

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
 Data File : BF109670.D
 Acq On : 9 Oct 2018 1:41
 Operator : JU/SJ
 Sample : J5287-17
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRACK-D-8

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-BF100818.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	4.904	473	479	491	rBV	44923	77177	3.56%	0.415%
2	5.322	546	550	580	rBV	1355663	1838684	84.75%	9.881%
3	6.351	721	725	741	rBV	1469773	2092451	96.45%	11.245%
4	6.469	741	745	770	rVB	1851977	2169501	100.00%	11.659%
5	6.698	781	784	806	rVB	382177	582907	26.87%	3.133%
6	6.851	806	810	836	rBV	1456956	1563467	72.07%	8.402%
7	7.263	876	880	902	rBV	936315	1314452	60.59%	7.064%
8	7.975	998	1001	1024	rBV	513738	719381	33.16%	3.866%
9	9.051	1180	1184	1197	rBV	2032778	1994869	91.95%	10.721%
10	9.445	1247	1251	1259	rBV	133209	148688	6.85%	0.799%
11	9.722	1294	1298	1322	rVB	635577	666628	30.73%	3.583%
12	10.510	1428	1432	1450	rBV	871585	1044474	48.14%	5.613%
13	11.198	1546	1549	1562	rBV	436502	570497	26.30%	3.066%
14	11.739	1637	1641	1648	rBV3	39392	49790	2.29%	0.268%
15	12.410	1751	1755	1761	rBV	39825	48623	2.24%	0.261%
