

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
 Data File : BF104693.D
 Acq On : 21 Apr 2018 00:40
 Operator : JU/SJ
 Sample : J2453-07
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-8_1.0-1.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.022	494	499	508	rBV	98548	132398	4.47%	0.500%
2	5.422	562	567	580	rBV	2638347	2833764	95.70%	10.709%
3	6.445	736	741	744	rBV	2654266	2783056	93.99%	10.517%
4	6.575	759	763	766	rBV	2883127	2845060	96.08%	10.751%
5	6.804	798	802	805	rBV	813461	636138	21.48%	2.404%
6	6.963	824	829	832	rBV	2547524	2319196	78.32%	8.764%
7	7.369	893	898	901	rBV	1754218	1748793	59.06%	6.609%
8	8.086	1016	1020	1026	rBV	933087	772839	26.10%	2.921%
9	9.163	1199	1203	1206	rBV	3363047	2961070	100.00%	11.190%
10	9.557	1266	1270	1278	rVB	208343	196697	6.64%	0.743%
11	9.763	1303	1305	1310	rBV	64960	56794	1.92%	0.215%
12	9.839	1315	1318	1333	rVB	806697	775213	26.18%	2.930%
13	10.263	1388	1390	1393	rVB	77079	64972	2.19%	0.246%
14	10.633	1449	1453	1463	rVB	1682065	1544629	52.16%	5.837%
15	10.739	1468	1471	1476	rBV	79909	72395	2.44%	0.274%
16	11.186	1544	1547	1550	rBV	42681	34596	1.17%	0.131%
17	11.333	1568	1572	1574	rBV	726852	707532	23.89%	2.674%
18	11.351	1574	1575	1582	rVB	126635	103367	3.49%	0.391%
19	11.863	1659	1662	1668	rVB3	31585	33162	1.12%	0.125%
20	12.545	1774	1778	1783	rBV	236860	201312	6.80%	0.761%
21	12.774	1811	1817	1822	rBV	196286	205484	6.94%	0.777%
22	12.921	1837	1842	1845	rBV	2734230	2641767	89.22%	9.983%
