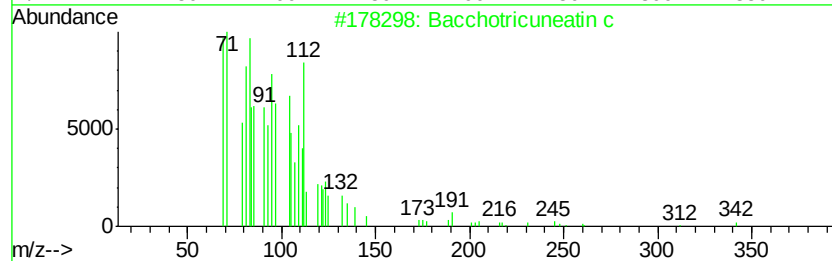
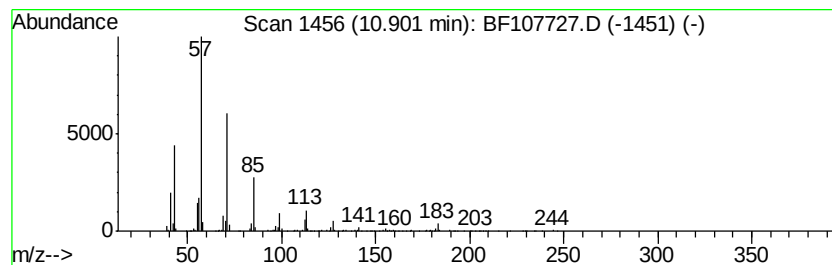
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bacchotricuneatin c Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.90	11.09 ng	793729	Phenanthrene-d10		11.49	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bacchotricuneatin c	342	C20H22O5	066563-30-2	96
2		Heptacosane	380	C27H56	000593-49-7	86
3		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	78
4		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78
5		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	72



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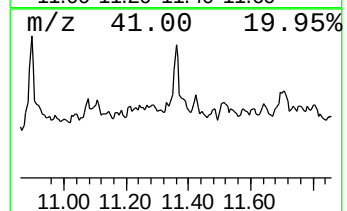
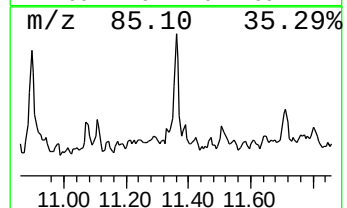
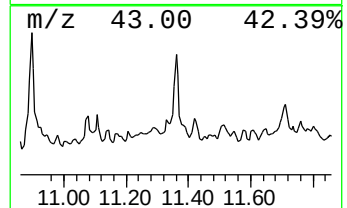
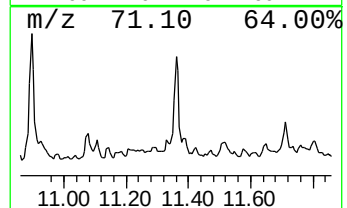
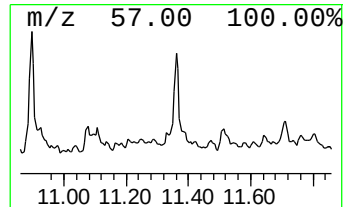
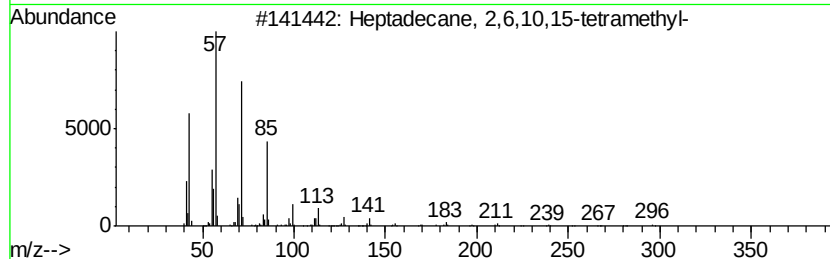
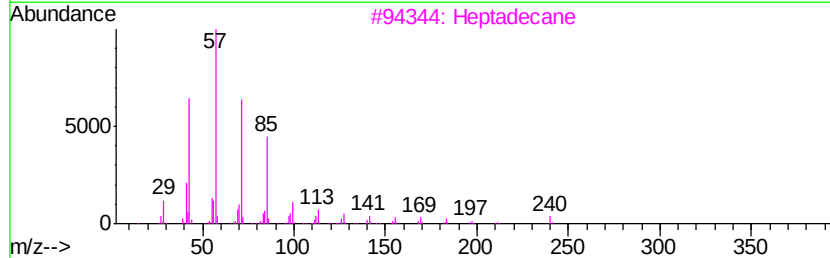
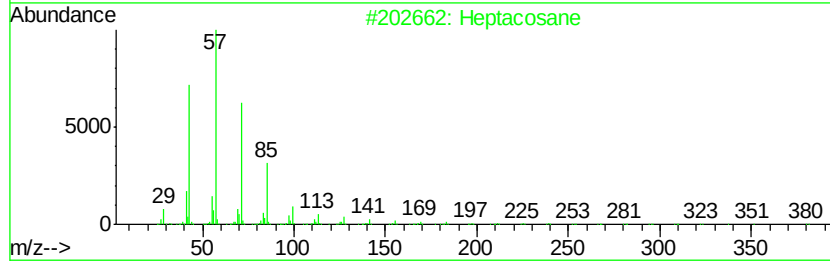
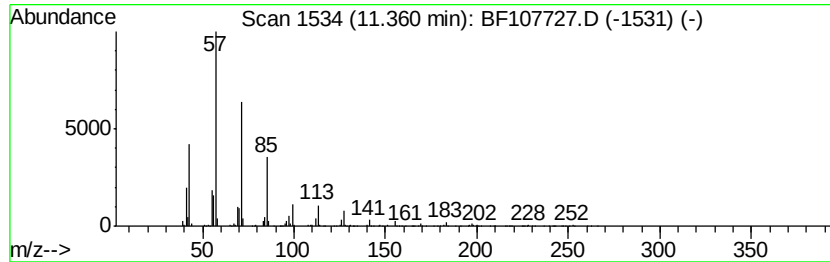
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	7.22 ng	516959	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4		Octadecane	254	C18H38	000593-45-3	90
