

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
 Data File : BF110005.D
 Acq On : 19 Oct 2018 16:28
 Operator : JU/SJ
 Sample : J5590-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LS-DRUM

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-BF101518.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	2.134	3	8	14	rVB	1074848	1728800	29.83%	3.408%
2	2.340	36	43	49	rVB	2554584	3417561	58.97%	6.737%
3	5.204	526	530	538	rVB	129440	140097	2.42%	0.276%
4	5.587	591	595	598	rBV	2519695	2218818	38.28%	4.374%
5	6.581	759	764	769	rBV2	1680438	1630006	28.12%	3.213%
6	6.734	785	790	794	rBV	4018985	4120458	71.10%	8.122%
7	6.969	826	830	833	rBV	1760033	1491826	25.74%	2.941%
8	7.128	852	857	860	rBV	4129084	3956315	68.26%	7.799%
9	7.534	919	926	929	rBV	3101326	3286730	56.71%	6.479%
10	7.698	950	954	957	rBV2	80265	84903	1.46%	0.167%
11	8.051	1006	1014	1019	rBV2	48796	64704	1.12%	0.128%
12	8.251	1043	1048	1051	rBV	2313155	1946297	33.58%	3.837%
13	9.328	1225	1231	1234	rBV	6041227	5795677	100.00%	11.425%
14	9.716	1292	1297	1300	rBV	507617	398427	6.87%	0.785%
15	10.010	1342	1347	1351	rBV2	2402244	2178844	37.59%	4.295%
16	10.545	1431	1438	1442	rBV2	93649	94140	1.62%	0.186%
17	10.804	1476	1482	1485	rBV	3405851	3410944	58.85%	6.724%
18	11.504	1596	1601	1604	rBV	2385994	2105238	36.32%	4.150%
19	12.010	1683	1687	1691	rBV	351696	324815	5.60%	0.640%
20	12.051	1691	1694	1697	rVB	53171	63625	1.10%	0.125%
21	12.798	1817	1821	1829	rBV2	84139	106151	1.83%	0.209%