23	13.480	1934	1937	1941	rBV	48166	52757	1.78%	0.199%
24	13.774	1981	1987	1991	rBV	139137	177371	5.99%	0.670%
25	13.815	1991	1994	2003	rVB2	130251	155635	5.26%	0.588%
26	13.974	2014	2021	2024	rBV	750912	789598	26.67%	2.984%
27	13.998	2024	2025	2033	rVB	98802	87137	2.94%	0.329%
28	14.127	2044	2047	2053	rBV2	85508	101185	3.42%	0.382%
29	14.439	2097	2100	2106	rBV	91437	99974	3.38%	0.378%
30	14.745	2149	2152	2156	rVB	83459	77725	2.62%	0.294%
31	14.815	2161	2164	2168	rVB	73300	70724	2.39%	0.267%
32	15.015	2195	2198	2201	rBV	63744	87103	2.94%	0.329%
33	15.080	2206	2209	2213	rVB	76045	85665	2.89%	0.324%
34	15.315	2246	2249	2255	rVB	44362	55952	1.89%	0.211%

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T-8_1.0-1.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.380	2257	2260	2265	rVV	49656	61136	2.06%	0.231%
36	15.445	2266	2271	2282	rVB	379450	580988	19.62%	2.196%
37	15.886	2342	2346	2350	rBV	38758	52097	1.76%	0.197%
38	18.797	2836	2841	2857	rVB4	68122	257009	8.68%	0.971%

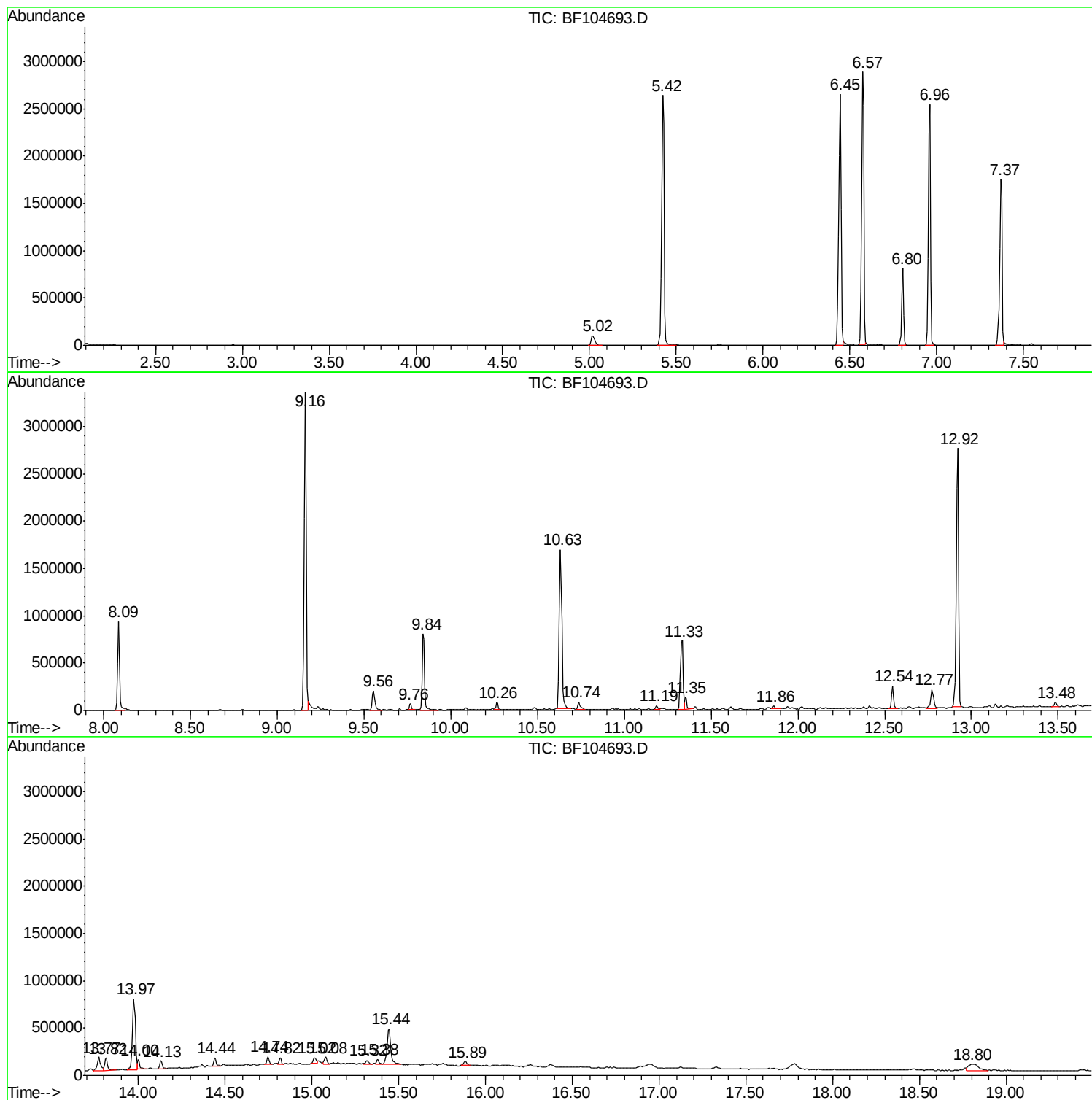
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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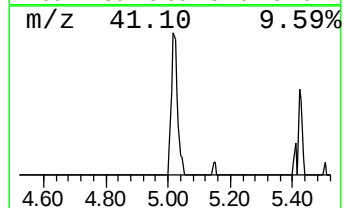
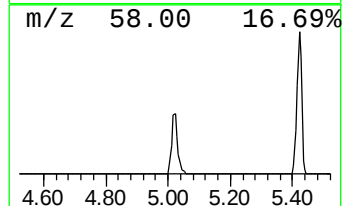
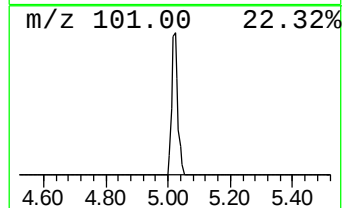
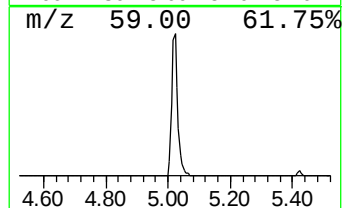
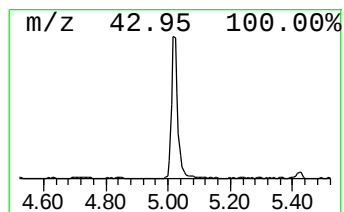
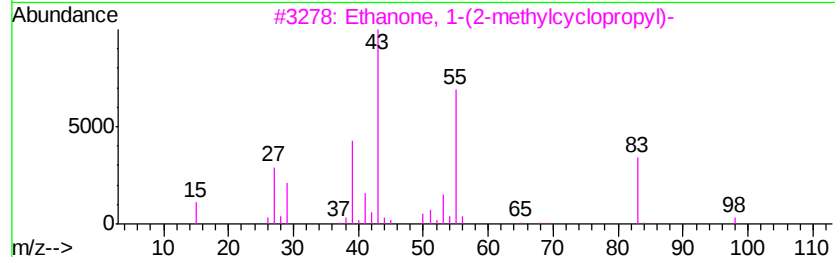
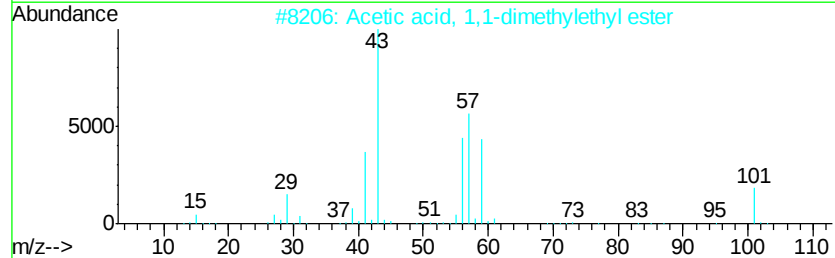
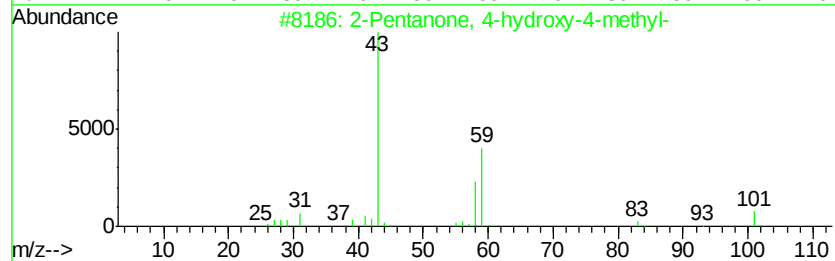
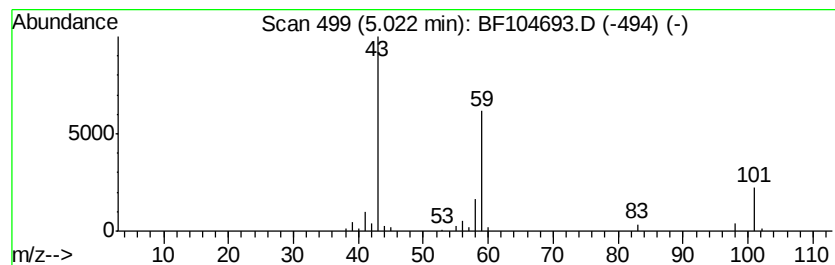