5		Tetracosane	338	C24H50	000646-31-1	90



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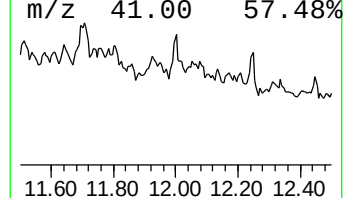
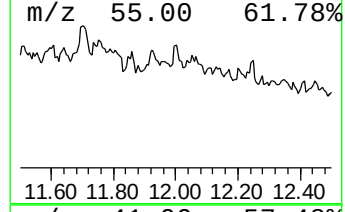
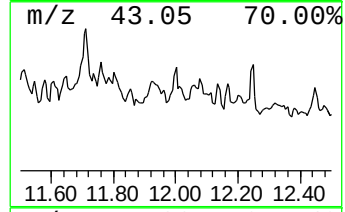
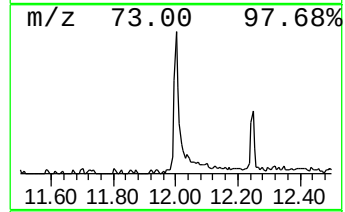
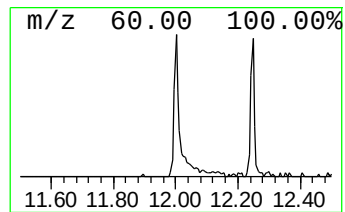
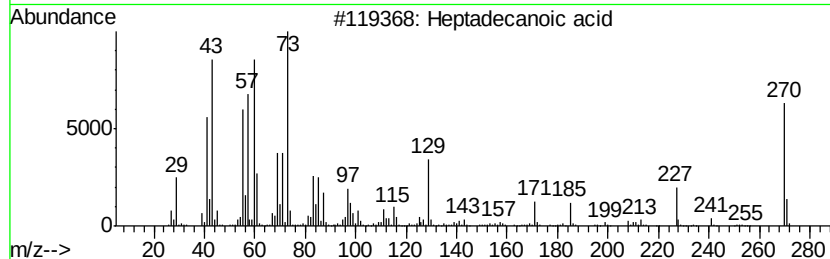
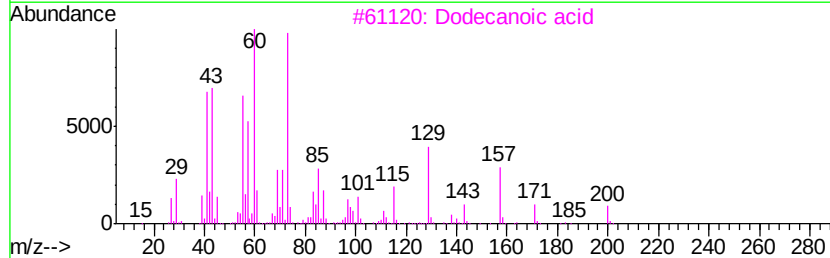
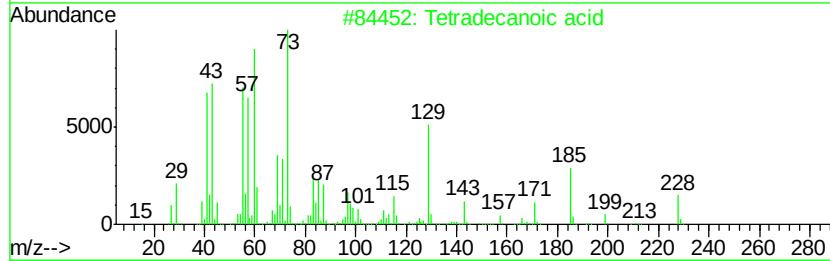
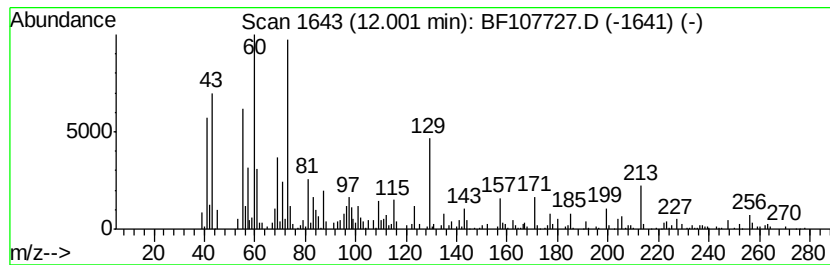
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Peak Number 6 Tetradecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.00	2.14 ng	153501	Phenanthrene-d10		11.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Heptadecanoic acid	270	C17H34O2	000506-12-7	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	42



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Misc :
ALS Vial : 29 Sample Multiplier: 1

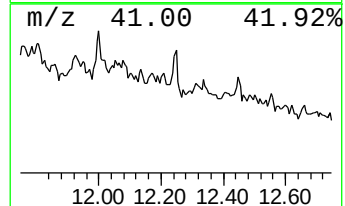
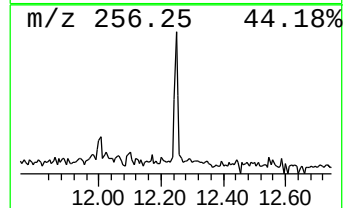
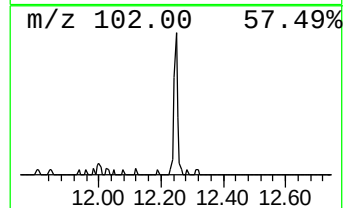
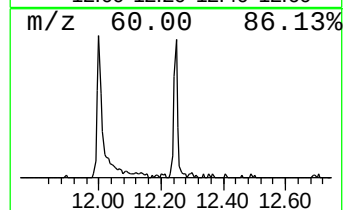
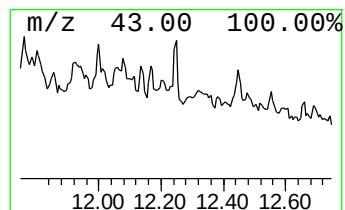
