

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
 Data File : BF109004.D
 Acq On : 14 Sep 2018 19:31
 Operator : JU/SJ
 Sample : J4906-25
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-PIT-4

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-BF091418.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	4.907	433	437	445	rVB	69030	93588	3.64%	0.376%
2	5.325	503	508	511	rBV	2259835	2104479	81.84%	8.459%
3	6.348	677	682	689	rBV	2293415	2329357	90.58%	9.363%
4	6.484	701	705	709	rBV	2450145	2276217	88.51%	9.150%
5	6.719	741	745	748	rBV	1097790	873808	33.98%	3.512%
6	6.748	748	750	754	rVB	40294	32492	1.26%	0.131%
7	6.878	768	772	775	rVB	2038853	1761295	68.49%	7.080%
8	7.278	831	840	843	rBV	1658276	1471685	57.23%	5.916%
9	7.372	852	856	861	rBV5	28066	40619	1.58%	0.163%
10	7.519	878	881	887	rVB3	49926	69845	2.72%	0.281%
11	7.648	900	903	908	rVB5	36627	47238	1.84%	0.190%
12	7.695	908	911	915	rBV2	50857	61345	2.39%	0.247%
13	7.736	915	918	921	rVB2	32255	34396	1.34%	0.138%
14	8.001	959	963	966	rBV	1405622	1181474	45.94%	4.749%
15	8.054	968	972	974	rVV3	48873	59693	2.32%	0.240%
16	8.078	974	976	979	rVV	144883	127634	4.96%	0.513%
17	8.130	983	985	988	rVB2	31630	30057	1.17%	0.121%
18	8.178	988	993	997	rBV4	28050	47228	1.84%	0.190%
19	8.307	1009	1015	1018	rBV5	53402	86895	3.38%	0.349%
20	8.360	1022	1024	1026	rBV2	44679	35195	1.37%	0.141%
21	8.389	1026	1029	1034	rVB5	23486	31372	1.22%	0.126%
22	8.442	1034	1038	1042	rBV2	115484	126546	4.92%	0.509%
23	8.554	1053	1057	1061	rBV6	34036	44866	1.74%	0.180%
24	8.707	1079	1083	1086	rVB2	68218	83236	3.24%	0.335%