16	12.610	1784	1789	1791	rBV3	14978	21986	1.01%	0.118%
17	12.633	1791	1793	1796	rBV	31613	27418	1.26%	0.147%
18	12.668	1796	1799	1801	rBV3	23243	31135	1.44%	0.167%
19	12.780	1814	1818	1822	rBV	1443103	1371169	63.20%	7.369%
20	13.263	1895	1900	1906	rBV	199864	217849	10.04%	1.171%
21	13.357	1913	1916	1919	rBV3	26926	22691	1.05%	0.122%
22	13.686	1969	1972	1982	rBV4	77540	144819	6.68%	0.778%
23	13.827	1991	1996	2004	rBV	559321	640933	29.54%	3.445%
24	13.998	2022	2025	2031	rBV	49469	45221	2.08%	0.243%
25	14.215	2056	2062	2065	rBV3	22607	32033	1.48%	0.172%
26	14.304	2074	2077	2080	rVB	58900	54813	2.53%	0.295%
27	14.592	2123	2126	2131	rBV	65388	65245	3.01%	0.351%
28	14.662	2135	2138	2141	rBV	40785	38604	1.78%	0.207%
29	14.833	2163	2167	2170	rBV	81373	115320	5.32%	0.620%
30	14.904	2176	2179	2187	rVB2	73529	95174	4.39%	0.511%
31	15.109	2210	2214	2220	rBV	45991	60997	2.81%	0.328%
32	15.168	2220	2224	2228	rVB	29457	40595	1.87%	0.218%
33	15.221	2228	2233	2237	rBV	351331	472822	21.79%	2.541%
34	15.645	2301	2305	2312	rBV	46996	74587	3.44%	0.401%