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.16 ng	132398	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetone	58	C3H6O	000067-64-1	9



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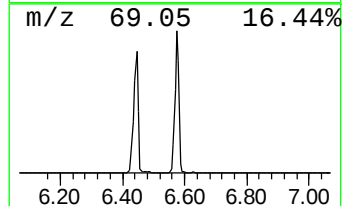
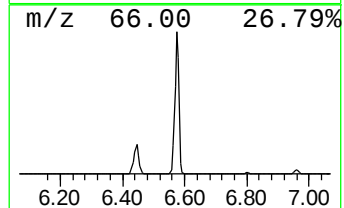
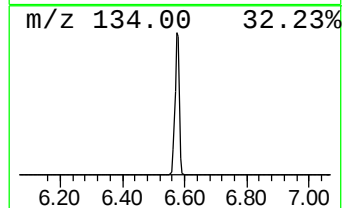
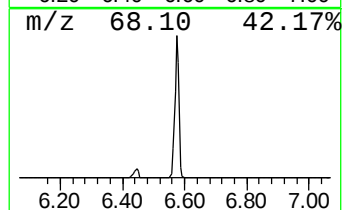
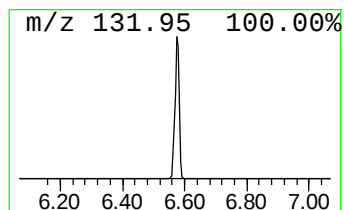
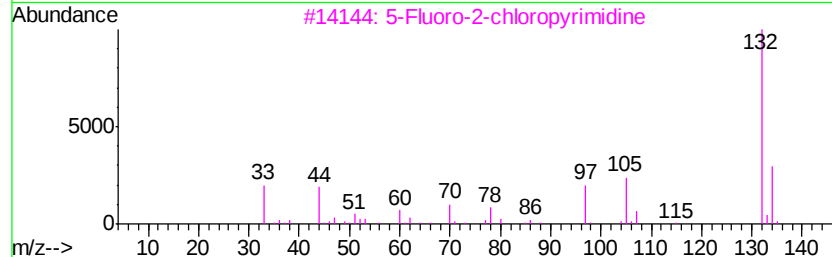
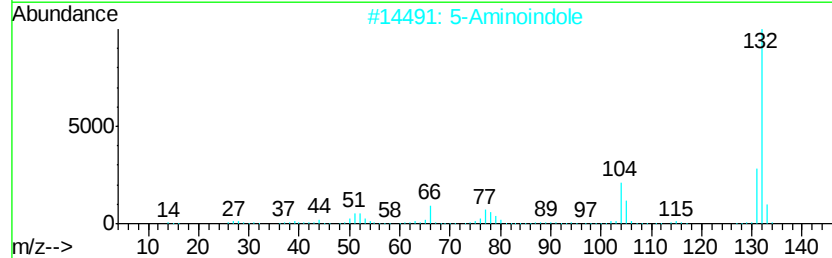
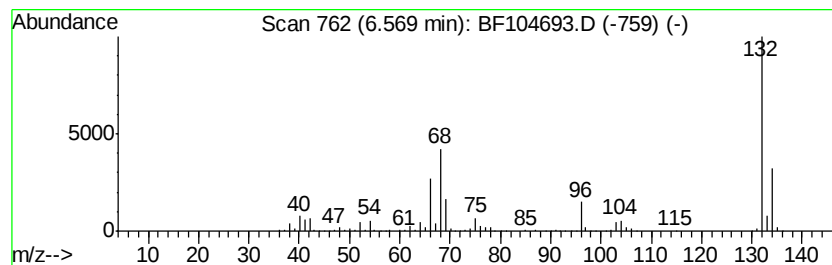
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	89.45 ng	2845060	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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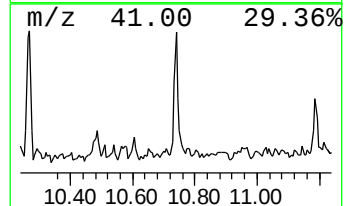
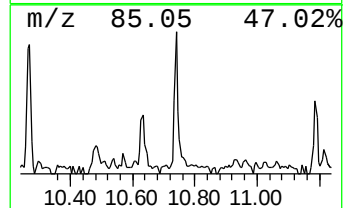
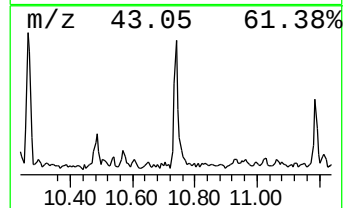
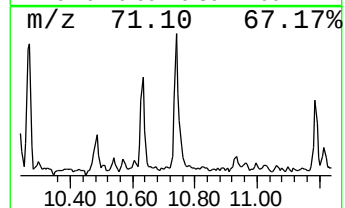
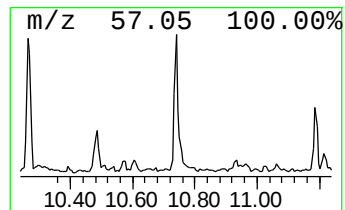
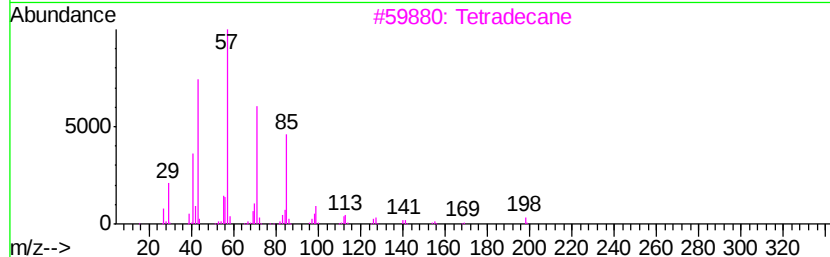
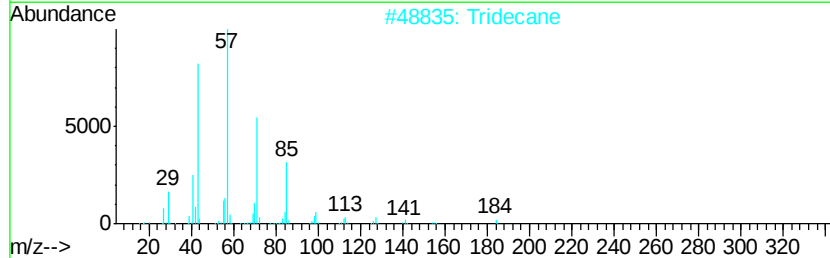
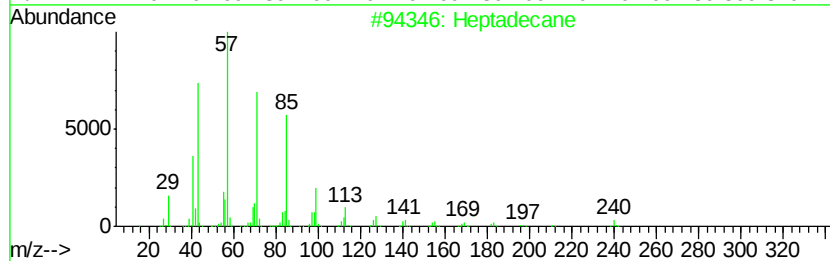
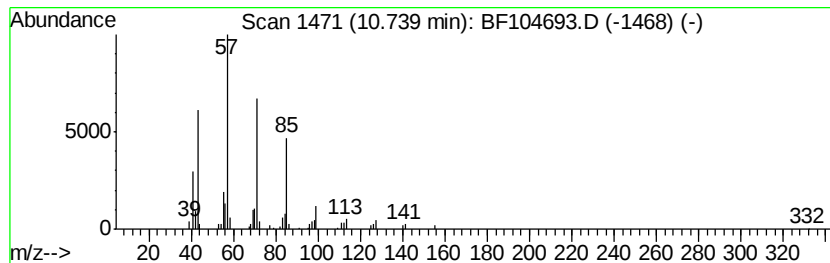
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.05 ng	72395	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Tridecane		184	C13H28	000629-50-5	90
3	Tetradecane		198	C14H30	000629-59-4	87
4	Dodecane, 2-methyl-		184	C13H28	001560-97-0	86
5	Heneicosane		296	C21H44	000629-94-7	80



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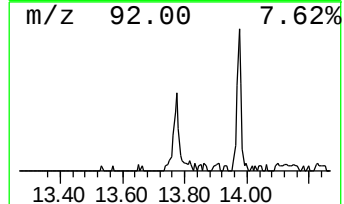
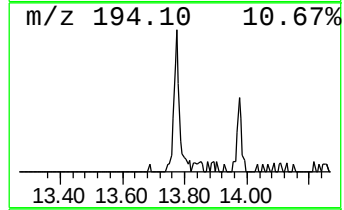