25	8.919	1116	1119	1121	rVB3	34001	32062	1.25%	0.129%
26	9.036	1136	1139	1142	rVB	86274	69286	2.69%	0.279%
27	9.078	1142	1146	1149	rBV	3078926	2571594	100.00%	10.337%
28	9.172	1158	1162	1166	rBV4	21411	35028	1.36%	0.141%
29	9.466	1209	1212	1215	rBV	309418	244536	9.51%	0.983%
30	9.489	1215	1216	1219	rVB	59509	38548	1.50%	0.155%
31	9.748	1256	1260	1264	rBV2	1500970	1352235	52.58%	5.436%
32	10.530	1389	1393	1407	rBV	1895396	1733684	67.42%	6.969%
33	10.683	1414	1419	1423	rVB	29751	39404	1.53%	0.158%
34	11.224	1507	1511	1514	rBV	1649908	1367452	53.18%	5.497%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

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-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.766	1599	1603	1606	rBV	159264	141117	5.49%	0.567%
36	12.218	1678	1680	1686	rBV3	26205	31089	1.21%	0.125%
37	12.430	1713	1716	1720	rBV	75119	82120	3.19%	0.330%
38	12.807	1776	1780	1784	rBV	2564727	2287159	88.94%	9.194%
39	13.848	1954	1957	1960	rBV	1036932	995057	38.69%	4.000%
40	15.259	2194	2197	2201	rVB	732205	806402	31.36%	3.242%

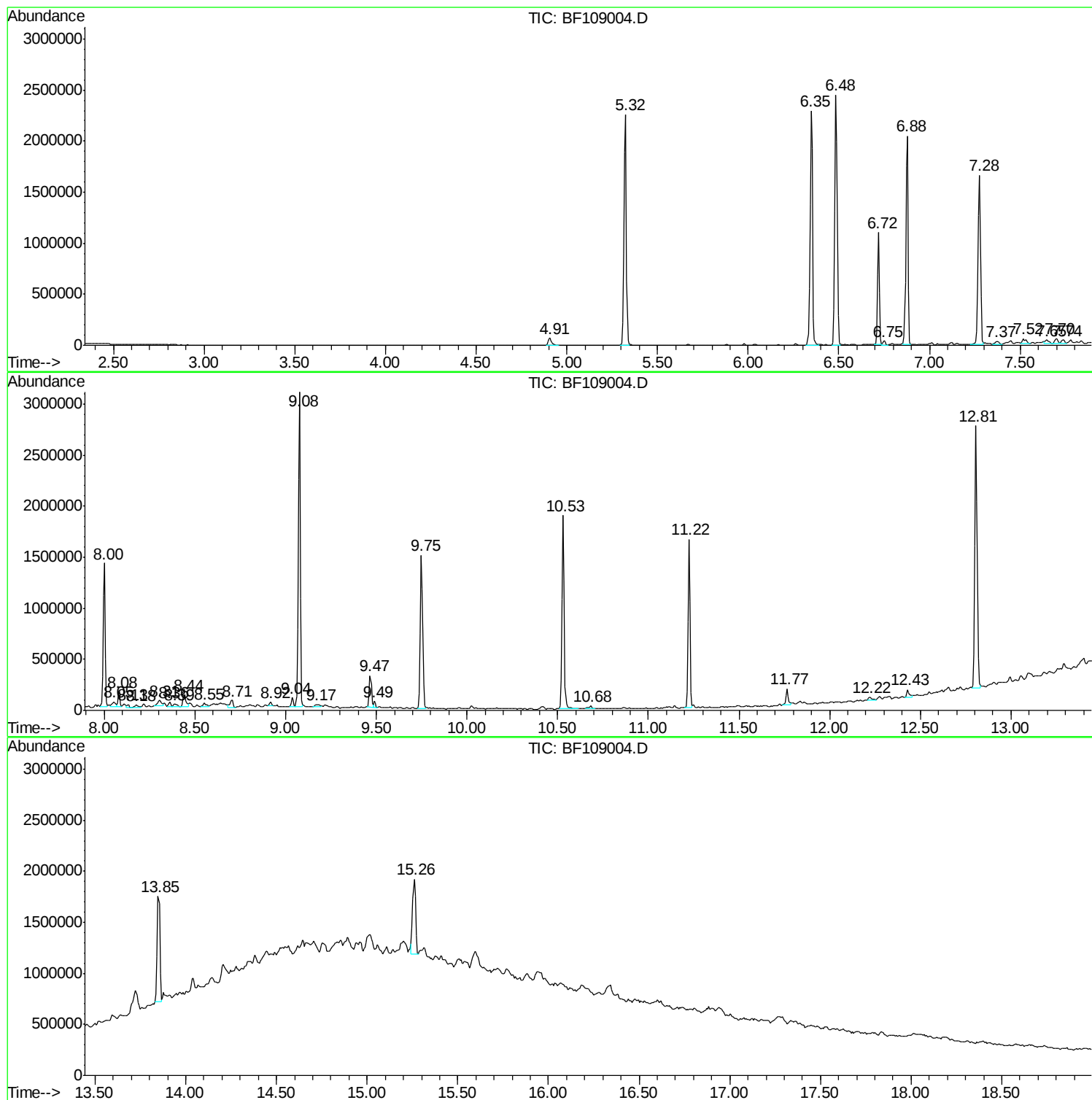
Sum of corrected areas: 24877333

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SP-PIT-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

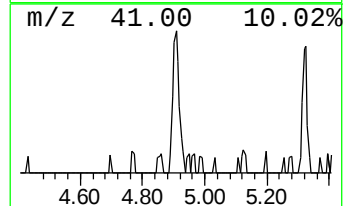
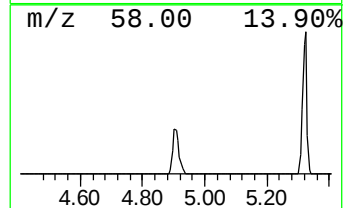
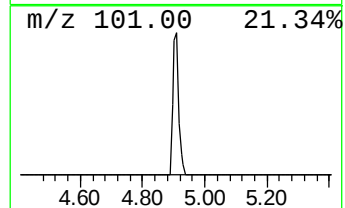
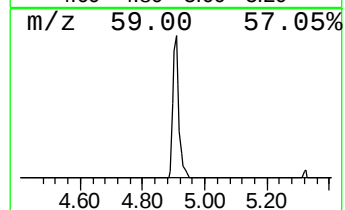
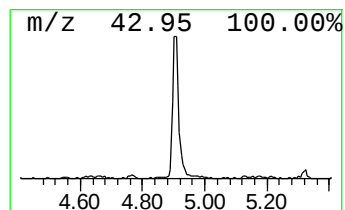
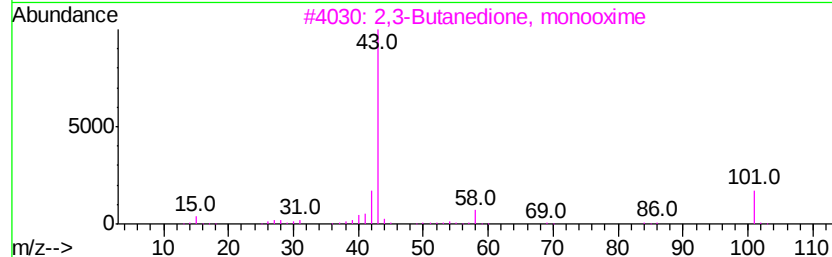
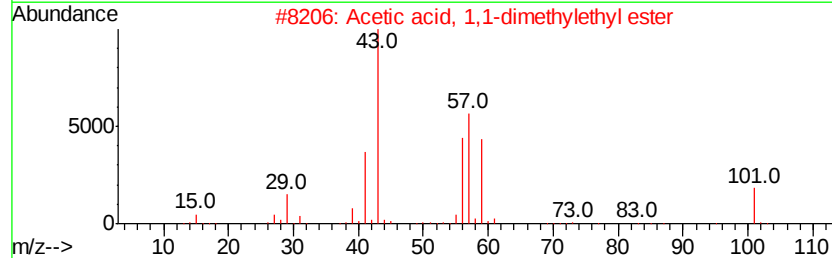
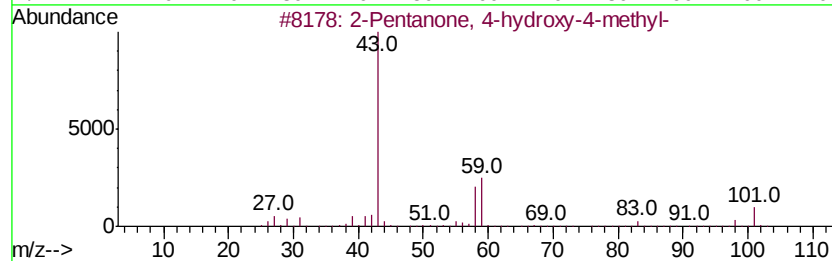