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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

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35	16.104	2378	2383	2388	rBV2	33299	56871	2.62%	0.306%
36	16.568	2457	2462	2470	rBV3	17209	43600	2.01%	0.234%
37	16.633	2470	2473	2479	rVB4	13446	24494	1.13%	0.132%
38	16.968	2526	2530	2538	rBV	12602	27456	1.27%	0.148%

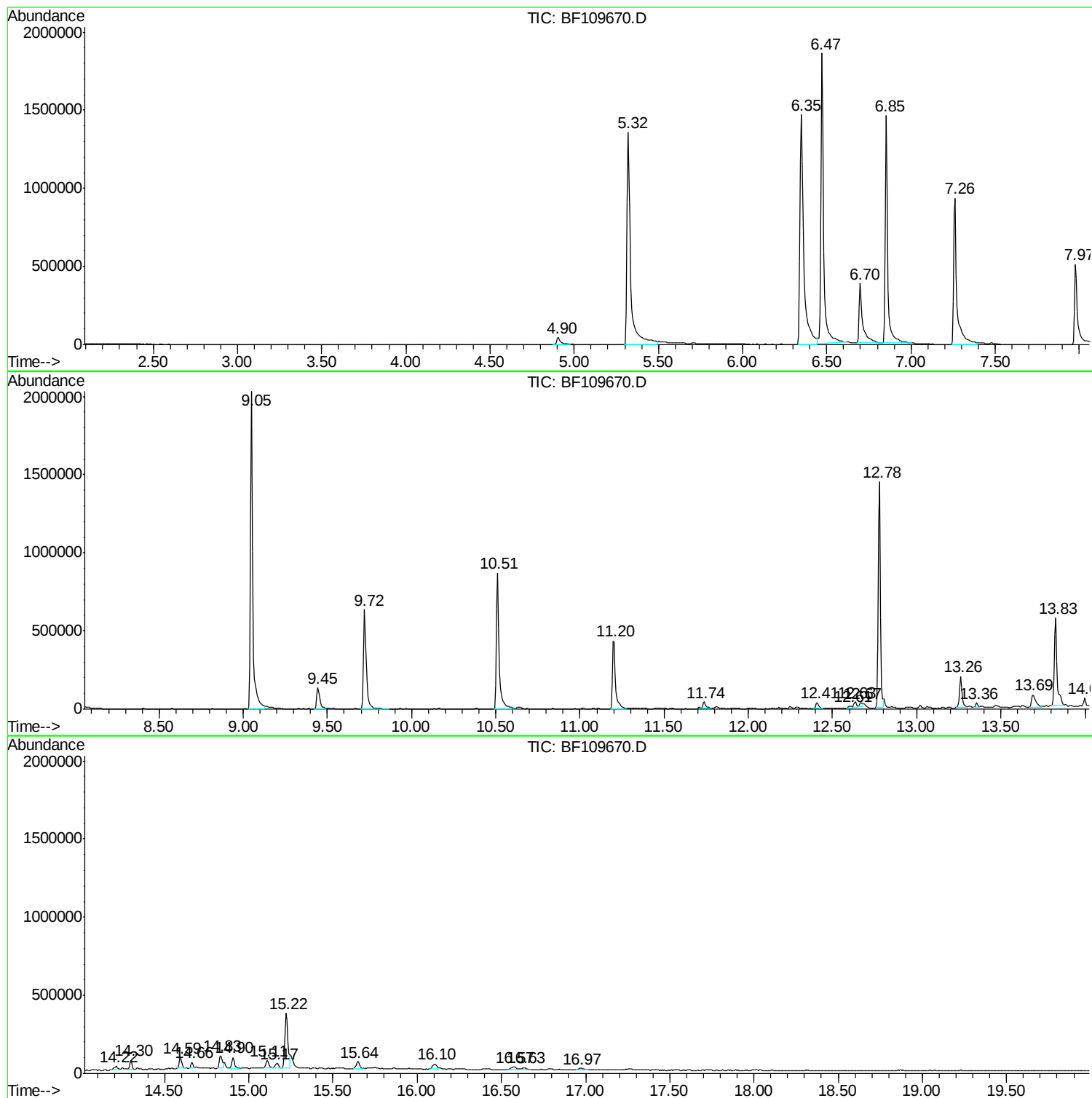
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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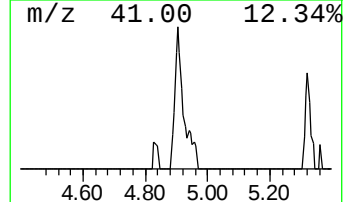
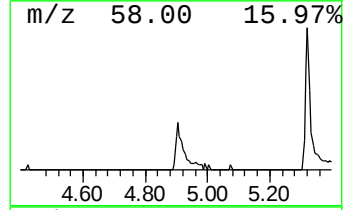
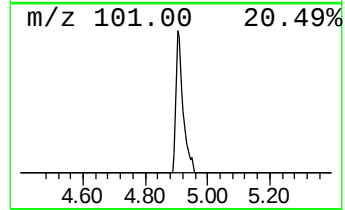
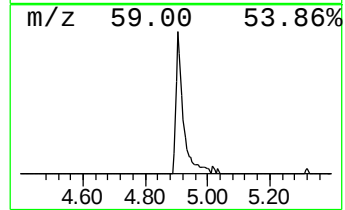
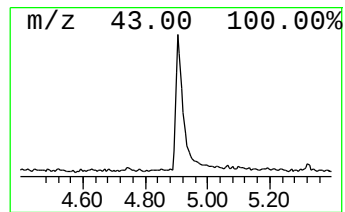
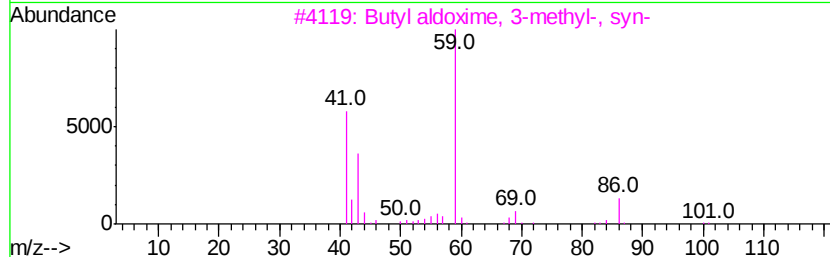
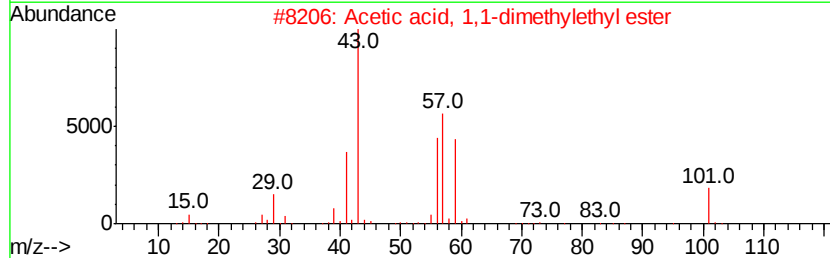
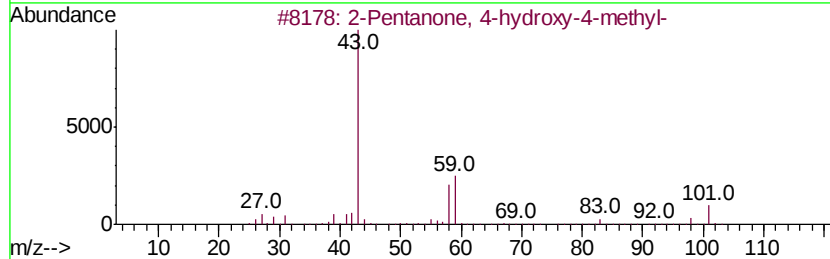
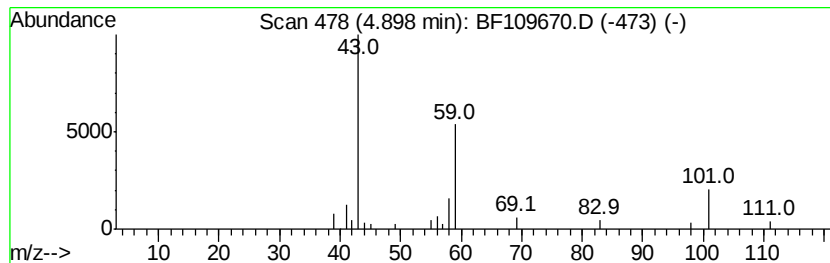
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.65 ng	77177	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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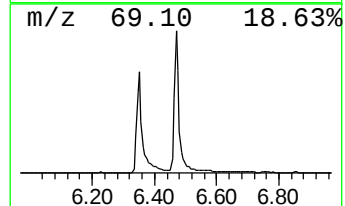
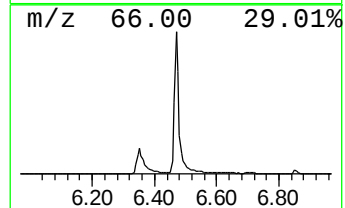