22	13.086	1865	1870	1874	rBV	4818344	4928826	85.04%	9.716%
23	13.963	2016	2019	2024	rBV	560269	525935	9.07%	1.037%
24	14.145	2046	2050	2053	rBV	1893545	1616380	27.89%	3.186%
25	14.286	2071	2074	2080	rVB	137972	123173	2.13%	0.243%
26	14.592	2122	2126	2135	rBV	263958	259058	4.47%	0.511%
27	14.915	2175	2181	2190	rBV	355181	400421	6.91%	0.789%
28	14.998	2190	2195	2200	rVB	492441	521550	9.00%	1.028%
29	15.268	2236	2241	2252	rBV	446328	526860	9.09%	1.039%
30	15.668	2303	2309	2318	rBV2	1253307	1740999	30.04%	3.432%
31	16.133	2382	2388	2394	rBV	332218	512105	8.84%	1.009%
32	16.668	2473	2479	2487	rBV	184265	323384	5.58%	0.637%
33	17.304	2581	2587	2595	rBV2	66209	145470	2.51%	0.287%
34	17.398	2595	2603	2614	rBV2	209065	467810	8.07%	0.922%

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.056	2709	2715	2722	rVB6	32410	73206	1.26%	0.144%
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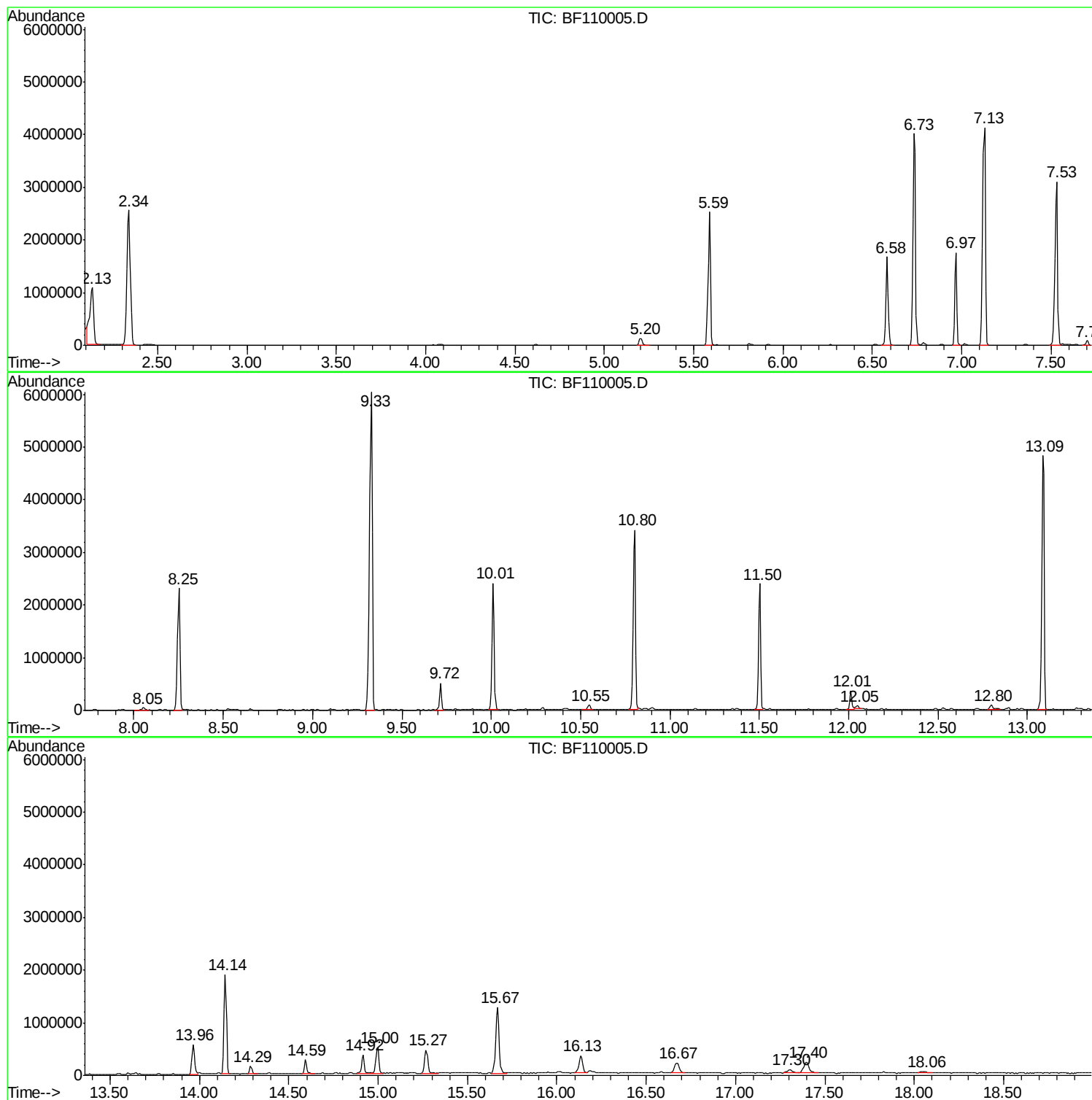
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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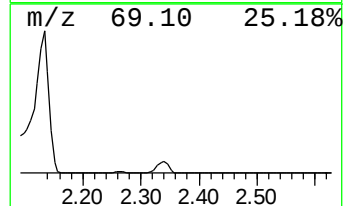
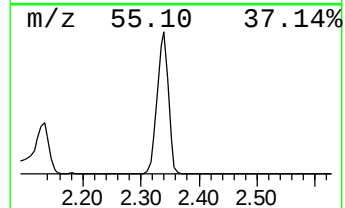
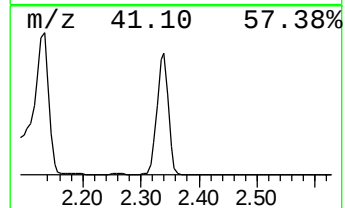
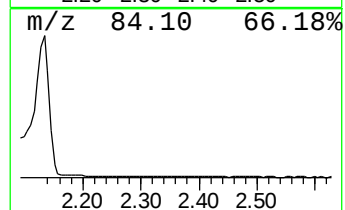
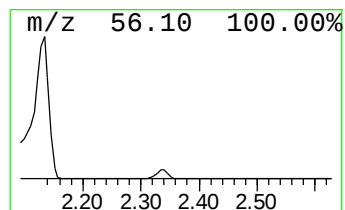
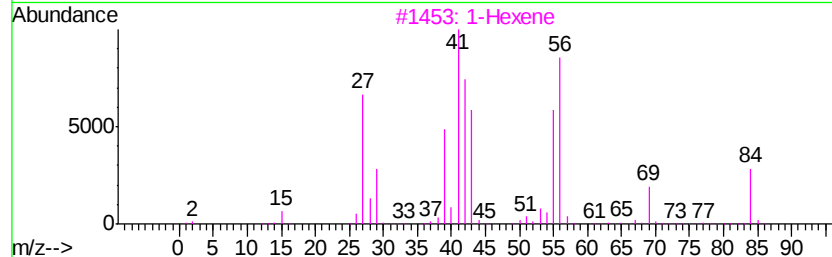
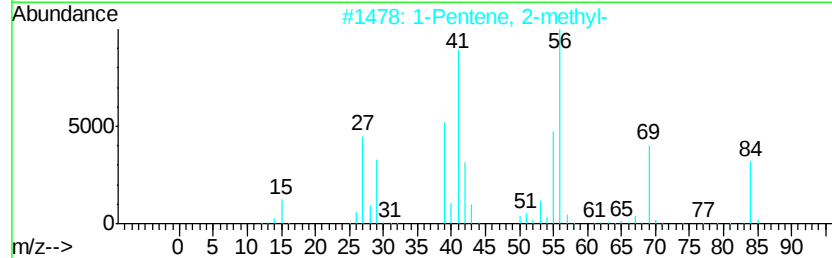
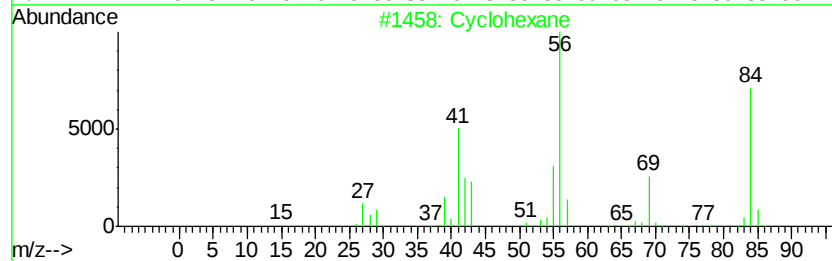
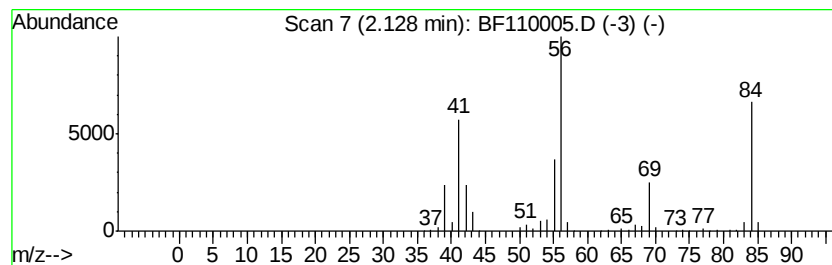