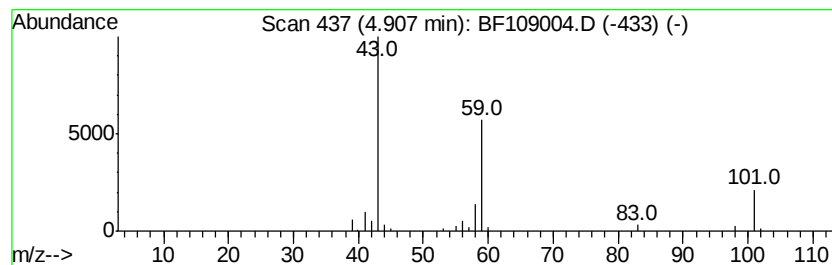
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.91	2.14 ng	93588	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

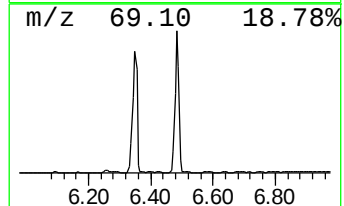
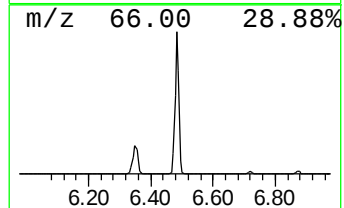
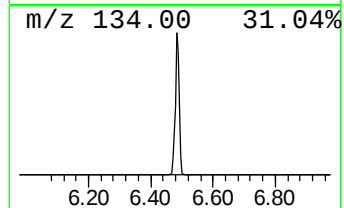
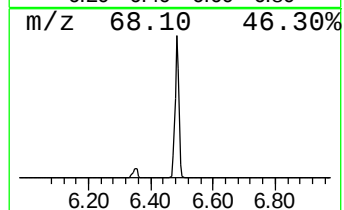
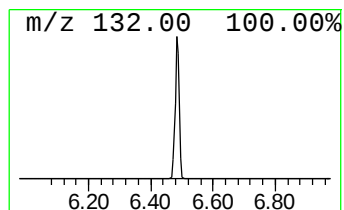
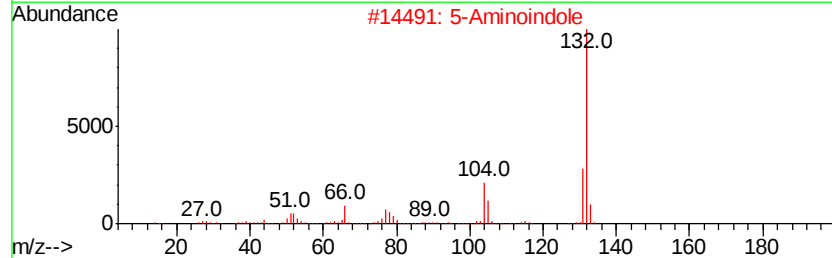
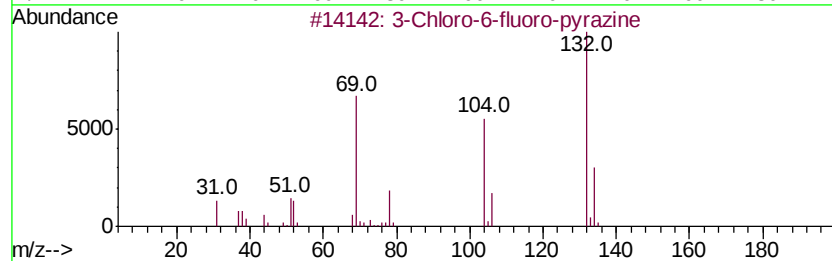
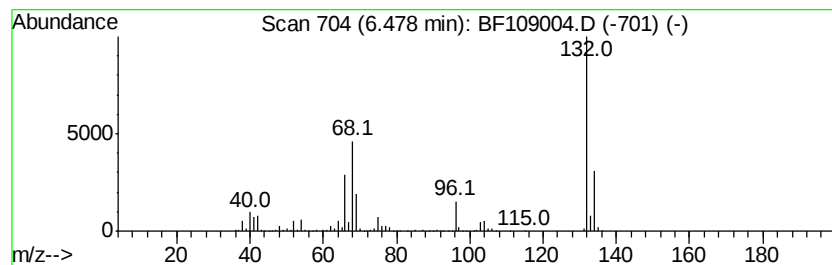
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	52.10 ng	2276220	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

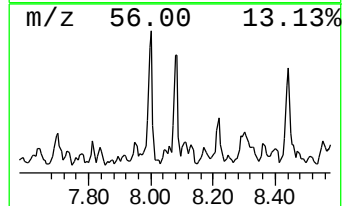
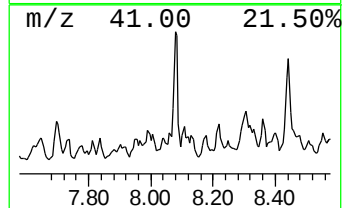
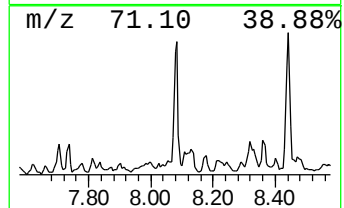
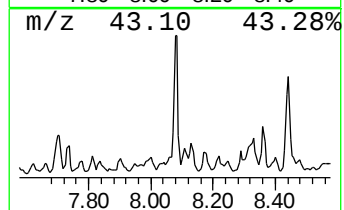