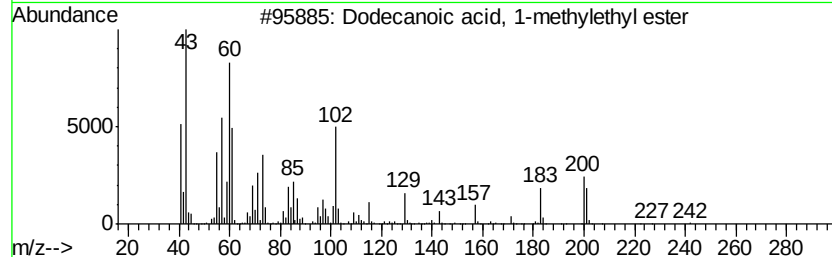
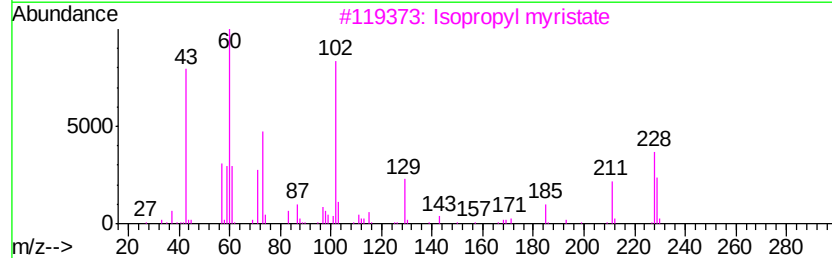
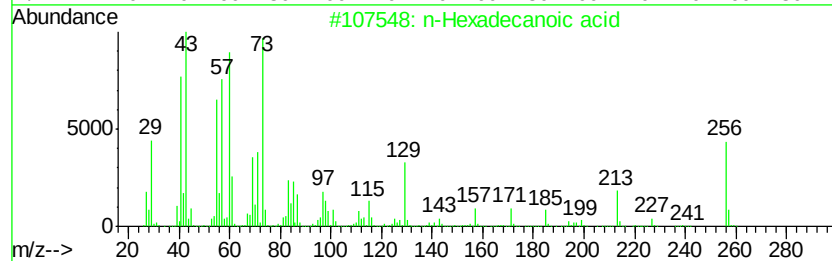
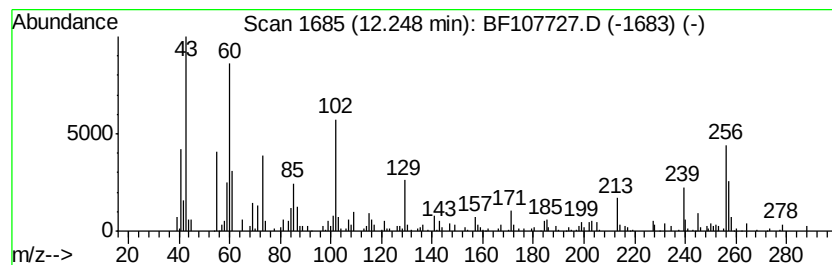
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.25	2.43 ng	173993	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2	Isopropyl myristate	270	C17H34O2	000110-27-0	43
3	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	37
4	Isopropyl palmitate	298	C19H38O2	000142-91-6	32
5	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107727.D
Acq On : 27 Jul 2018 5:03
Operator : JU/SJ
Sample : J4146-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

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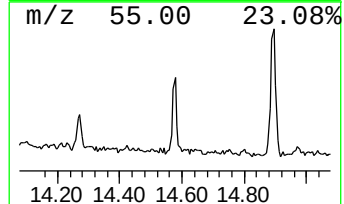
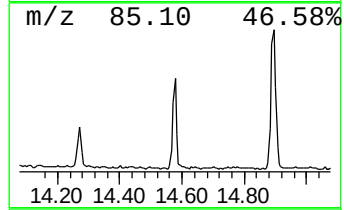
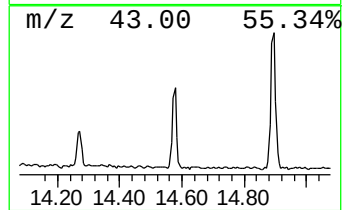
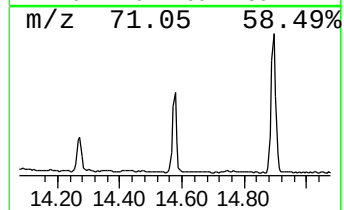
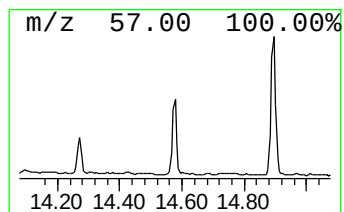
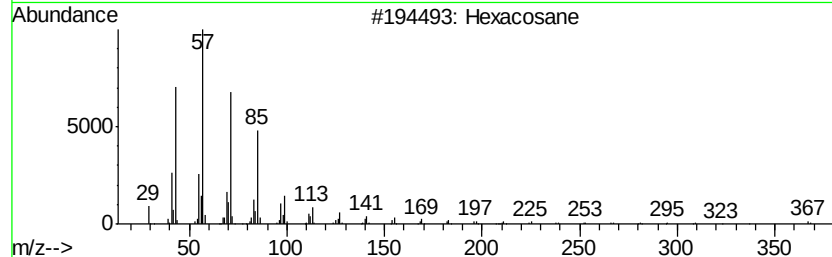
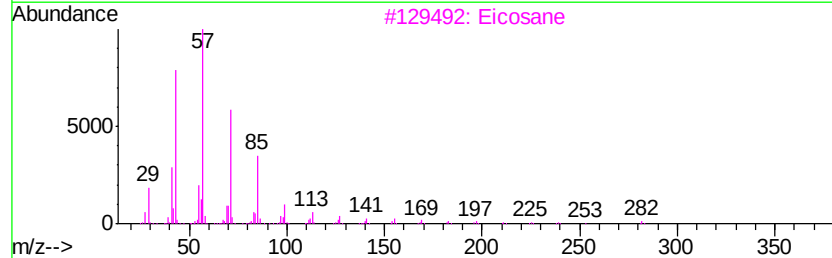
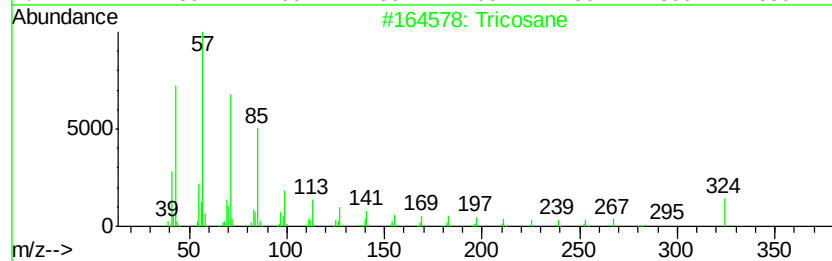
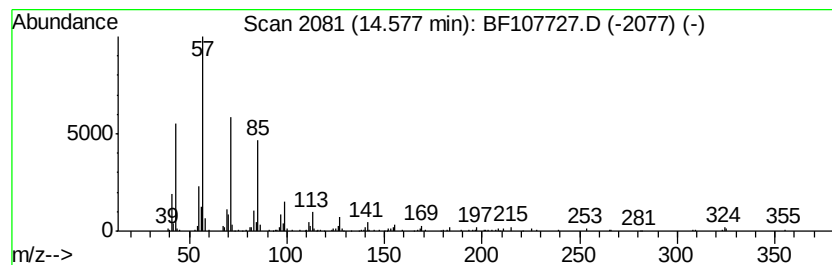