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	23.18 ng	1728800	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane	84	C6H12	000110-82-7	91
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3		1-Hexene	84	C6H12	000592-41-6	59
4		1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	56
5		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53



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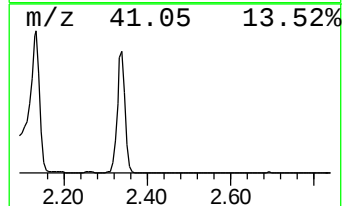
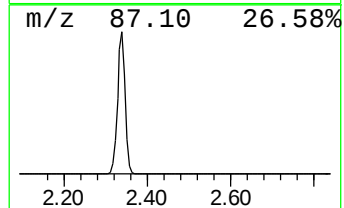
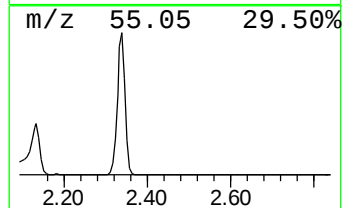
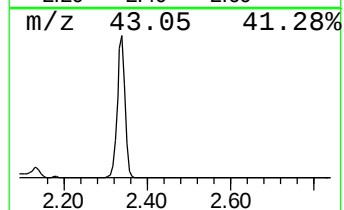
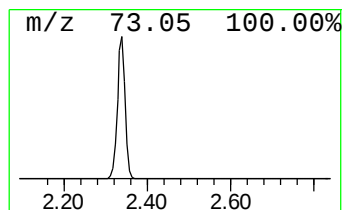
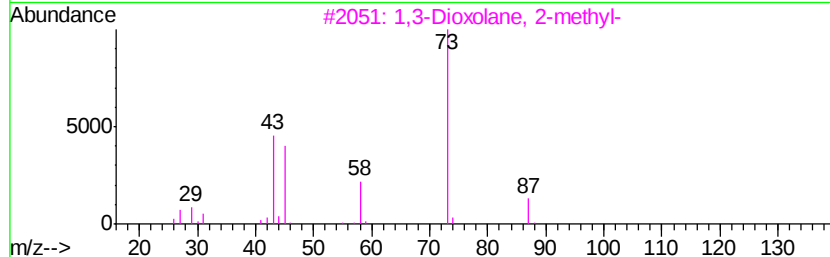
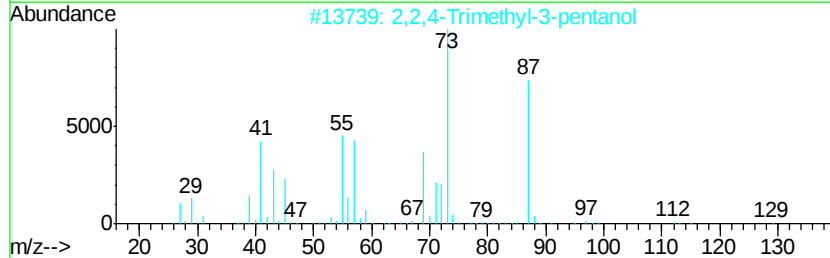
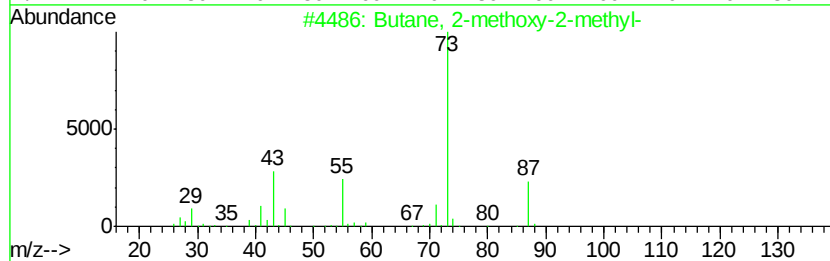
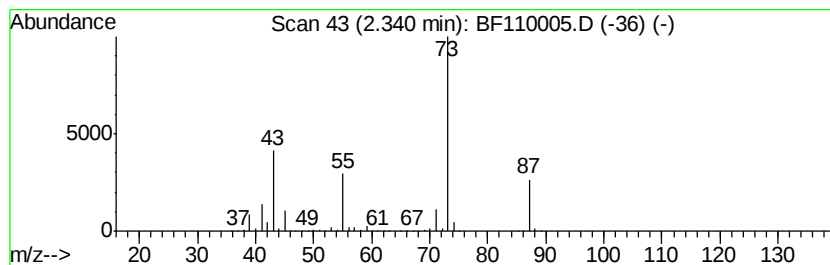
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	45.82 ng	3417560	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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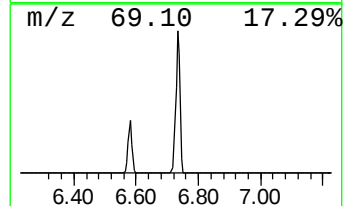
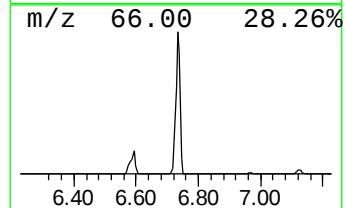
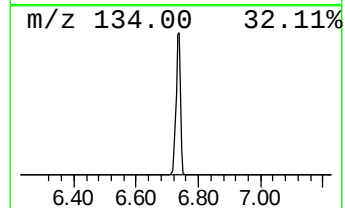
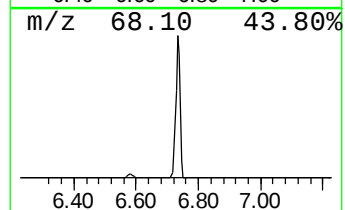
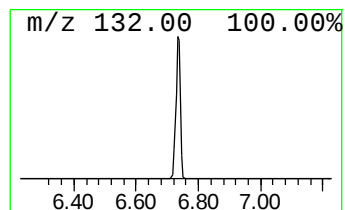
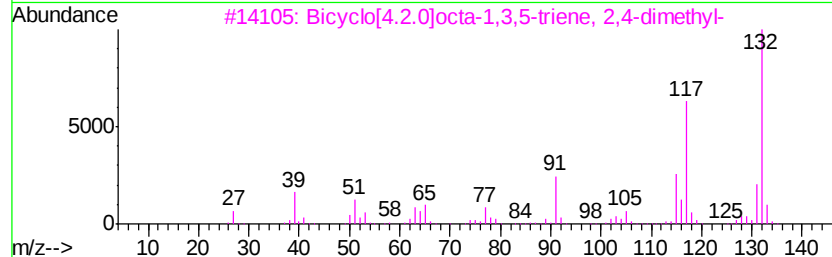
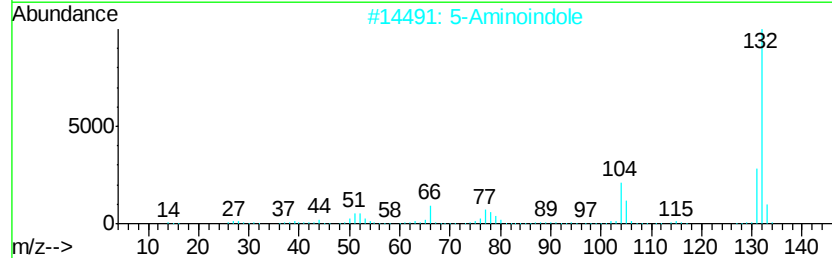
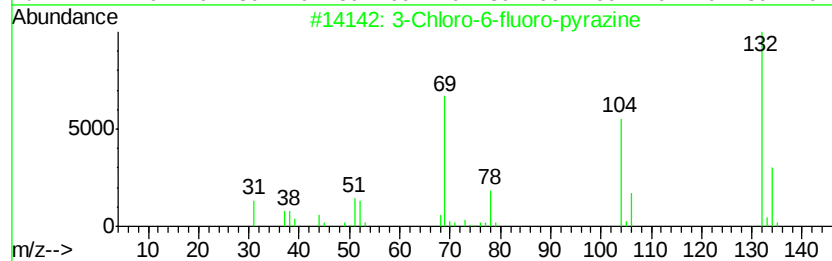
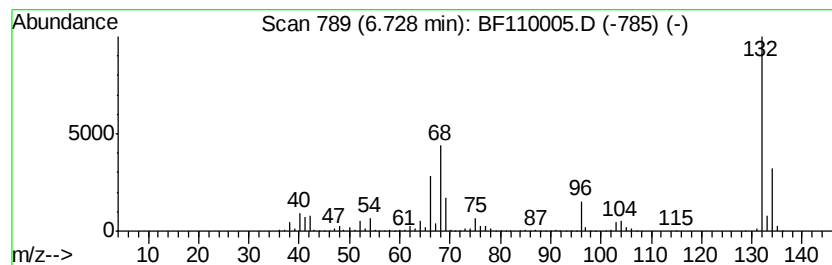
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	55.24 ng	4120460	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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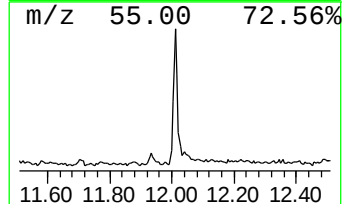