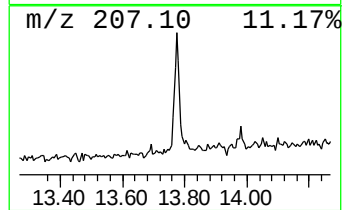
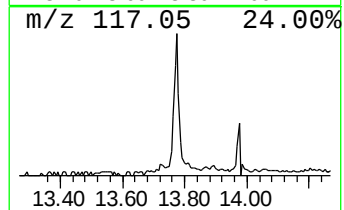
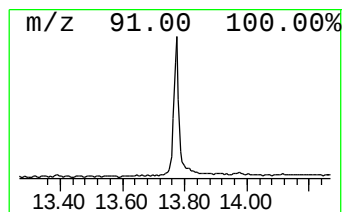
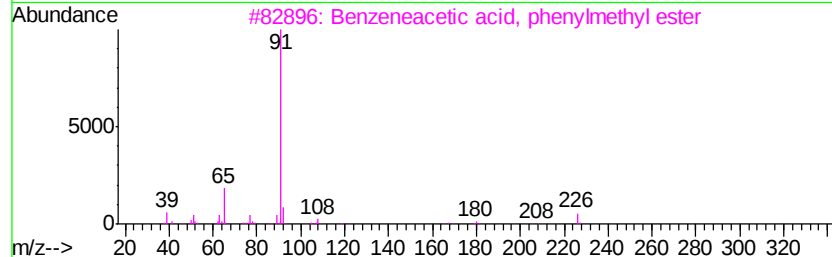
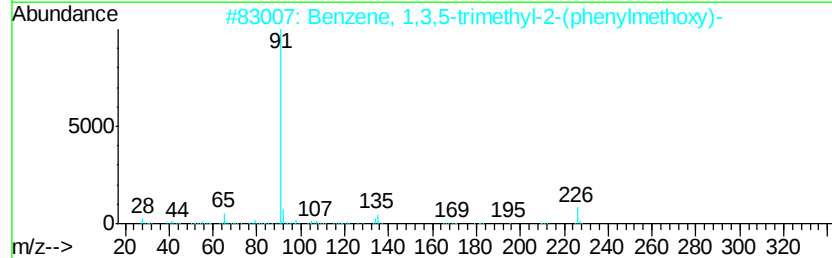
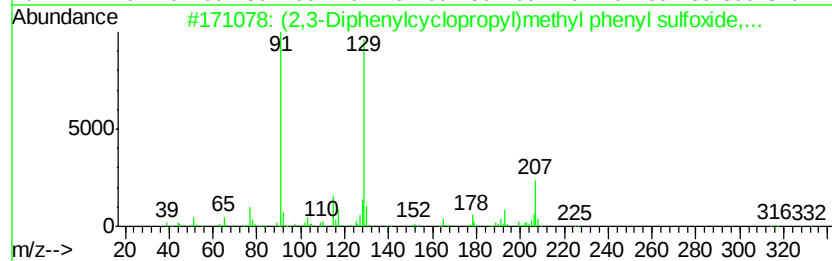
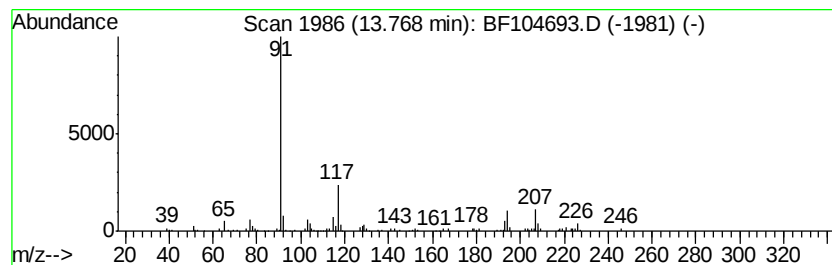
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.49 ng	177371	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	17
2		Benzene, 1,3,5-trimethyl-2-(phen...	226	C16H18O	019578-76-8	14
3		Benzeneacetic acid, phenylmethyl...	226	C15H14O2	000102-16-9	14
4		Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	12
5		Benzylidene-l-ornithine	220	C12H16N2O2	025693-00-9	10



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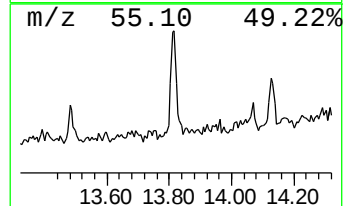
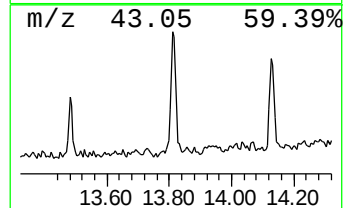
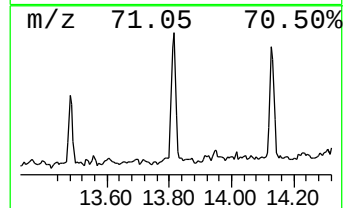
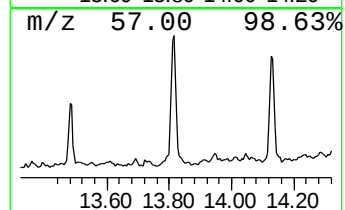
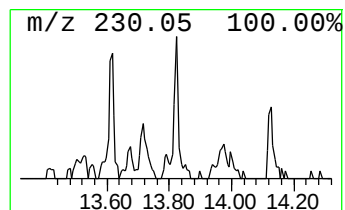
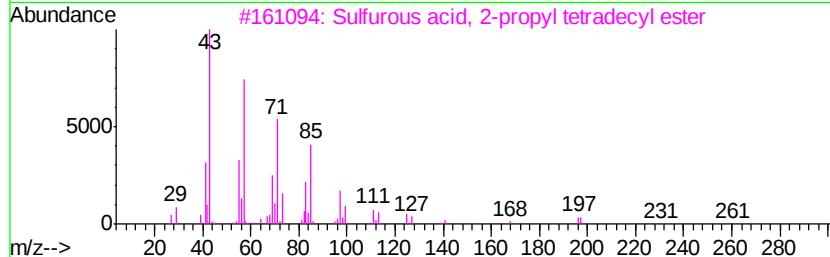
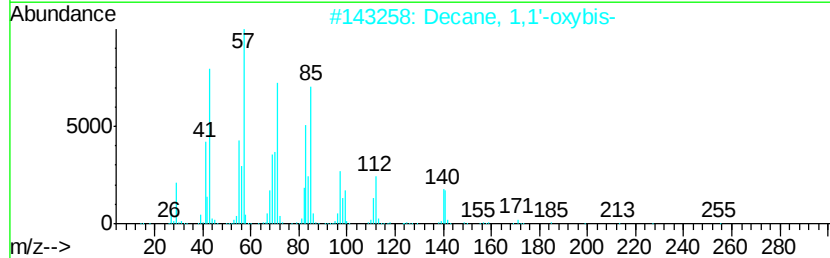
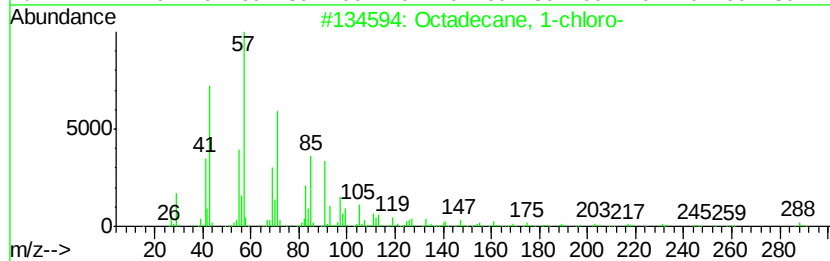
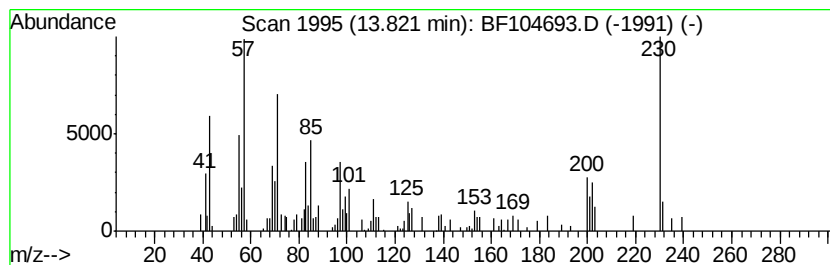
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	3.94 ng	155635	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
2	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	80
3	Sulfurous acid, 2-propyl tetradecyl...	320	C17H36O3S	1000309-12-5	80
4	Tritetracontane	605	C43H88	007098-21-7	72
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