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tricosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	4.48 ng	255146	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	97
2		Eicosane	282	C20H42	000112-95-8	96
3		Hexacosane	366	C26H54	000630-01-3	94
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\BF072618\
Data File : BF107727.D
Acq On : 27 Jul 2018 5:03
Operator : JU/SJ
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Misc :
ALS Vial : 29 Sample Multiplier: 1

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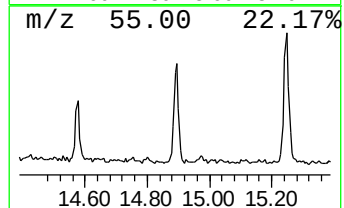
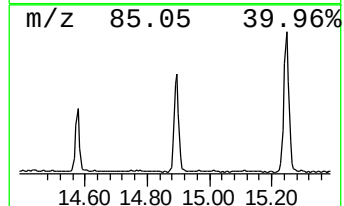
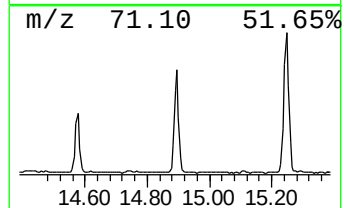
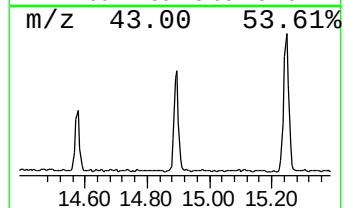
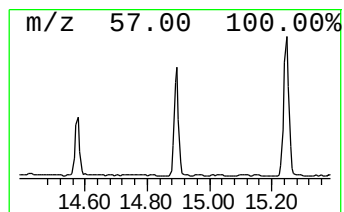
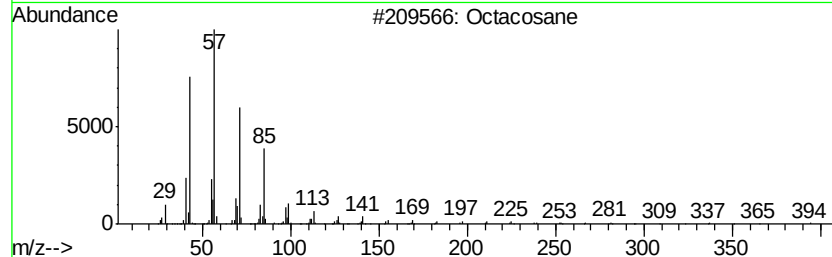
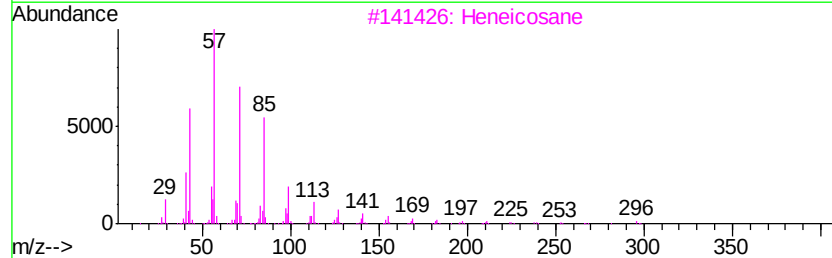
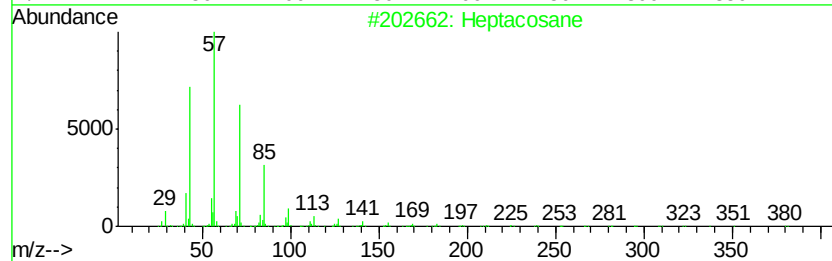
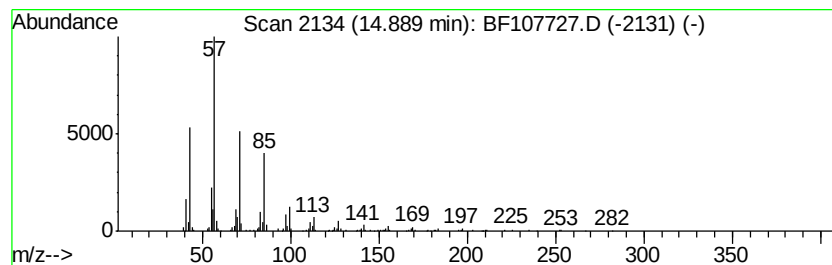
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	7.88 ng	449359	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107727.D
Acq On : 27 Jul 2018 5:03
Operator : JU/SJ
Sample : J4146-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

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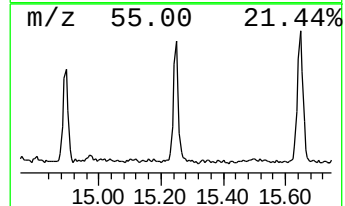