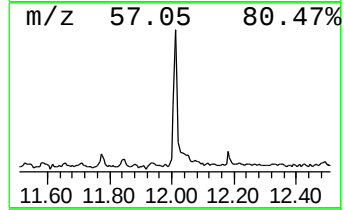
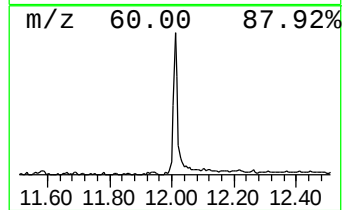
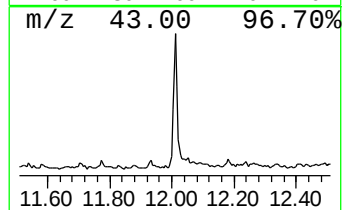
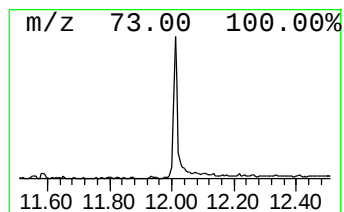
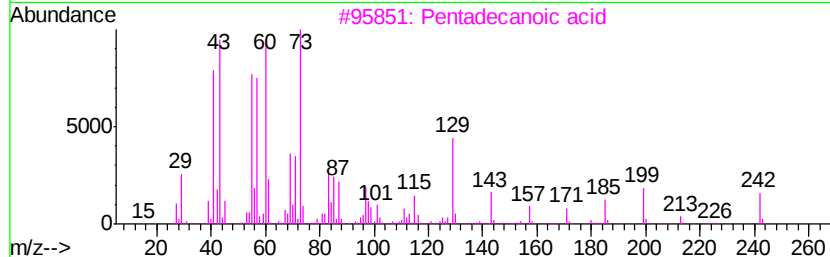
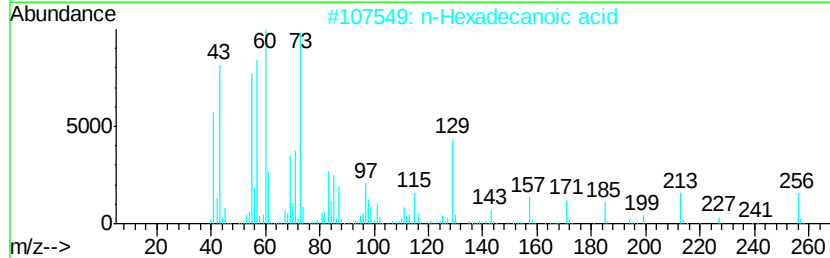
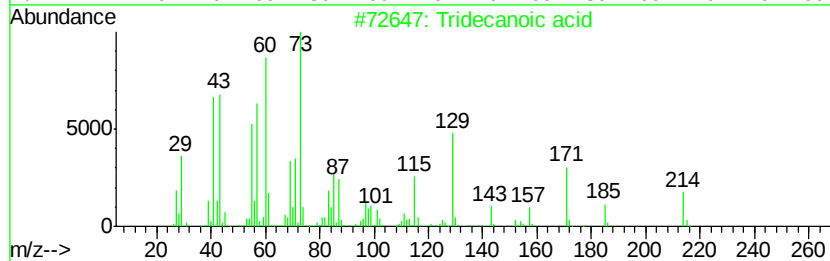
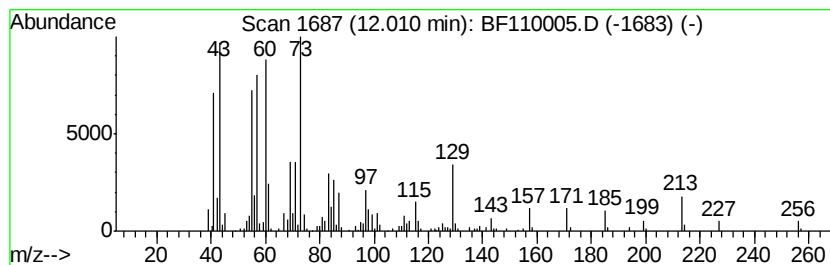
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Tridecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.09 ng	324815	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



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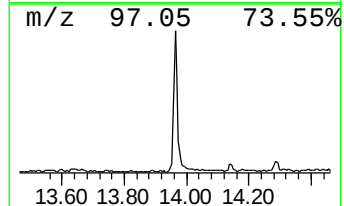
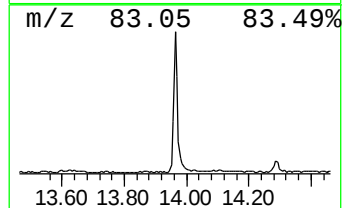
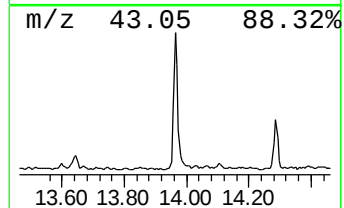
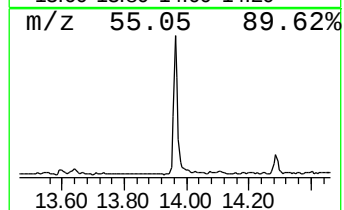
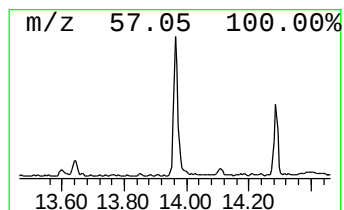
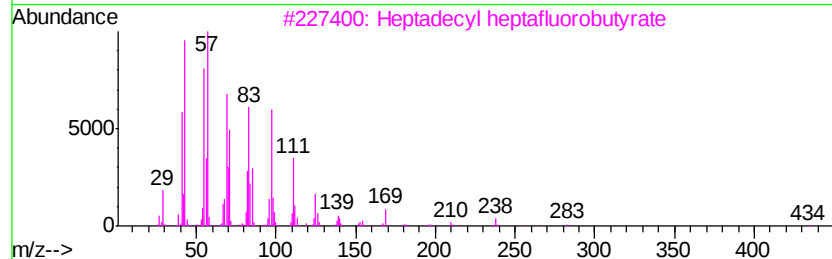
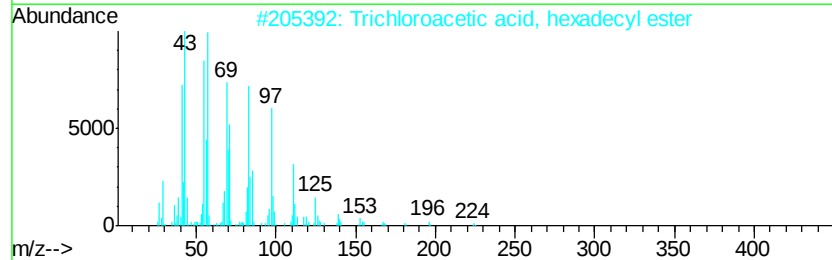
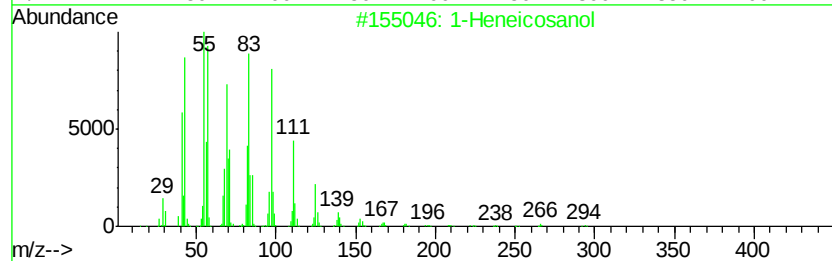
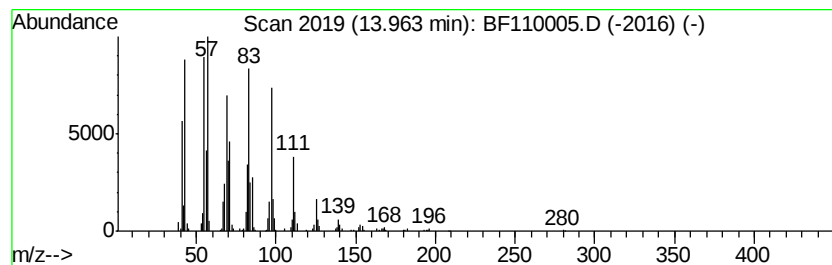
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	6.51 ng	525935	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	91



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Data File : BF110005.D
Acq On : 19 Oct 2018 16:28
Operator : JU/SJ
Sample : J5590-09
Misc :
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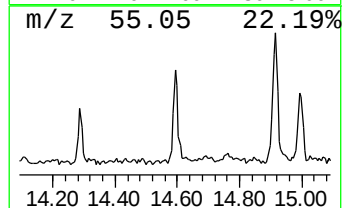
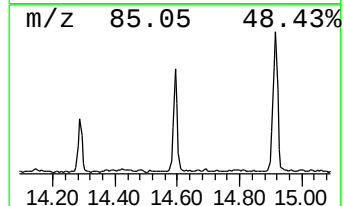
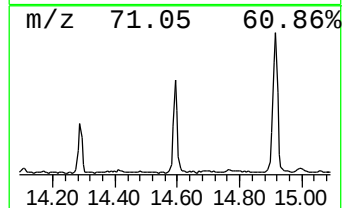