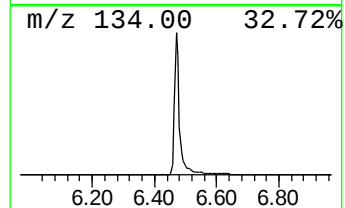
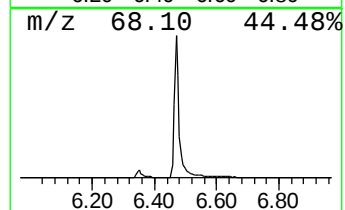
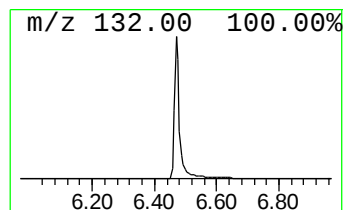
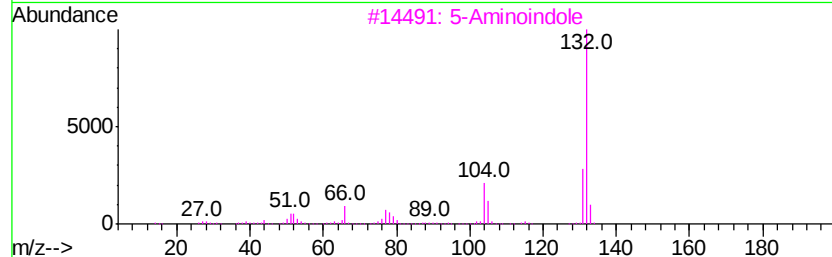
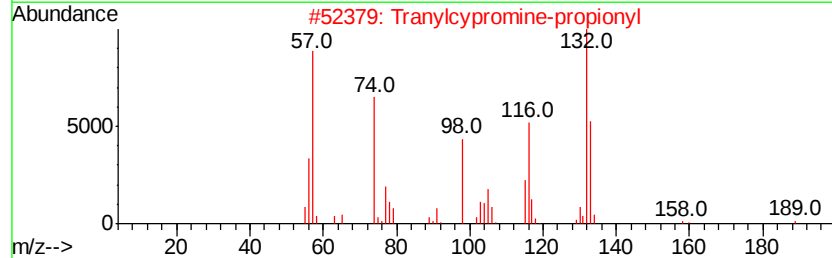
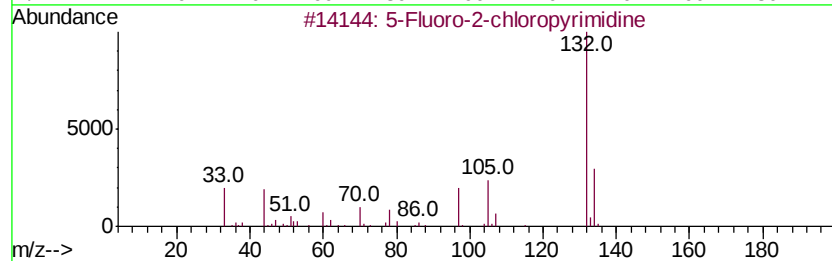
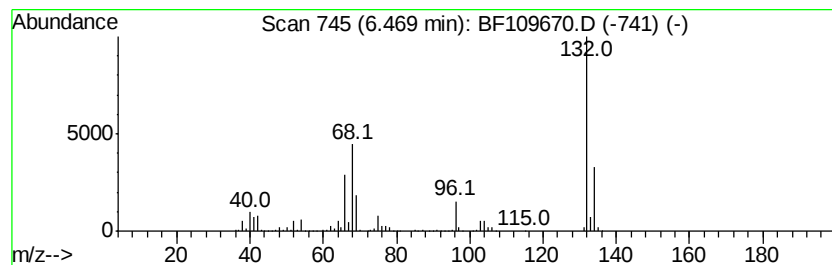
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	74.44 ng	2169500	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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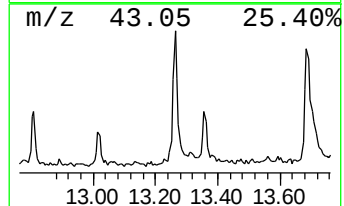
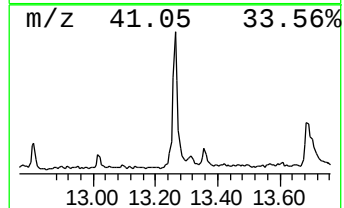
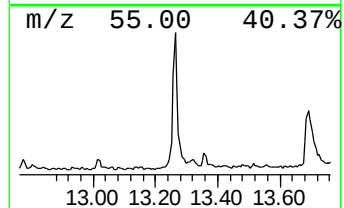
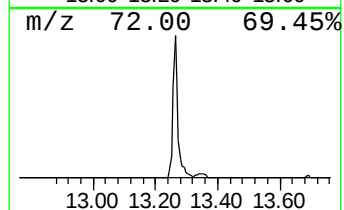
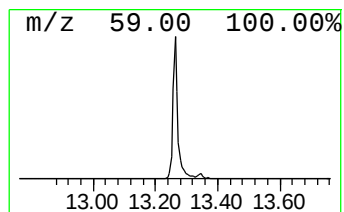
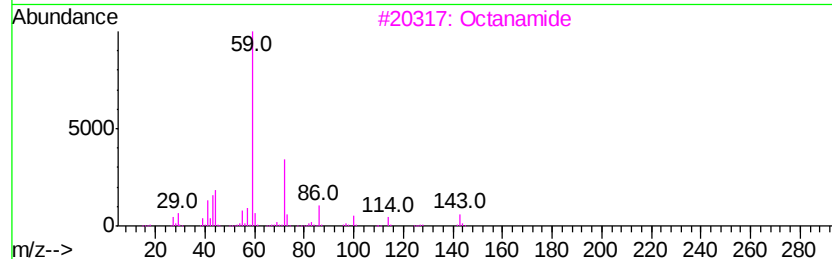
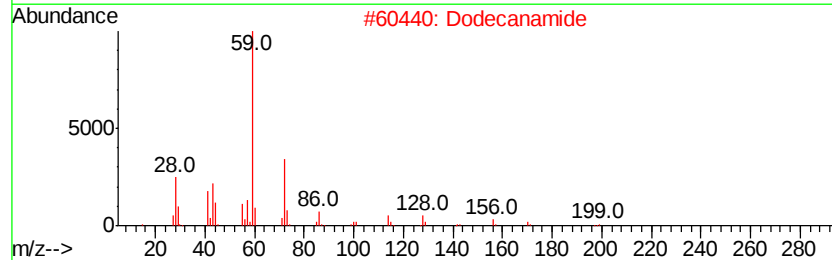
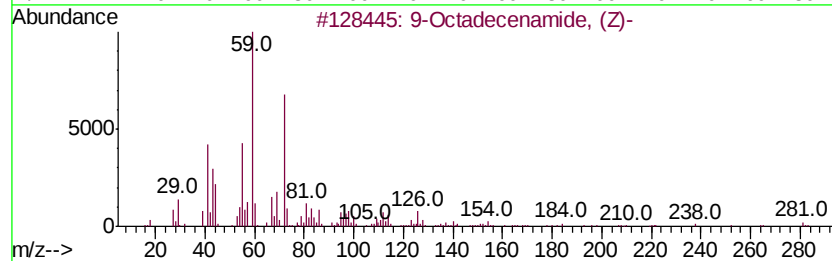
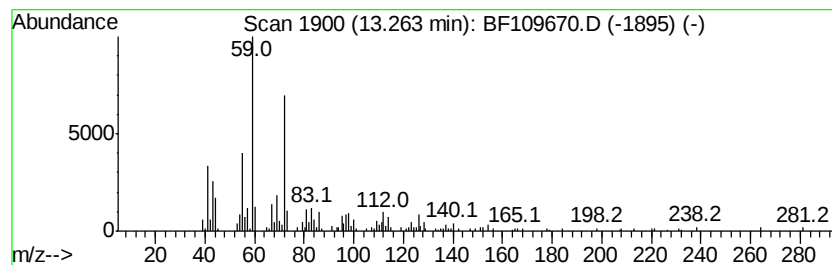
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	6.80 ng	217849	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Dodecanamide	199	C12H25NO	001120-16-7	59
3		Octanamide	143	C8H17NO	000629-01-6	59
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
5		Hexadecanamide	255	C16H33NO	000629-54-9	53