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Acq On : 21 Apr 2018 00:40
Operator : JU/SJ
Sample : J2453-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

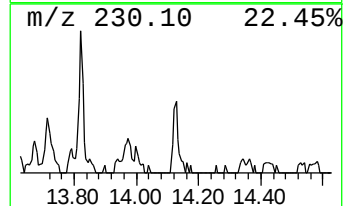
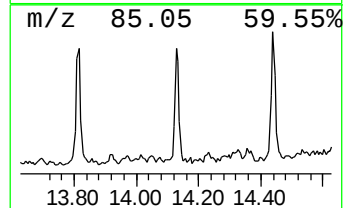
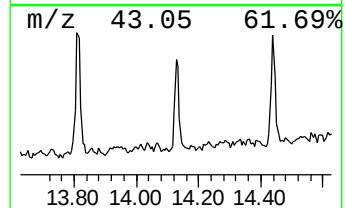
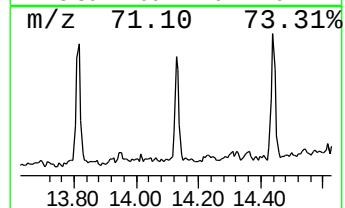
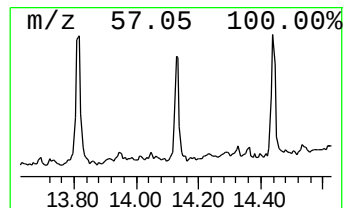
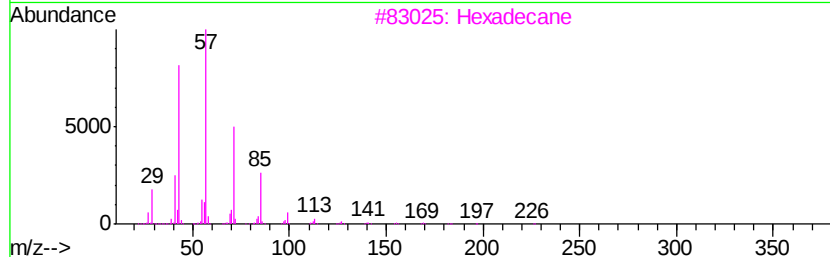
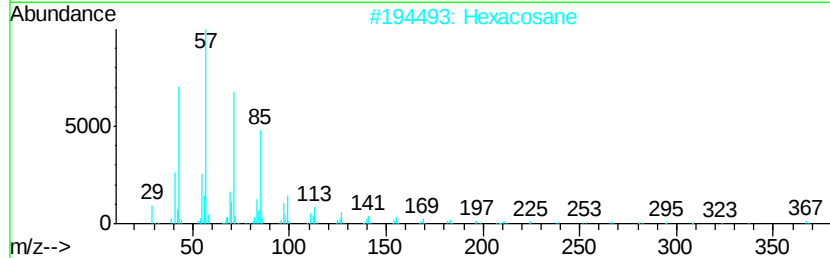
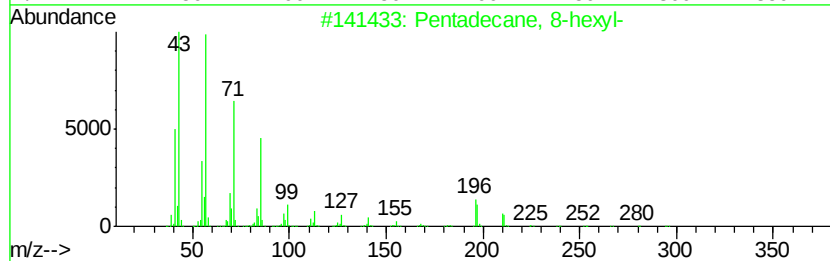
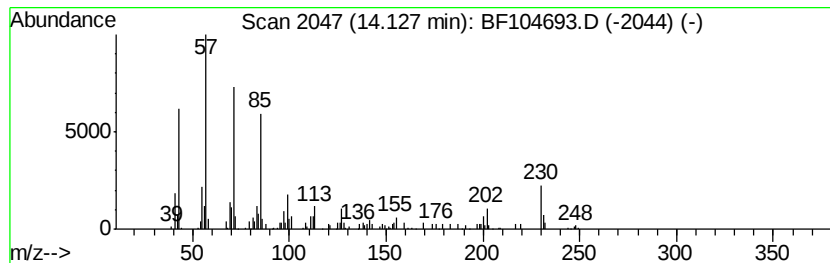
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ClientSampleId :
T-8_1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.13	2.56 ng	101185	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	80
2	Hexacosane	366	C26H54	000630-01-3	80
3	Hexadecane	226	C16H34	000544-76-3	80
4	Heptadecane	240	C17H36	000629-78-7	74
5	Octadecane	254	C18H38	000593-45-3	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
Data File : BF104693.D
Acq On : 21 Apr 2018 00:40
Operator : JU/SJ
Sample : J2453-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

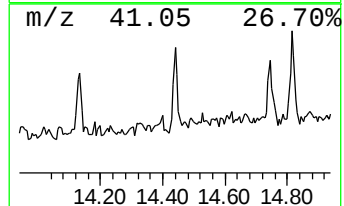
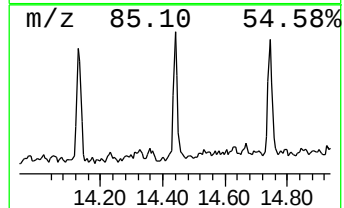
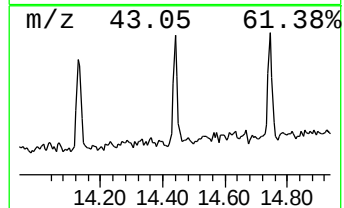
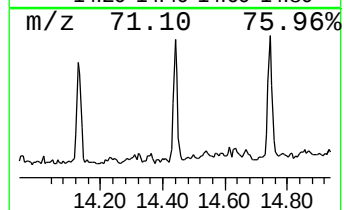
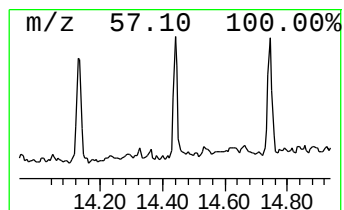
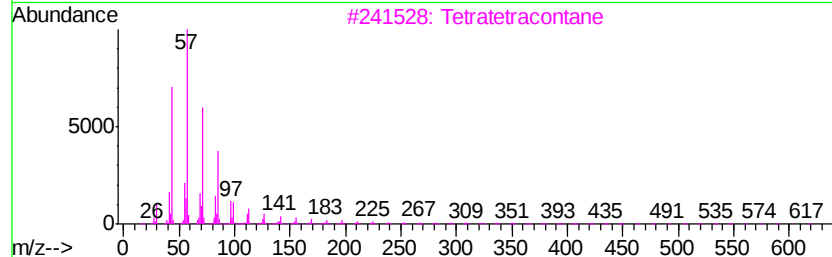
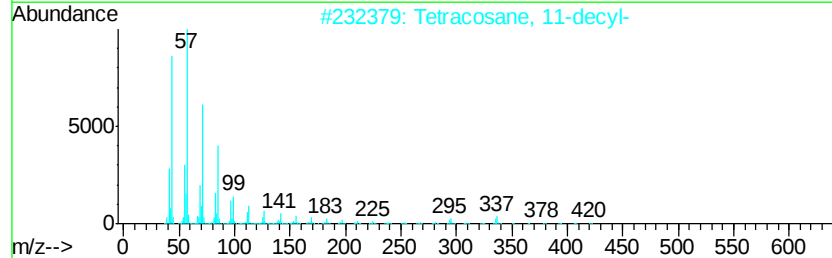
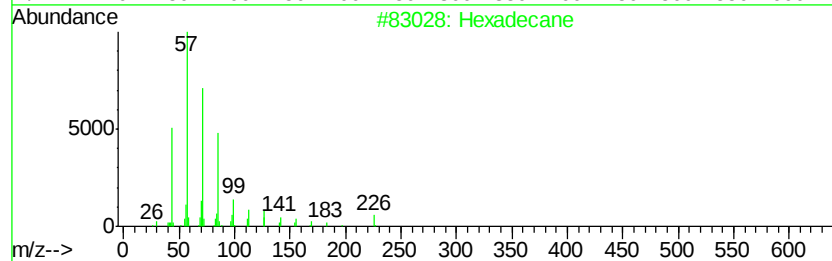
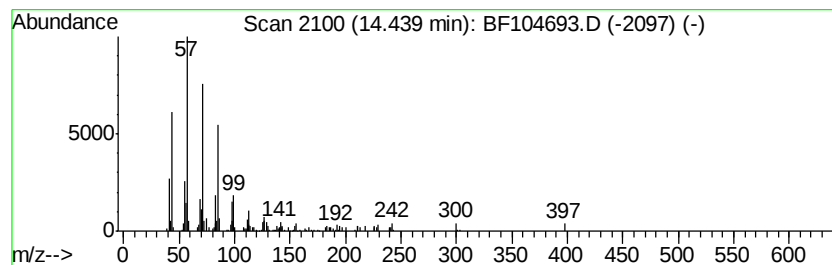
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ClientSampleId :