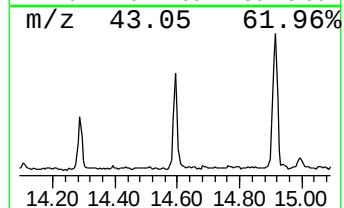
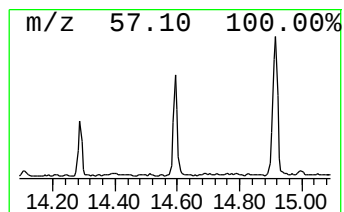
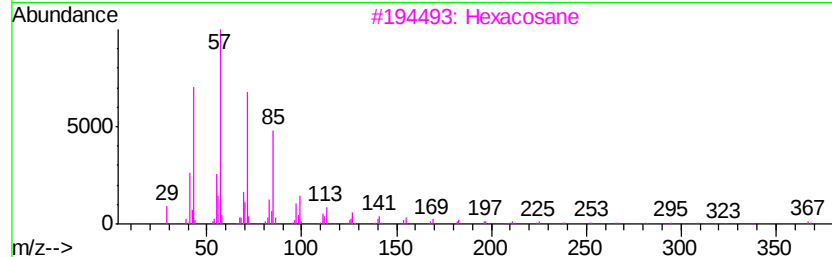
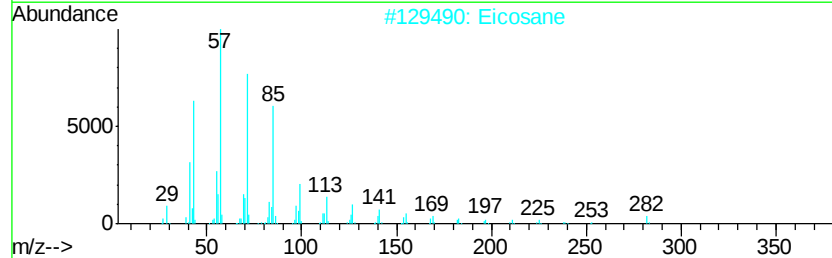
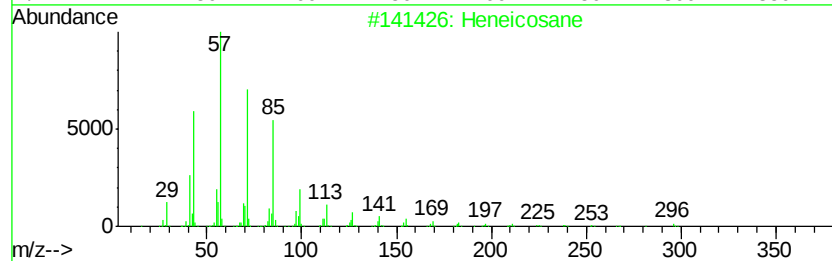
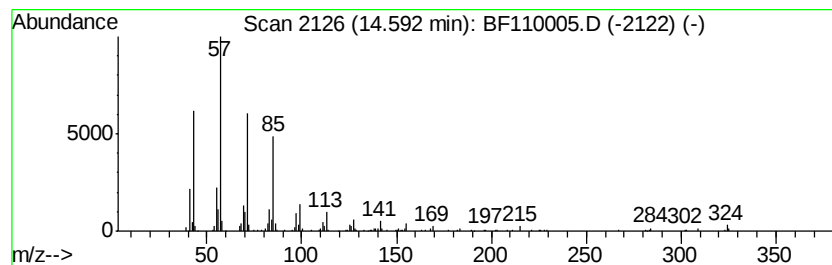
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	3.21 ng	259058	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Eicosane	282	C20H42	000112-95-8	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110005.D
Acq On : 19 Oct 2018 16:28
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ClientSampleId :
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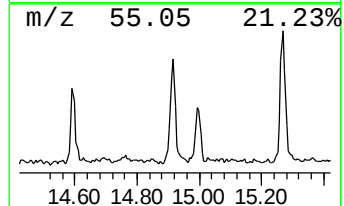
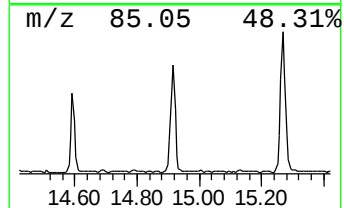
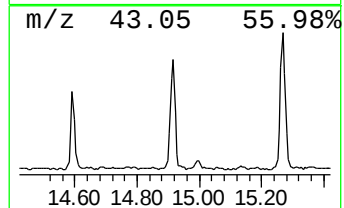
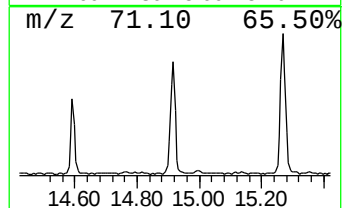
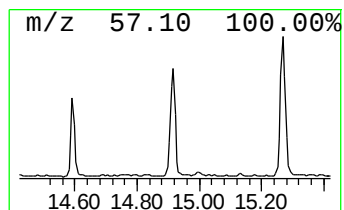
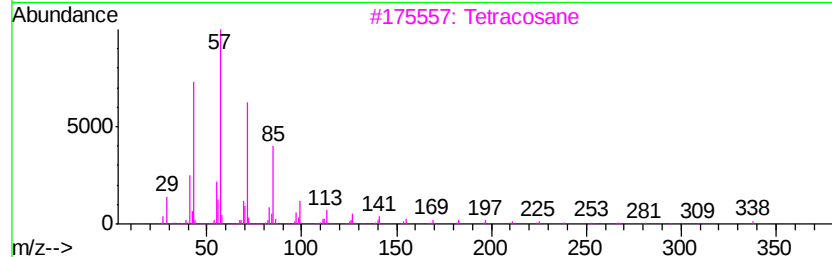
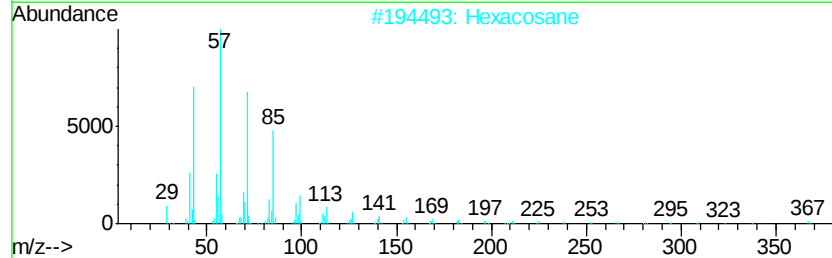
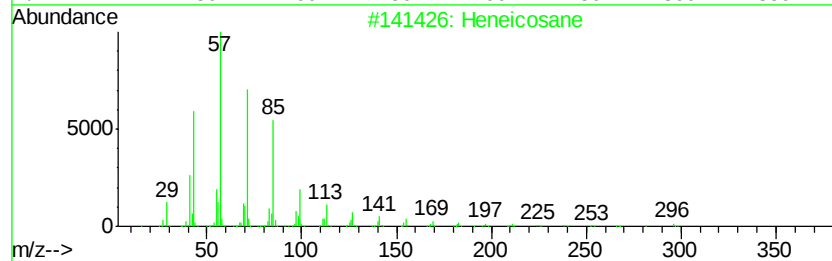
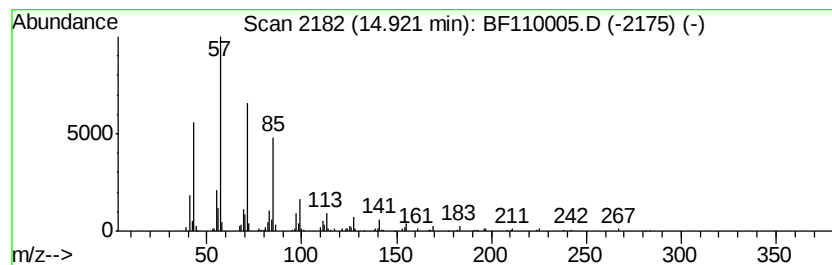
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.60 ng	400421	Perylene-d12	15.67

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	Tetracosane		338	C24H50	000646-31-1	91
4	Octacosane		394	C28H58	000630-02-4	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110005.D
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Instrument :
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ClientSampleId :
LS-DRUM

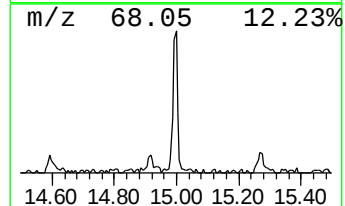
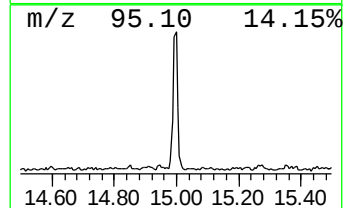