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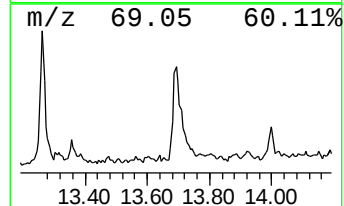
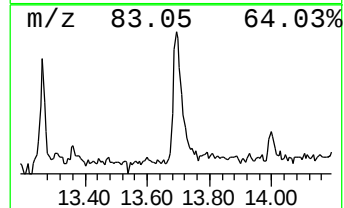
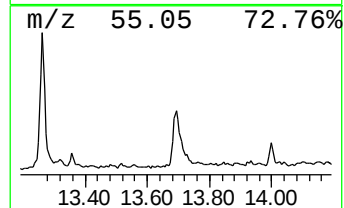
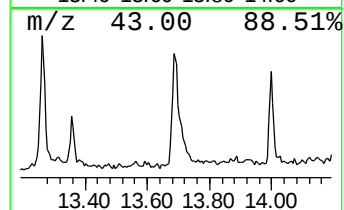
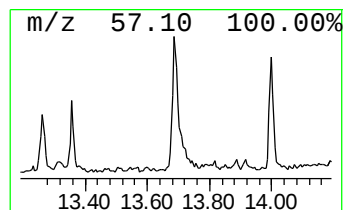
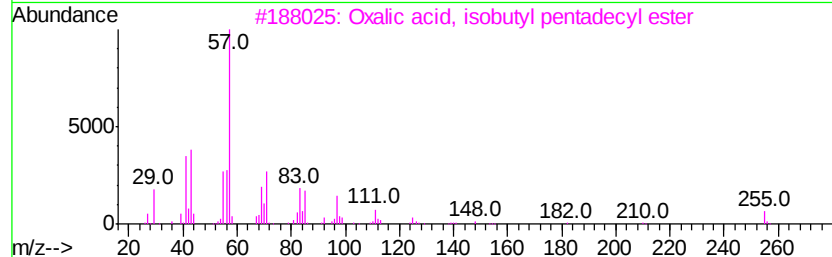
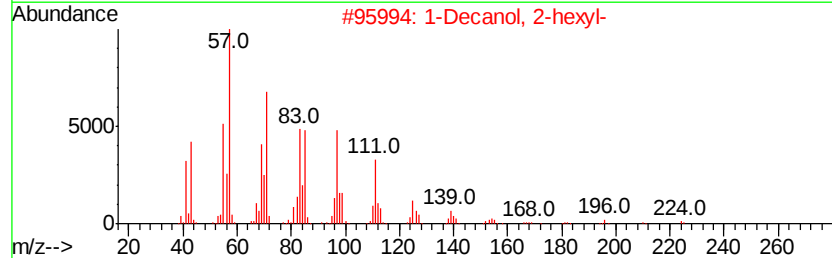
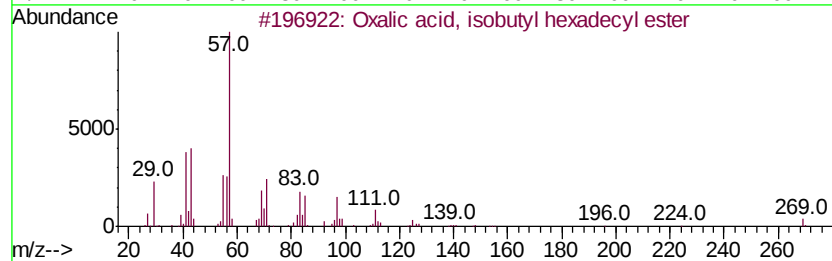
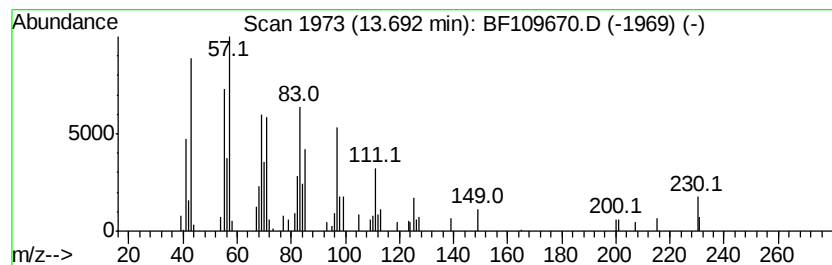
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	4.52 ng	144819	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
3		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
4		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
5		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	86



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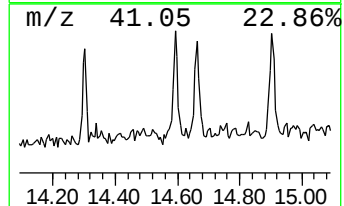
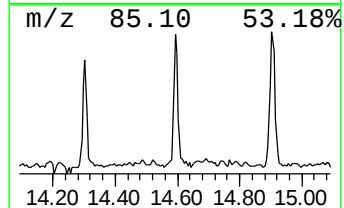
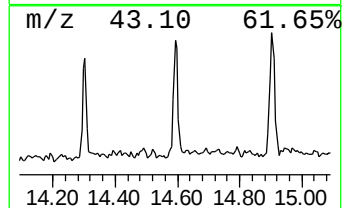
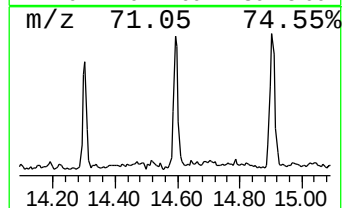
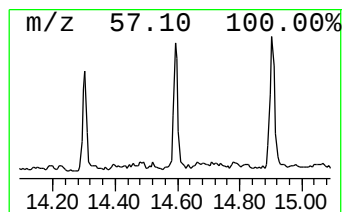
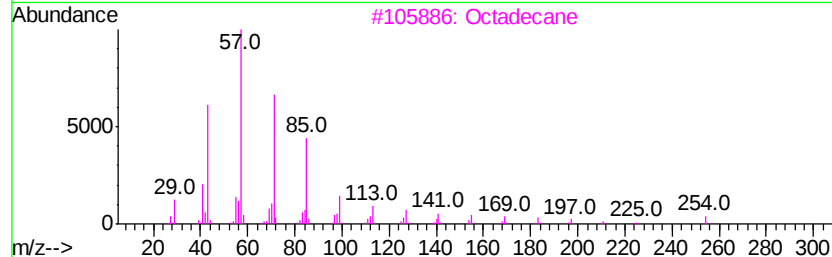
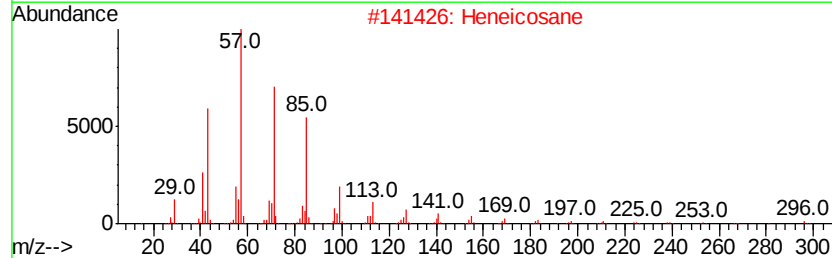
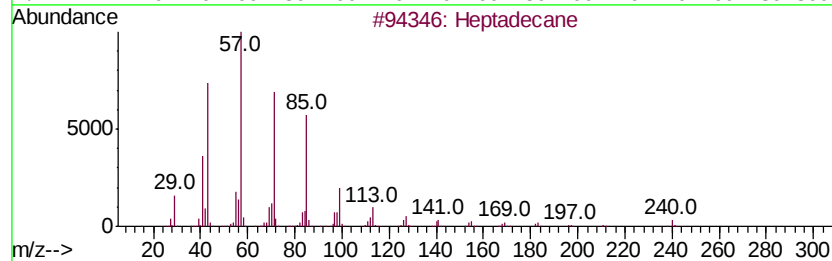