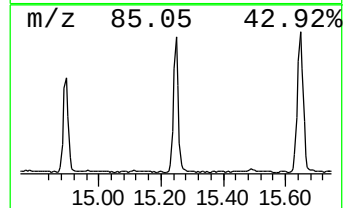
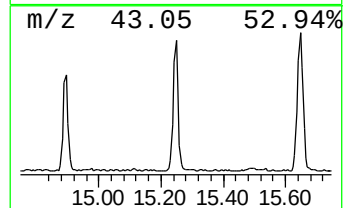
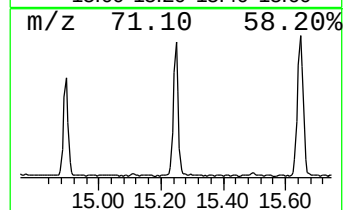
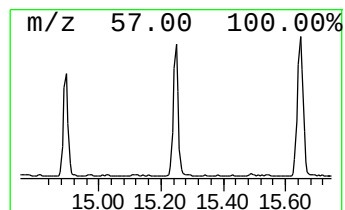
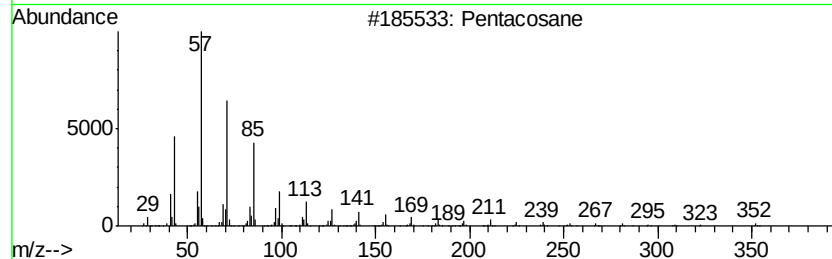
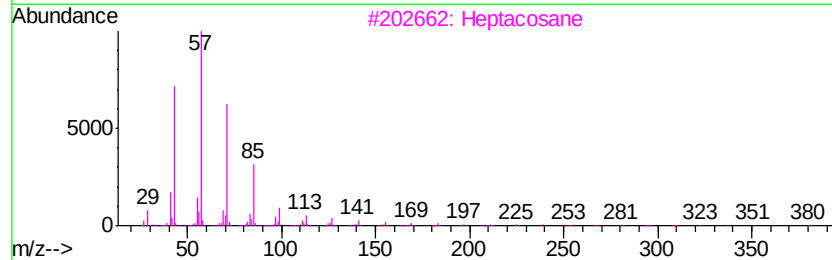
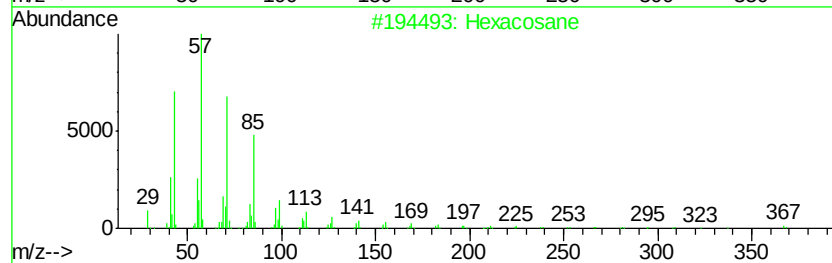
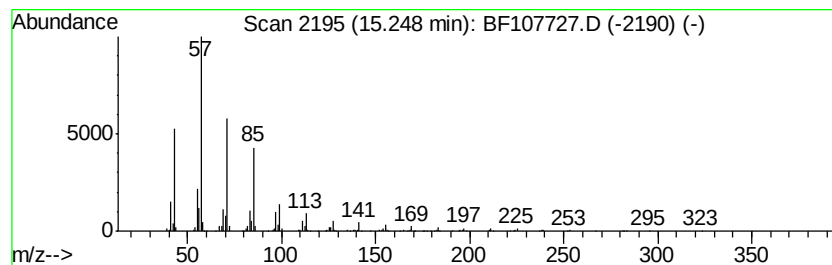
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	13.30 ng	634896	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Heptacosane	380	C27H56	000593-49-7	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
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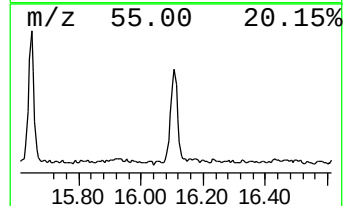
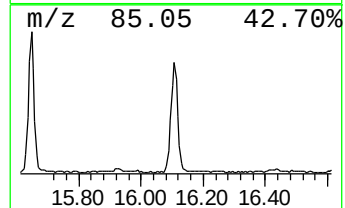
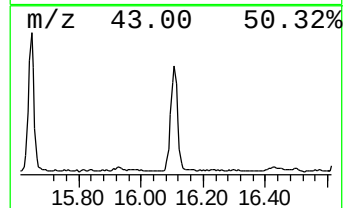
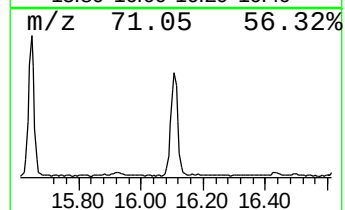
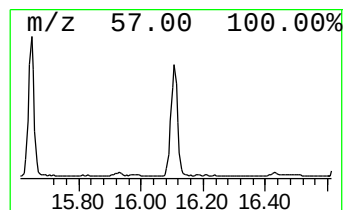
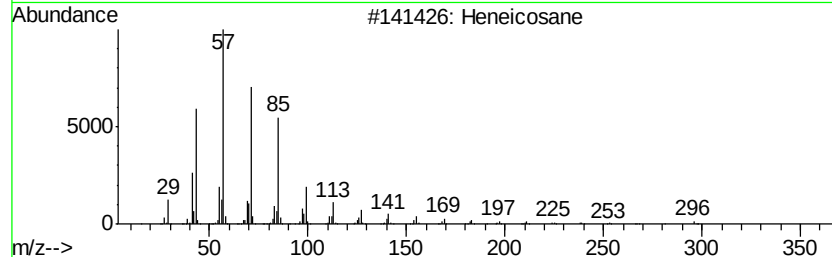
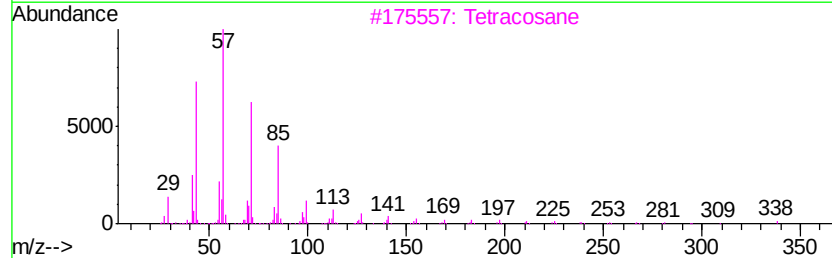
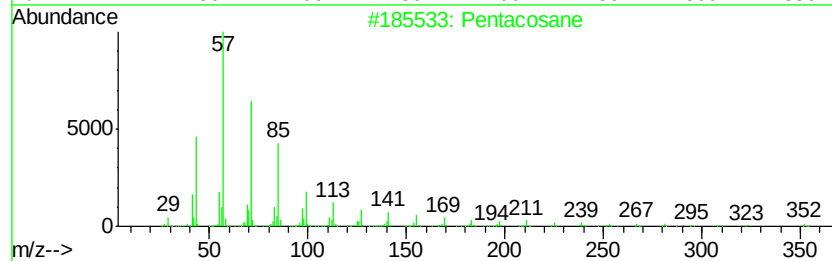
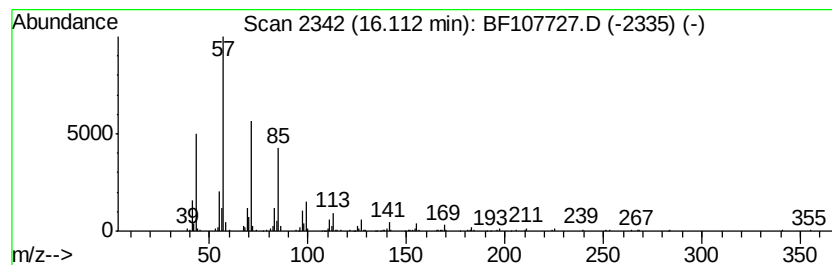
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	14.78 ng	705577	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107727.D