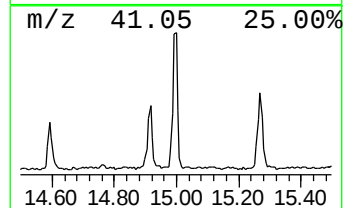
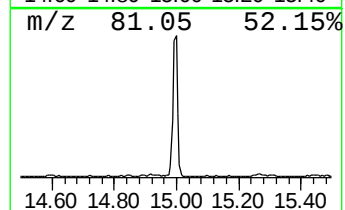
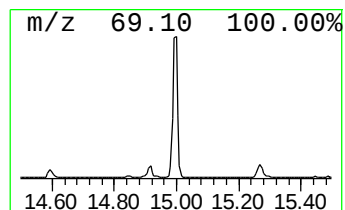
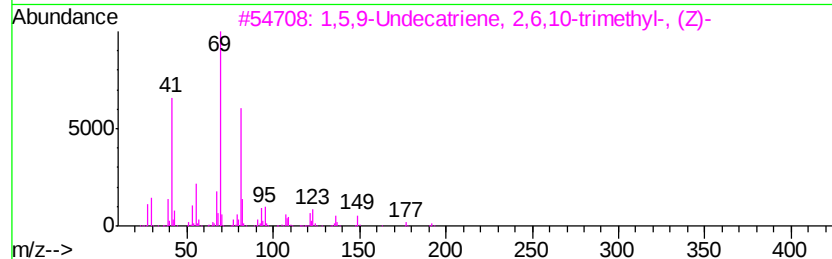
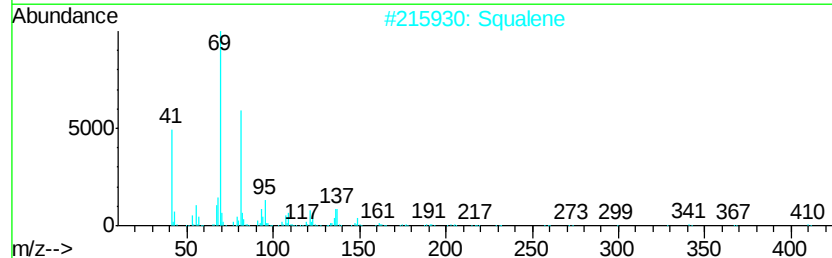
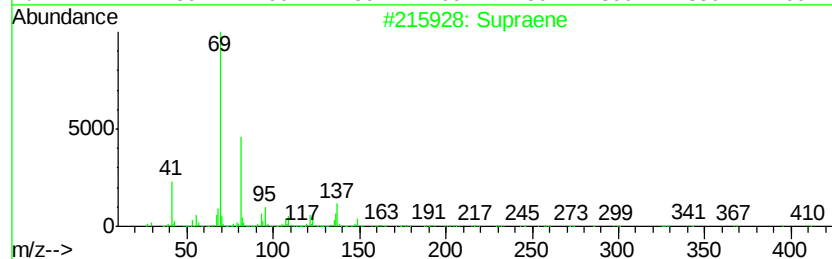
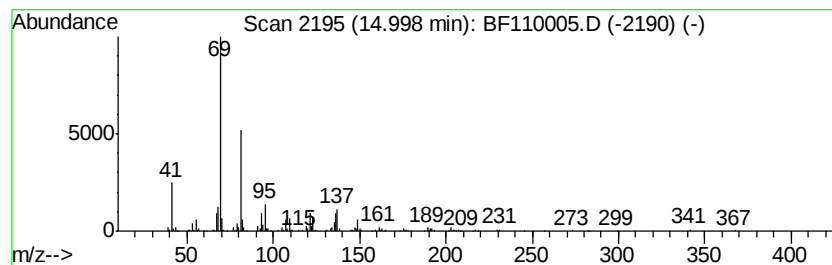
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	5.99 ng	521550	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110005.D
Acq On : 19 Oct 2018 16:28
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Sample : J5590-09
Misc :
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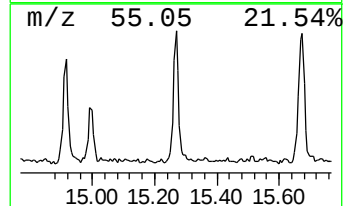
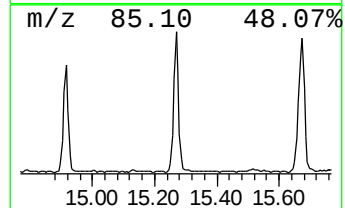
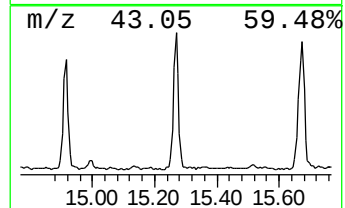
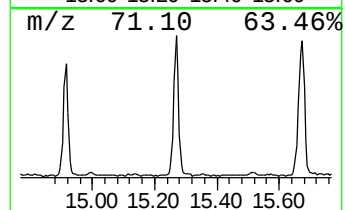
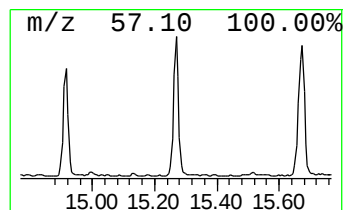
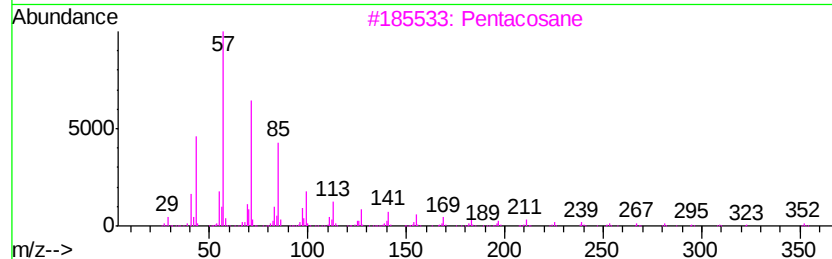
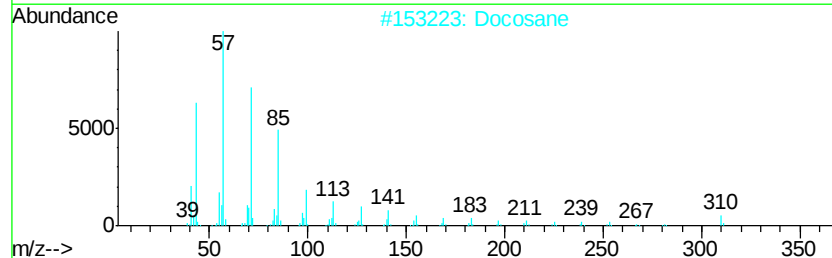
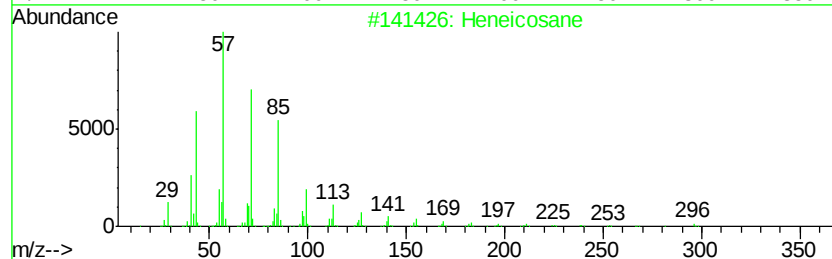
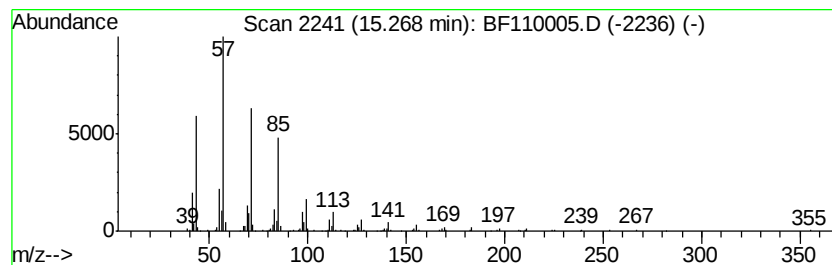
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	6.05 ng	526860	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Docosane	310	C22H46	000629-97-0	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110005.D
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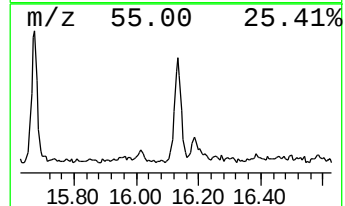
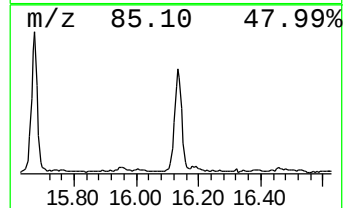
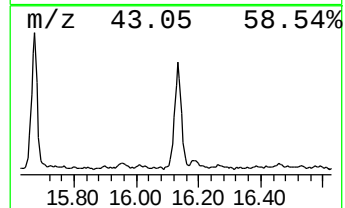
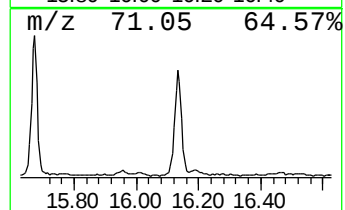
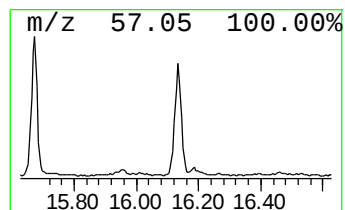
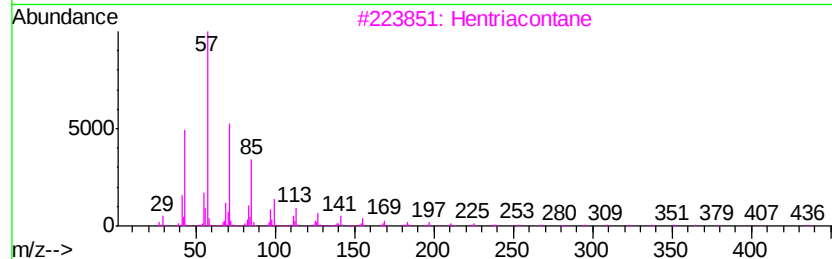