T-8_1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.53 ng	99974	Chrysene-d12	13.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane		226 C16H34	000544-76-3 94
2	Tetracosane, 11-decyl-		479 C34H70	055429-84-0 90
3	Tetratetracontane		619 C44H90	007098-22-8 90
4	Hexacosane		366 C26H54	000630-01-3 90
5	2-methyloctacosane		408 C29H60	1000376-72-8 90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
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Acq On : 21 Apr 2018 00:40
Operator : JU/SJ
Sample : J2453-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-8_1.0-1.5

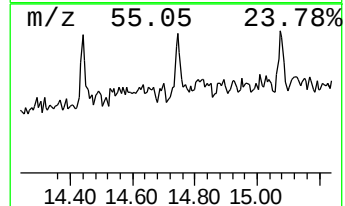
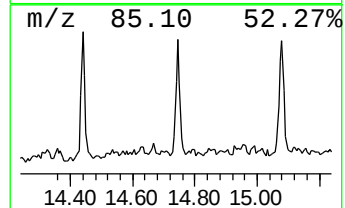
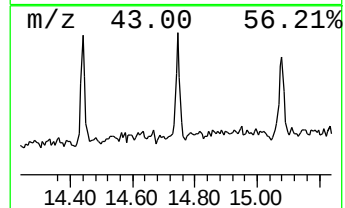
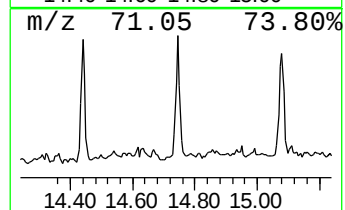
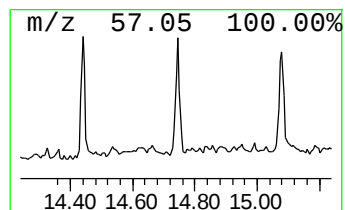
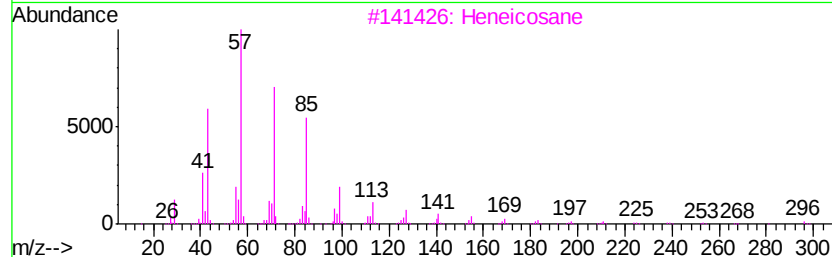
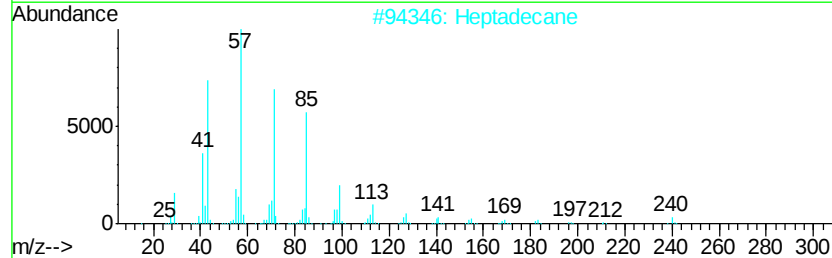
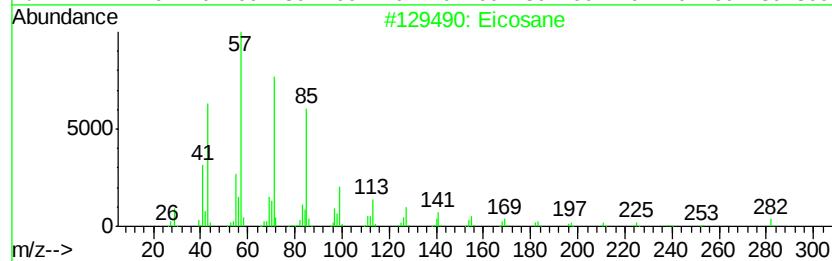
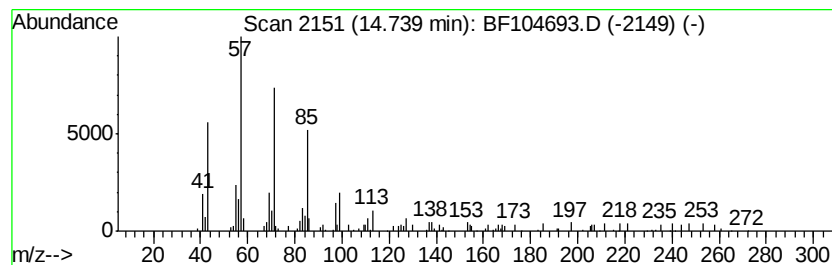
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.68 ng	77725	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexadecane	226	C16H34	000544-76-3	90
5		Tetracontane	563	C40H82	004181-95-7	90



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Data File : BF104693.D
Acq On : 21 Apr 2018 00:40
Operator : JU/SJ
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Instrument :
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ClientSampleId :
T-8_1.0-1.5

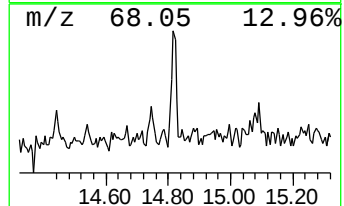
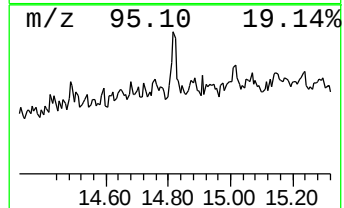