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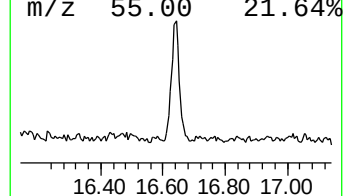
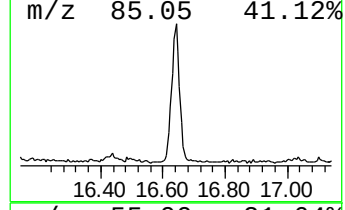
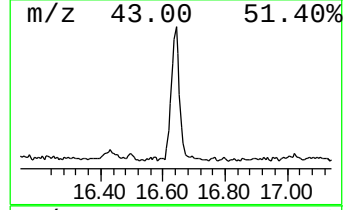
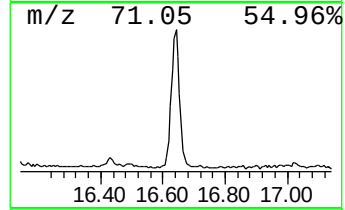
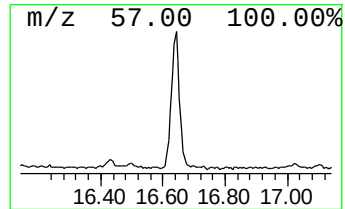
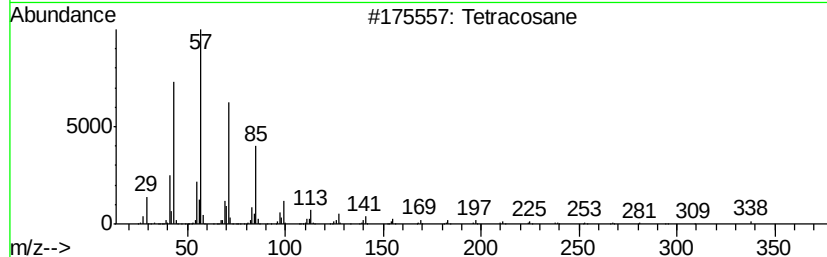
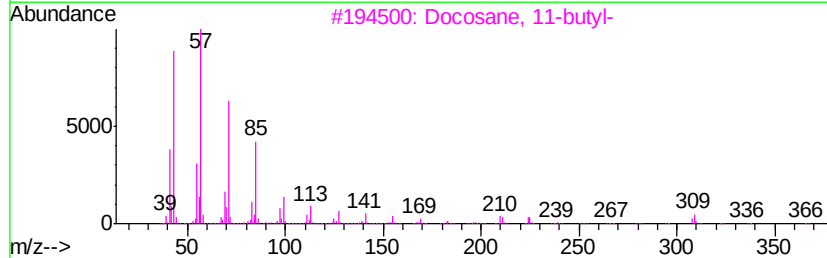
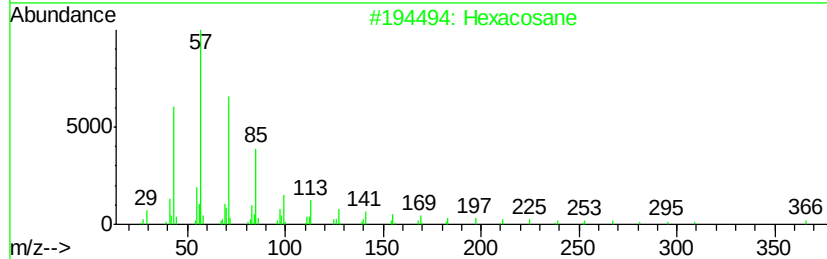
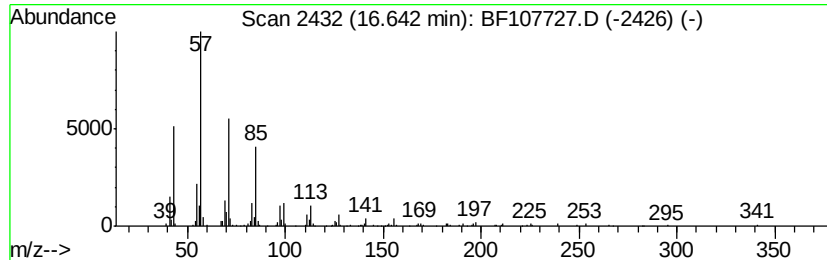
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	9.16 ng	437128	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3		Tetracosane	338	C24H50	000646-31-1	90
4		Nonadecane	268	C19H40	000629-92-5	87
5		Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107727.D
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Operator : JU/SJ
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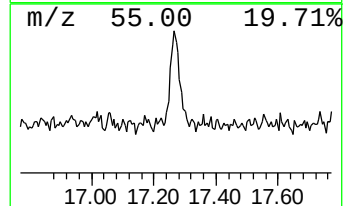
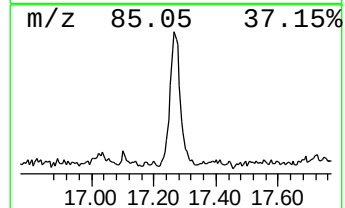
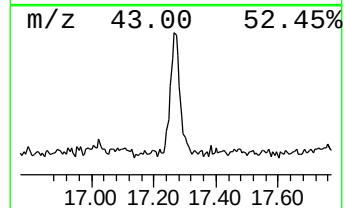
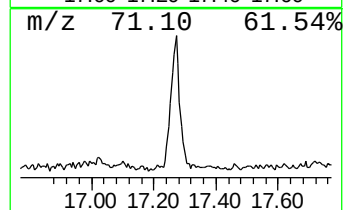
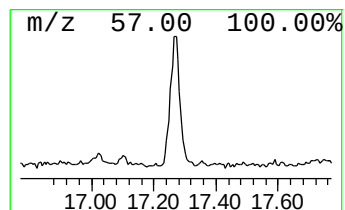
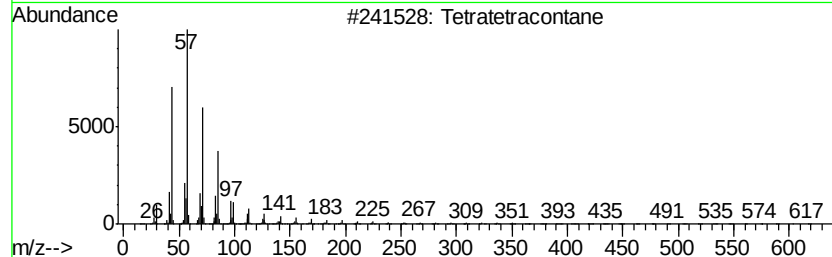
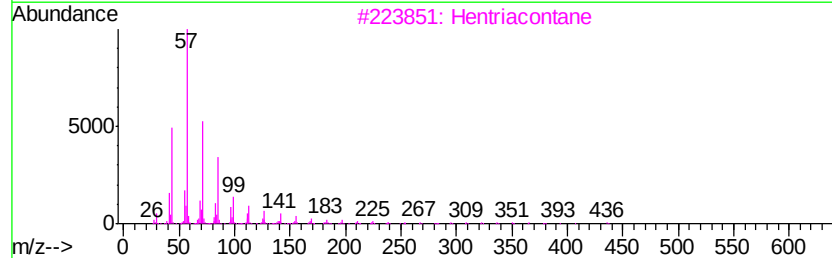
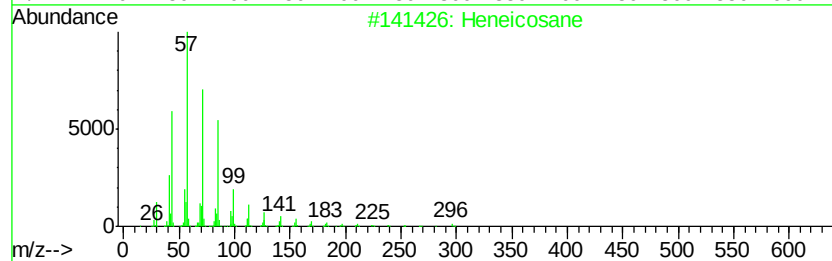