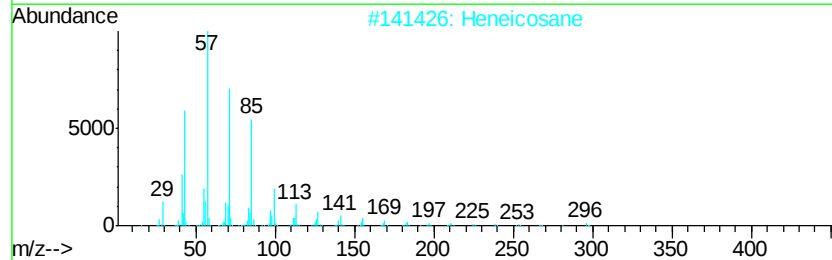
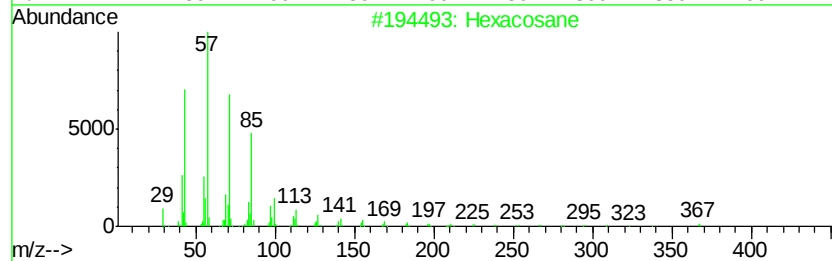
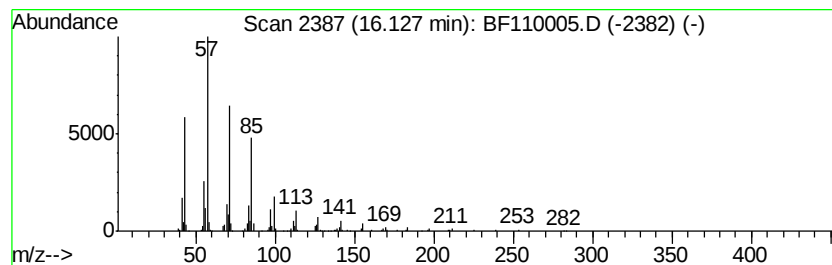
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	5.88 ng	512105	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Octadecane	254	C18H38	000593-45-3	90
5			Triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110005.D
Acq On : 19 Oct 2018 16:28
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ALS Vial : 10 Sample Multiplier: 1

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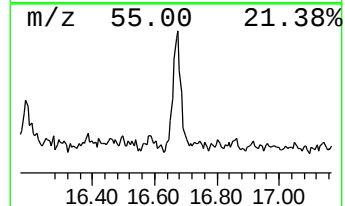
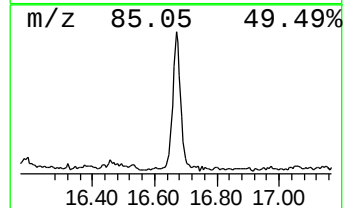
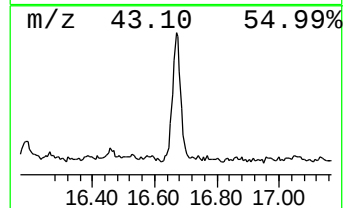
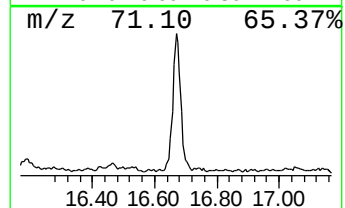
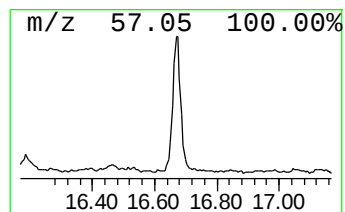
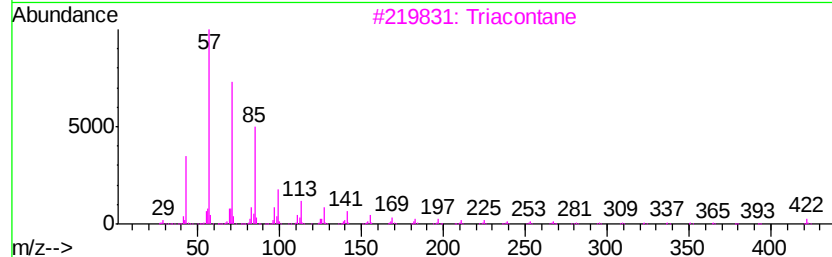
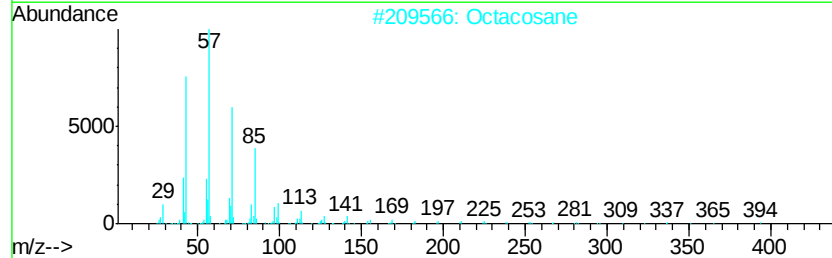
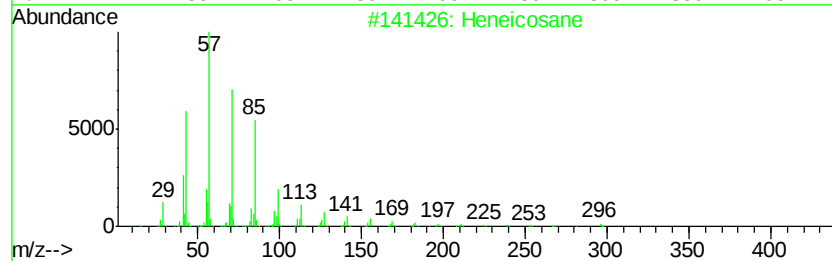
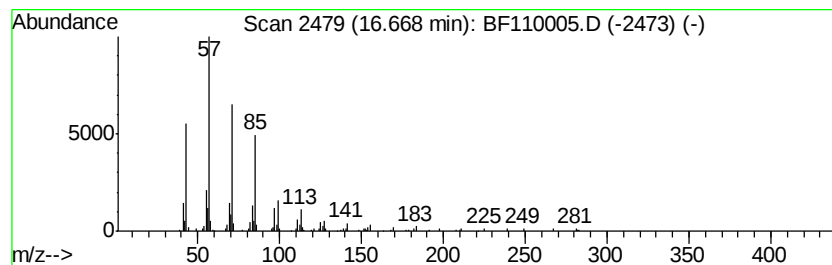
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	3.71 ng	323384	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Tetracosane	338	C24H50	000646-31-1	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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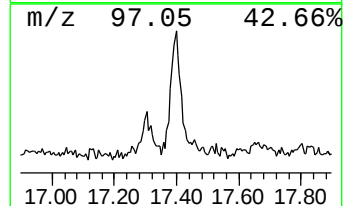
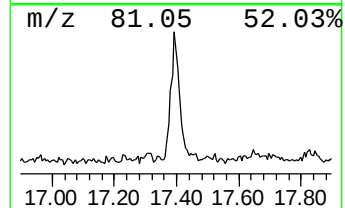
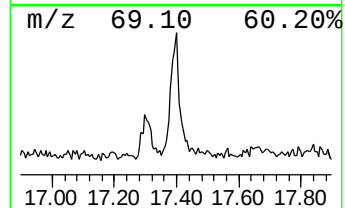
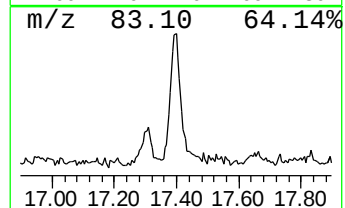
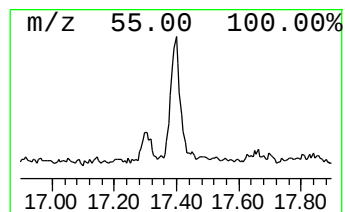
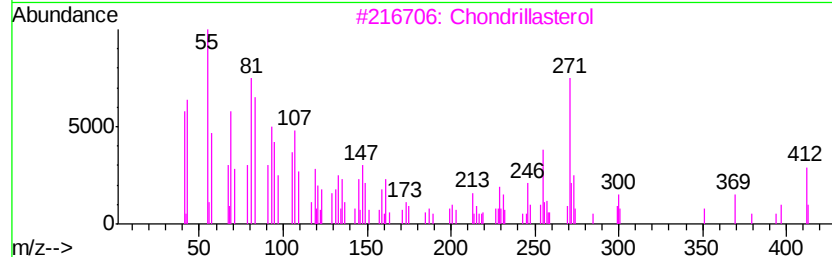
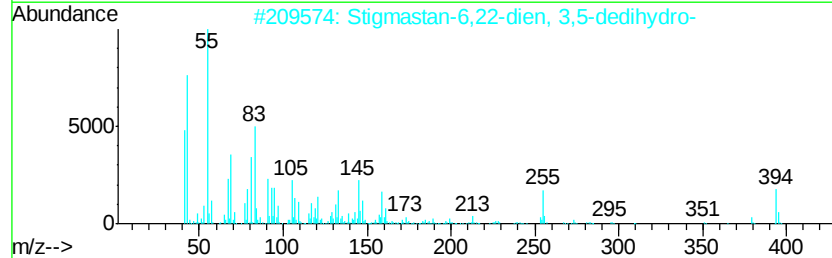