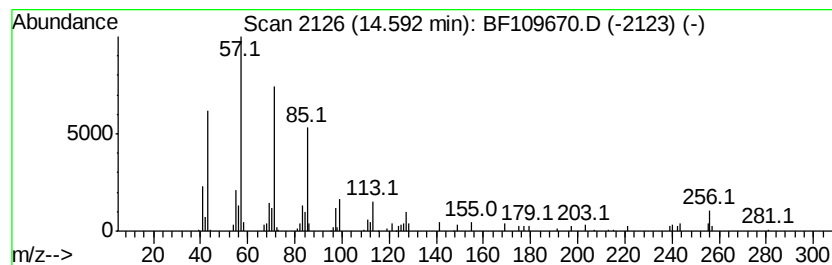
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.76 ng	65245	Perylene-d12	15.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	93
2	Heneicosane		296	C21H44	000629-94-7	87
3	Octadecane		254	C18H38	000593-45-3	87
4	Hexacosane		366	C26H54	000630-01-3	87
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109670.D
Acq On : 9 Oct 2018 1:41
Operator : JU/SJ
Sample : J5287-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-8

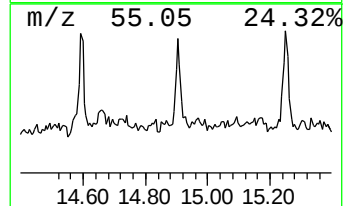
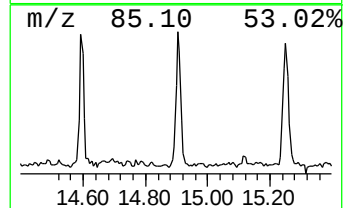
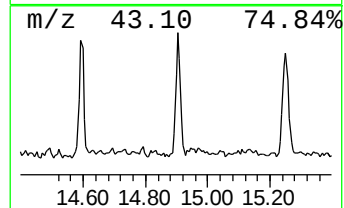
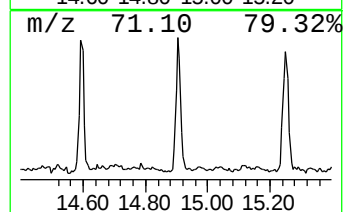
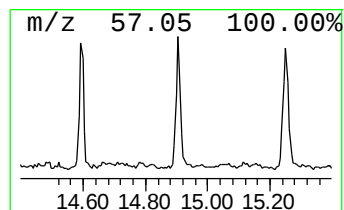
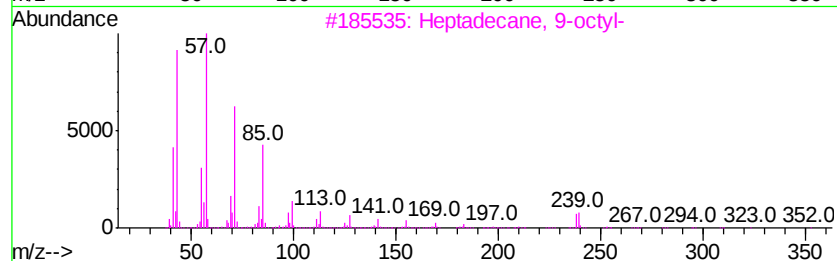
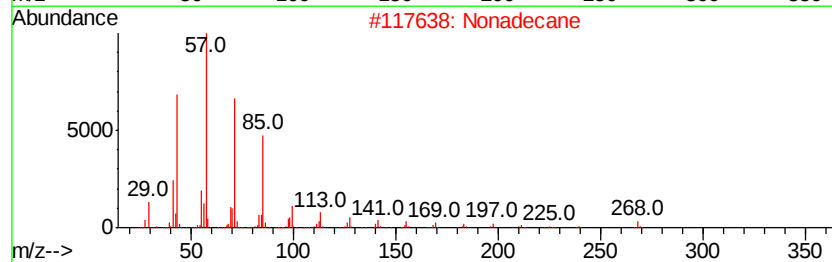
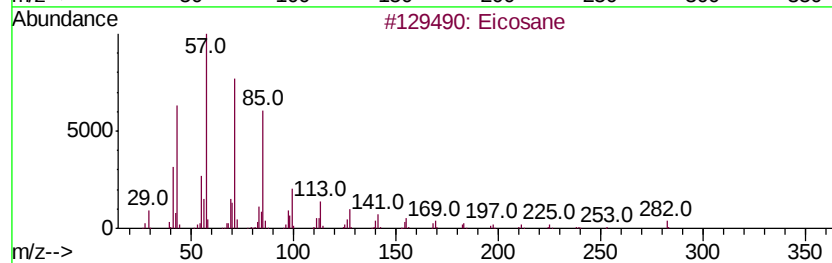
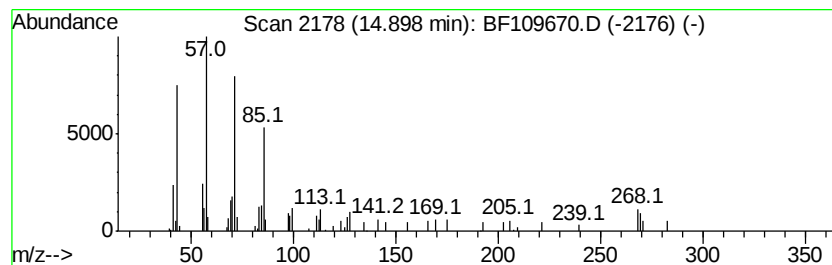
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	4.03 ng	95174	Perylene-d12	15.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	98
2	Nonadecane		268	C19H40	000629-92-5	94
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87