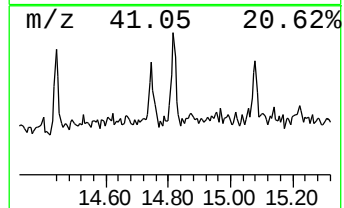
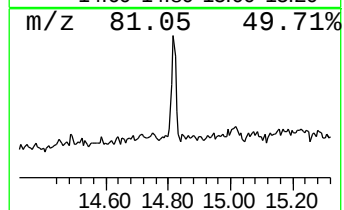
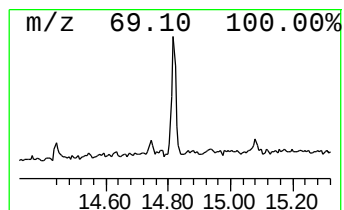
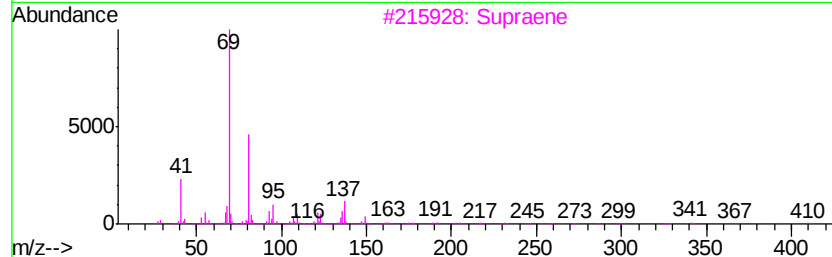
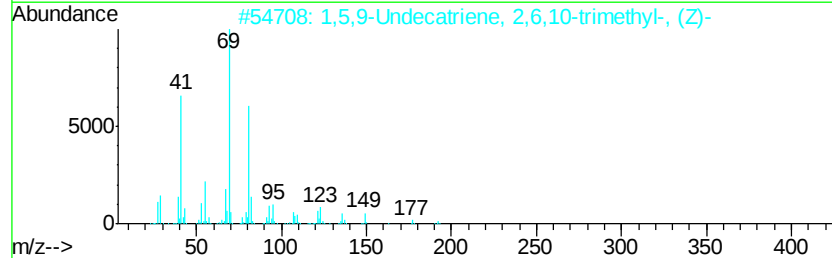
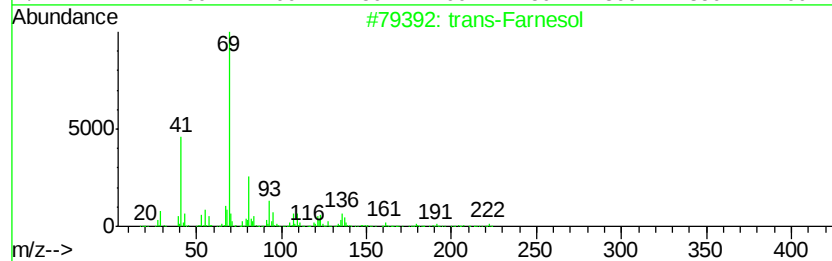
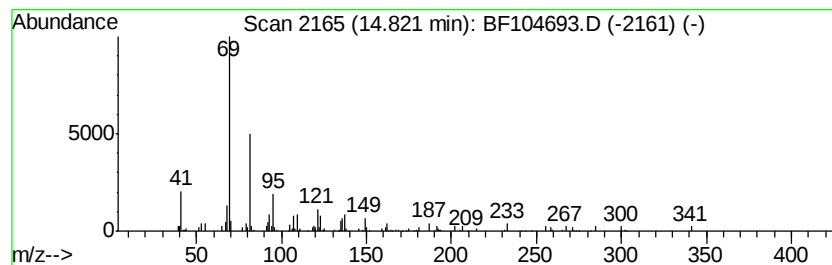
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 trans-Farnesol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.43 ng	70724	Perylene-d12	15.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Farnesol	222	C15H26O	000106-28-5	87
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
3			Supraene	410	C30H50	007683-64-9	80
4			Farnesol isomer a	222	C15H26O	1000108-92-4	80
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
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Acq On : 21 Apr 2018 00:40
Operator : JU/SJ
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Misc :
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Instrument :
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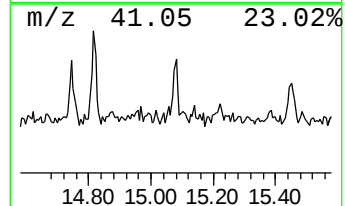
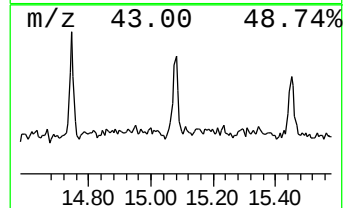
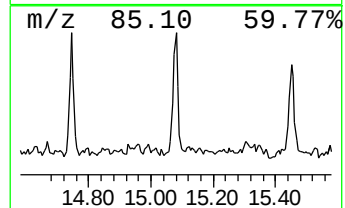
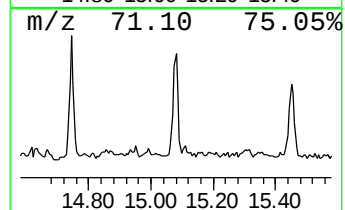
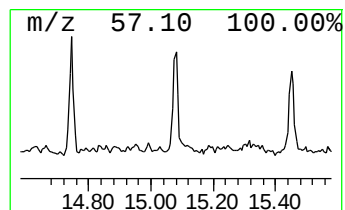
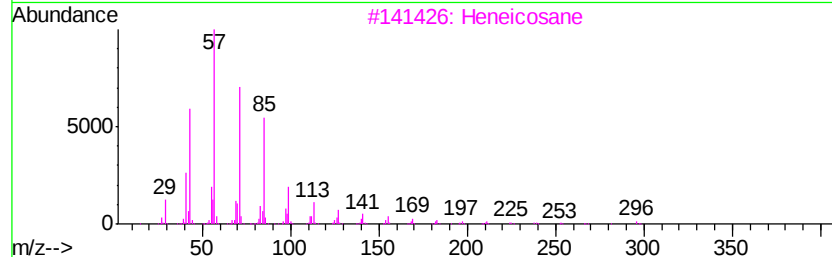
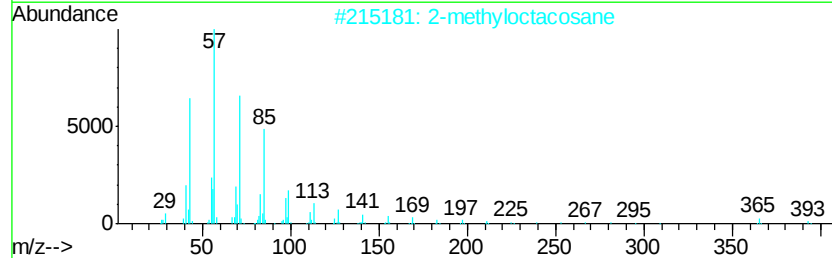
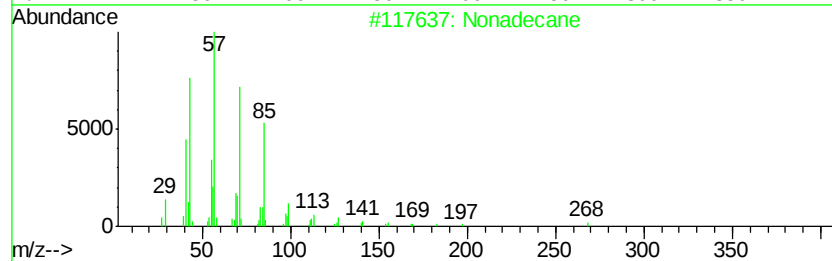
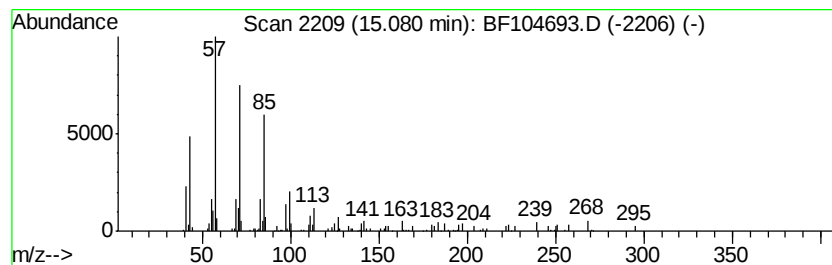
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.95 ng	85665	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	90