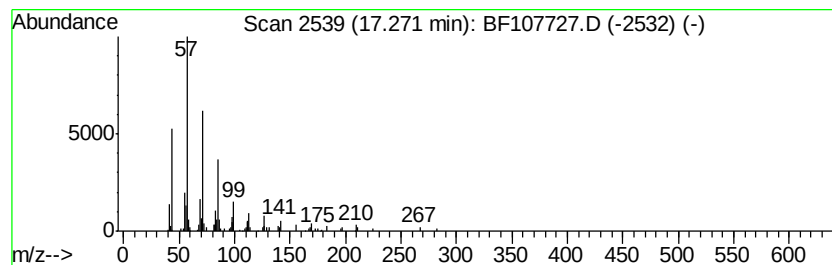
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	4.28 ng	204231	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Triacontane	422	C30H62	000638-68-6	90
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107727.D
Acq On : 27 Jul 2018 5:03
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Sample : J4146-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

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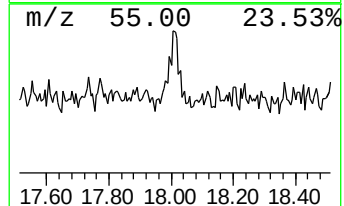
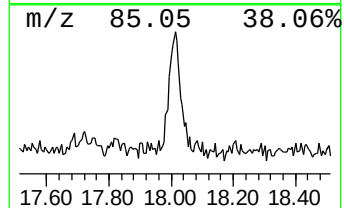
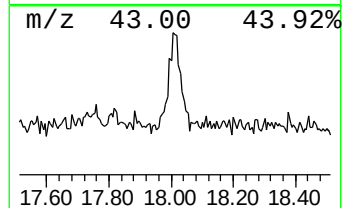
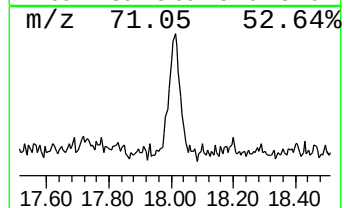
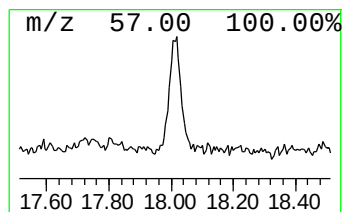
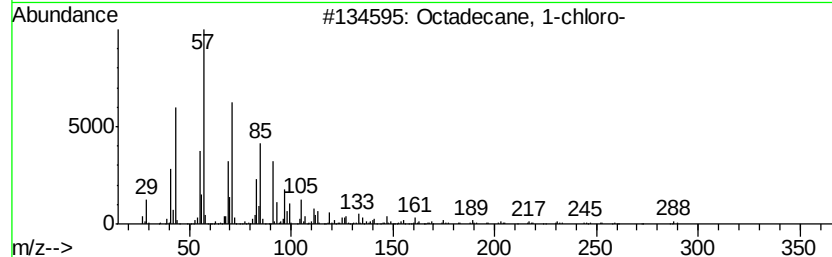
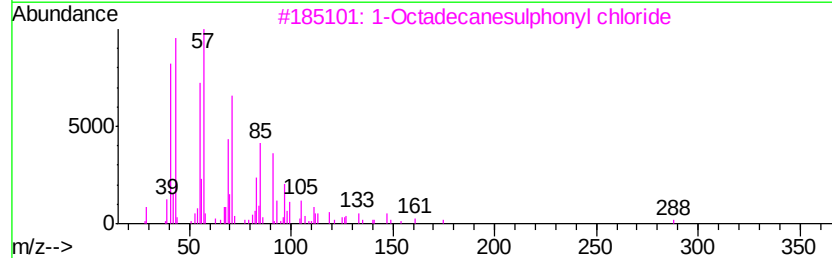
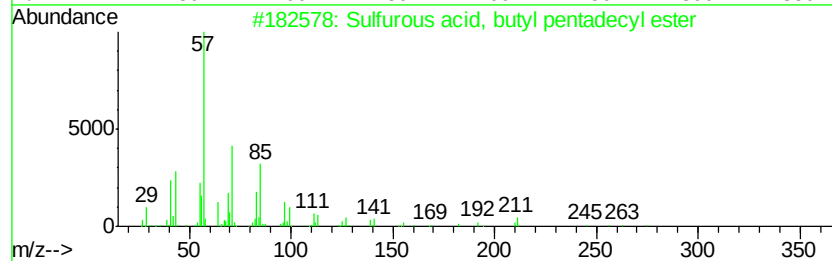
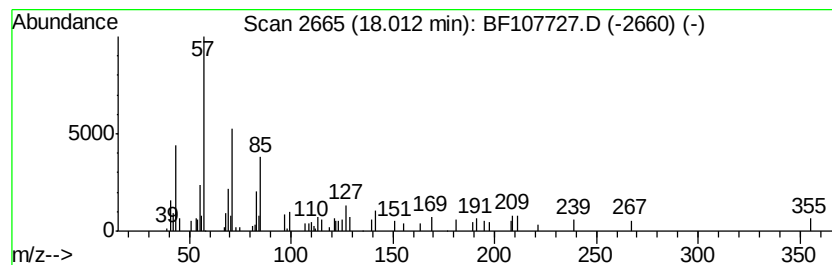
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Sulfurous acid, butyl penta... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	2.21 ng	105426	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	72
2		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