4	Hexacosane		366	C26H54	000630-01-3	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109670.D
Acq On : 9 Oct 2018 1:41
Operator : JU/SJ
Sample : J5287-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-8

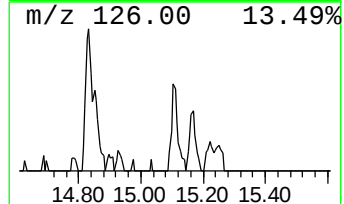
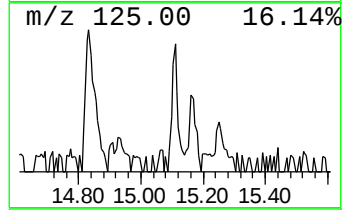
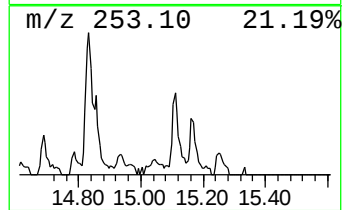
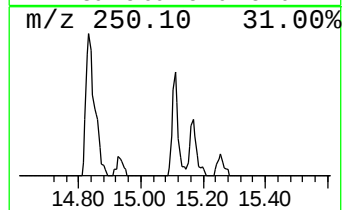
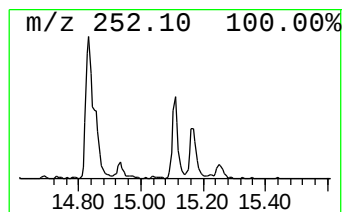
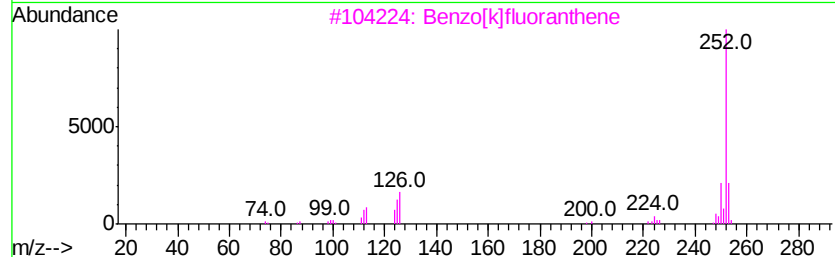
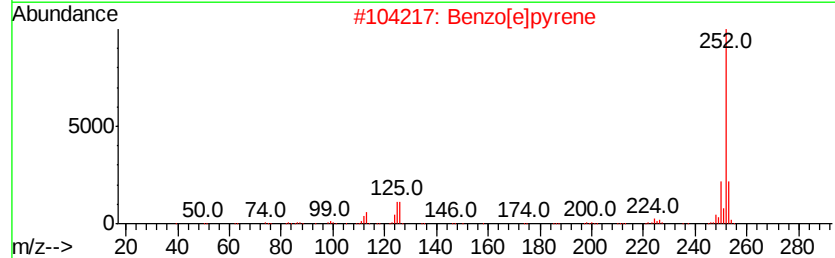
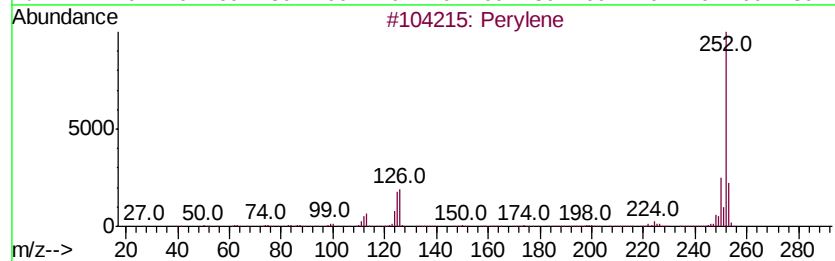
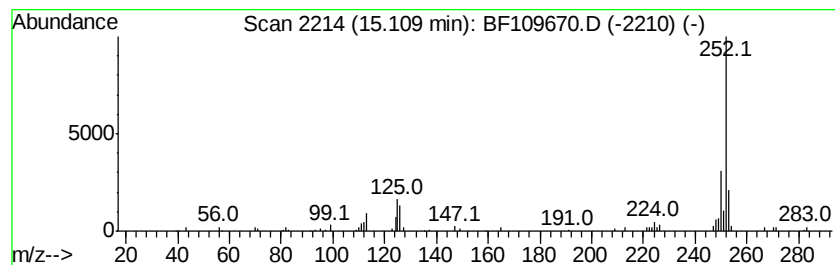
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	2.58 ng	60997	Perylene-d12	15.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	95
2	Benzo[e]pyrene		252	C20H12	000192-97-2	95
3	Benzo[k]fluoranthene		252	C20H12	000207-08-9	93
4	Benzo[e]acephenanthrylene		252	C20H12	000205-99-2	93
5	Benzo[a]pyrene		252	C20H12	000050-32-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109670.D
Acq On : 9 Oct 2018 1:41
Operator : JU/SJ
Sample : J5287-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-8

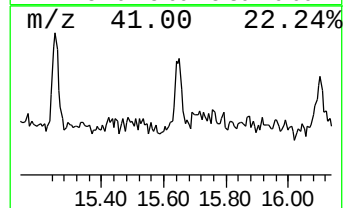
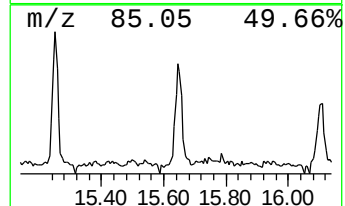