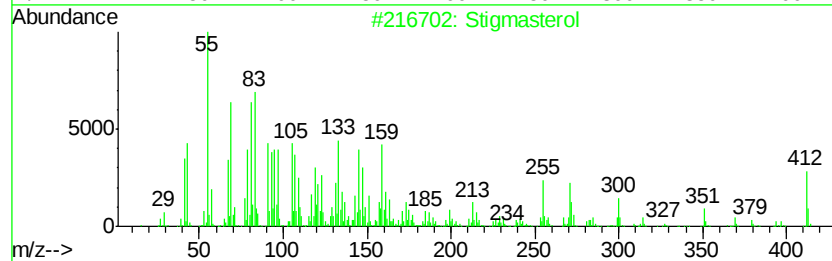
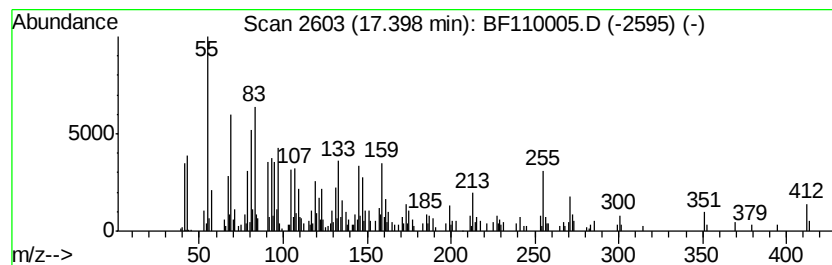
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Stigmasterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.40	5.37 ng	467810	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmasterol	412	C29H48O	000083-48-7	99
2		Stigmastan-6,22-dien, 3,5-dedihi...	394	C29H46	107304-12-1	52
3		Chondrillasterol	412	C29H48O	000481-17-4	50
4		Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	49
5		Cholesta-6,22,24-triene, 4,4-dim...	394	C29H46	1000128-66-9	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110005.D
Acq On : 19 Oct 2018 16:28
Operator : JU/SJ
Sample : J5590-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LS-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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
Cyclohexane	2.13	23.2	ng	1728800	1	6.97	1491830	20.0
Butane, 2-methoxy...	2.34	45.8	ng	3417560	1	6.97	1491830	20.0
unknown6.73	6.73	55.2	ng	4120460	1	6.97	1491830	20.0
Tridecanoic acid	12.01	3.1	ng	324815	4	11.50	2105240	20.0
1-Heneicosanol	13.96	6.5	ng	525935	5	14.14	1616380	20.0
Eicosane	14.59	3.2	ng	259058	5	14.14	1616380	20.0
Heneicosane	14.92	4.6	ng	400421	6	15.67	1741000	20.0
Supraene	15.00	6.0	ng	521550	6	15.67	1741000	20.0
Docosane	15.27	6.0	ng	526860	6	15.67	1741000	20.0
Hexacosane	16.13	5.9	ng	512105	6	15.67	1741000	20.0
Octacosane	16.67	3.7	ng	323384	6	15.67	1741000	20.0
Stigmasterol	17.40	5.4	ng	467810	6	15.67	1741000	20.0