2		2-methyloctacosane	408	C29H60	1000376-72-8	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		10-Methylnonadecane	282	C20H42	056862-62-5	86
5		Tridecane, 3-methyl-	198	C14H30	006418-41-3	80



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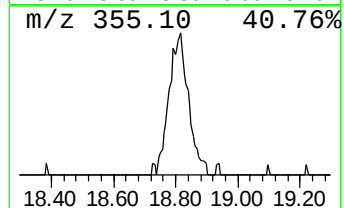
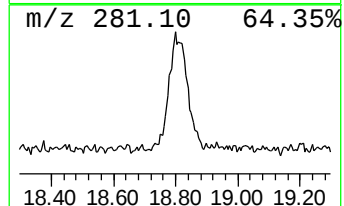
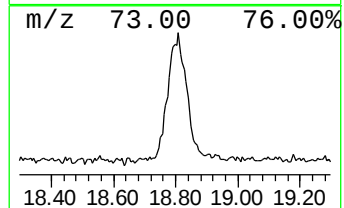
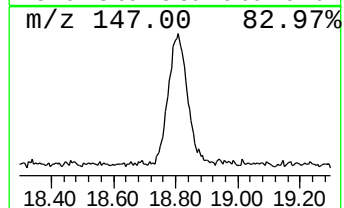
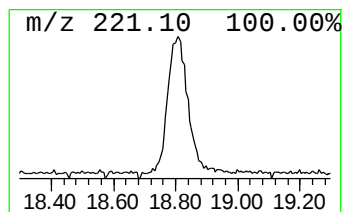
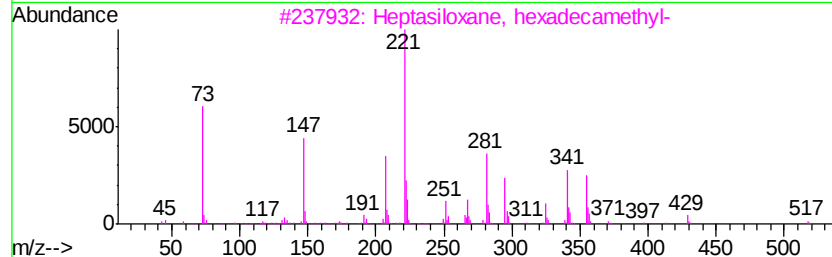
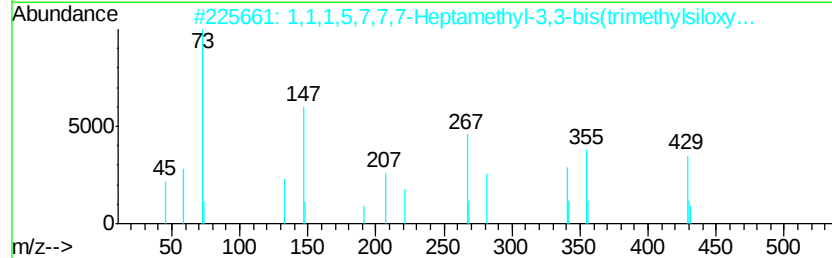
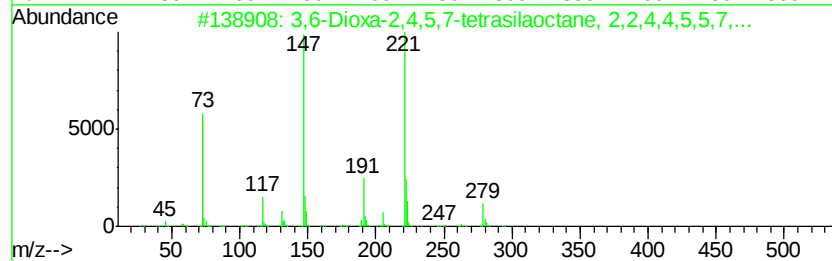
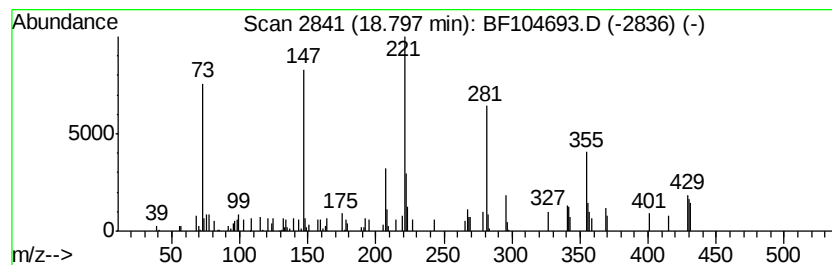
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.80	8.85 ng	257009	Perylene-d12	15.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	47
2			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
4			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22
5			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.57	6.57	89.5	ng	2845060	1	6.80	636138	20.0
Heptadecane	10.74	2.0	ng	72395	4	11.33	707532	20.0
unknown13.77	13.77	4.5	ng	177371	5	13.97	789598	20.0
Octadecane, 1-chl...	13.82	3.9	ng	155635	5	13.97	789598	20.0
Pentadecane, 8-he...	14.13	2.6	ng	101185	5	13.97	789598	20.0
Hexadecane	14.44	2.5	ng	99974	5	13.97	789598	20.0
Eicosane	14.74	2.7	ng	77725	6	15.44	580988	20.0
trans-Farnesol	14.82	2.4	ng	70724	6	15.44	580988	20.0
Nonadecane	15.08	3.0	ng	85665	6	15.44	580988	20.0
unknown18.80	18.80	8.8	ng	257009	6	15.44	580988	20.0