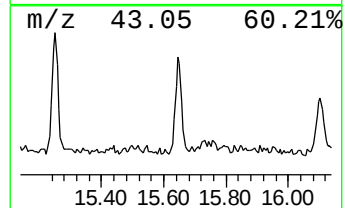
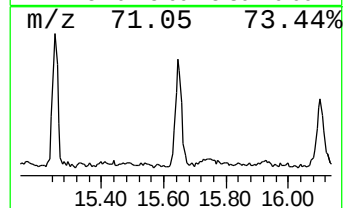
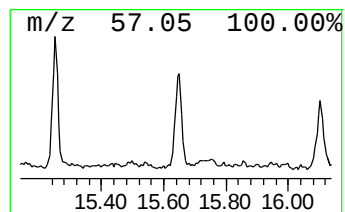
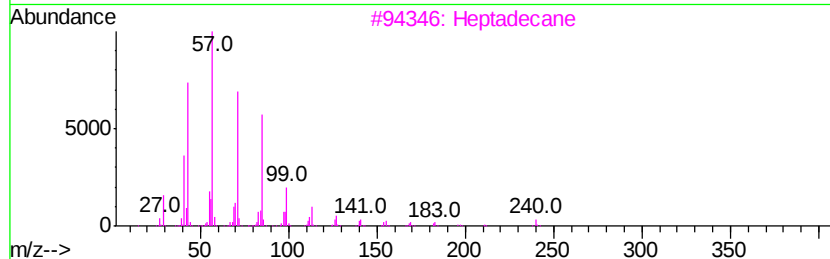
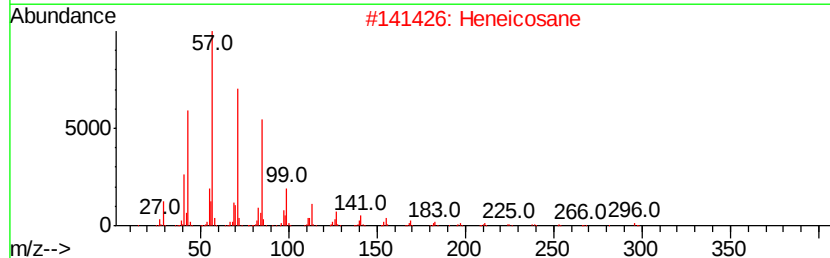
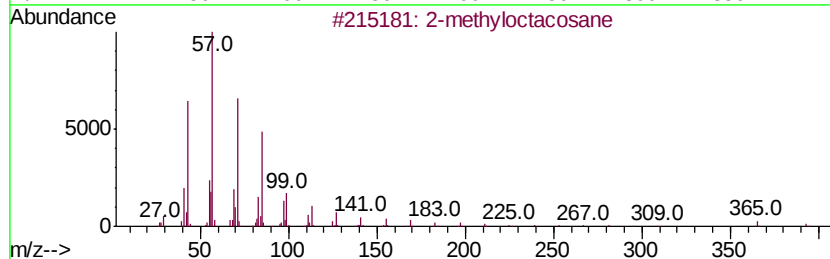
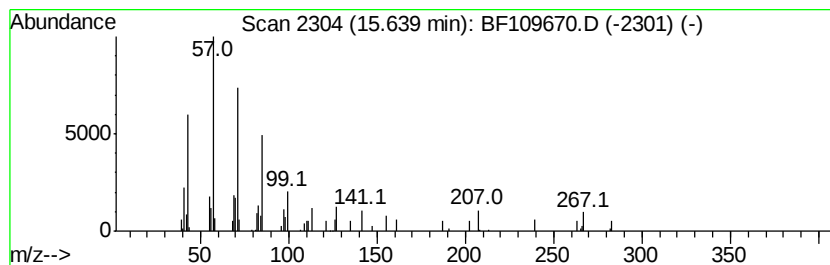
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.15 ng	74587	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane	240	C17H36	000629-78-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
Data File : BF109670.D
Acq On : 9 Oct 2018 1:41
Operator : JU/SJ
Sample : J5287-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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
2-Pentanone, 4-hy...	4.90	2.6	ng	77177	1	6.70	582907	20.0
unknown6.47	6.47	74.4	ng	2169500	1	6.70	582907	20.0
9-Octadecenamide, ...	13.26	6.8	ng	217849	5	13.83	640933	20.0
Oxalic acid, isob...	13.69	4.5	ng	144819	5	13.83	640933	20.0
Heptadecane	14.59	2.8	ng	65245	6	15.22	472822	20.0
Eicosane	14.90	4.0	ng	95174	6	15.22	472822	20.0
Perylene	15.11	2.6	ng	60997	6	15.22	472822	20.0
2-methyloctacosane	15.64	3.1	ng	74587	6	15.22	472822	20.0