3		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
4		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	64
5		Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107727.D
 Acq On : 27 Jul 2018 5:03
 Operator : JU/SJ
 Sample : J4146-01
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SES-CS-PH4-COA-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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
unknown6.73	6.73	55.4	ng	2954300	1	6.96	1067340	20.0
Undecane, 3,6-dim...	10.63	5.8	ng	397229	3	10.00	1382150	20.0
Bacchotricuneatin c	10.90	11.1	ng	793729	4	11.49	1431550	20.0
Heptacosane	11.36	7.2	ng	516959	4	11.49	1431550	20.0
Tetradecanoic acid	12.00	2.1	ng	153501	4	11.49	1431550	20.0
n-Hexadecanoic acid	12.25	2.4	ng	173993	4	11.49	1431550	20.0
Tricosane	14.58	4.5	ng	255146	5	14.14	1140160	20.0
Octacosane	14.89	7.9	ng	449359	5	14.14	1140160	20.0
Hexacosane	15.25	13.3	ng	634896	6	15.67	954686	20.0
Pentacosane	16.11	14.8	ng	705577	6	15.67	954686	20.0
Tetracosane	16.64	9.2	ng	437128	6	15.67	954686	20.0
triacontane	17.27	4.3	ng	204231	6	15.67	954686	20.0
Sulfurous acid, b...	18.01	2.2	ng	105426	6	15.67	954686	20.0