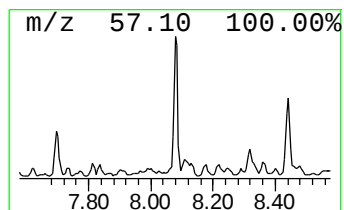
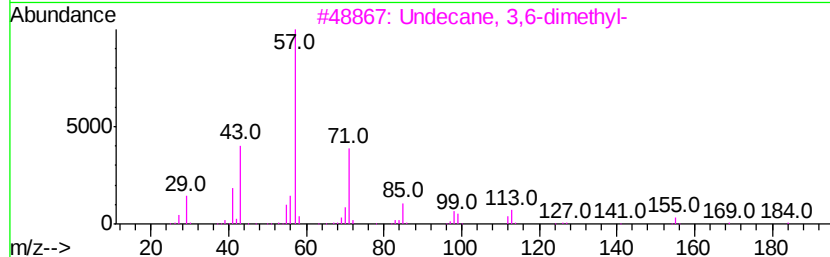
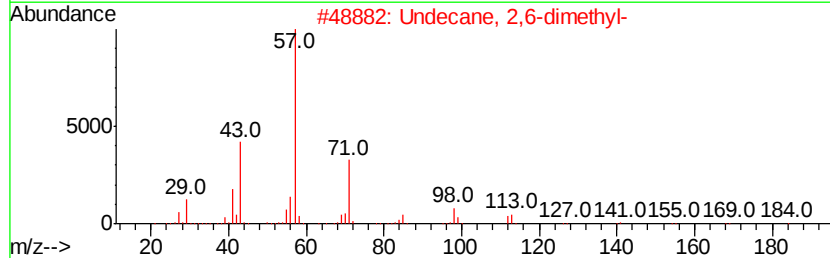
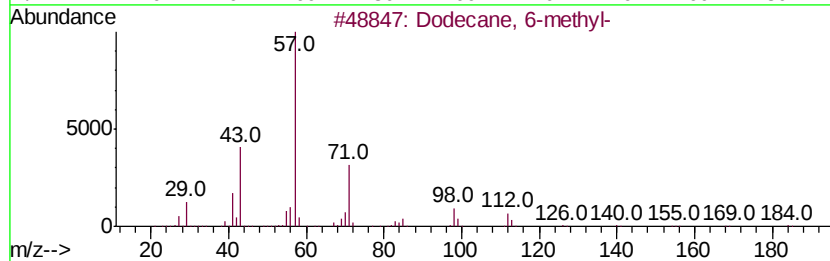
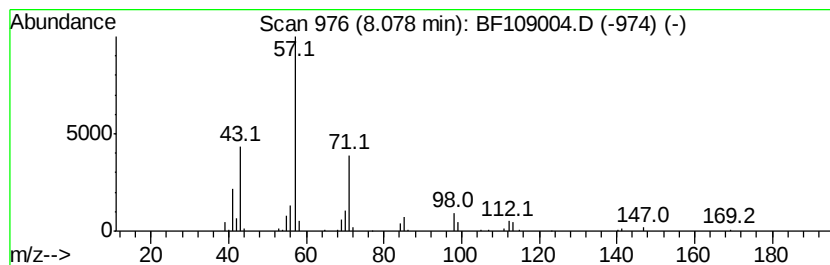
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecane, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.08	2.16 ng	127634	Naphthalene-d8	8.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 6-methyl-	184	C13H28	006044-71-9	90
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

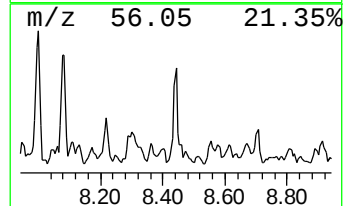
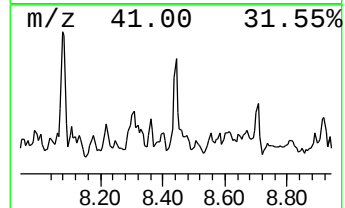
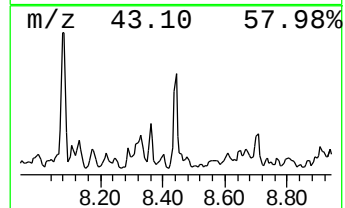
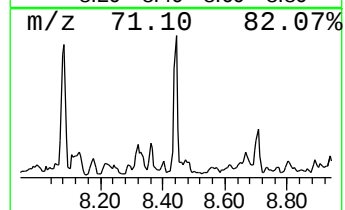
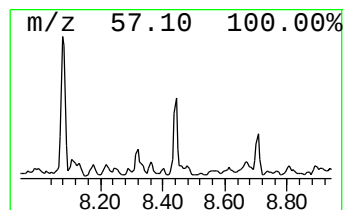
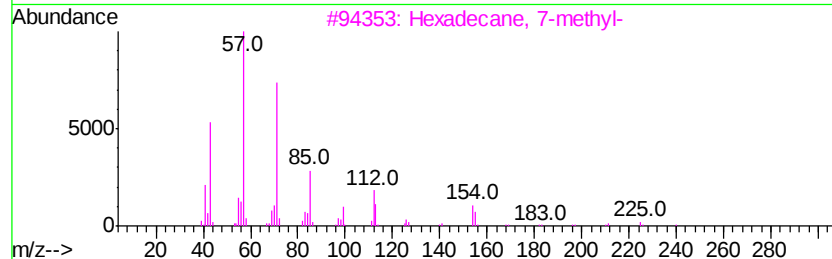
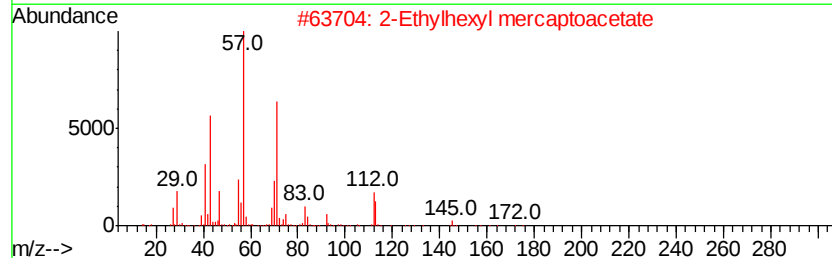
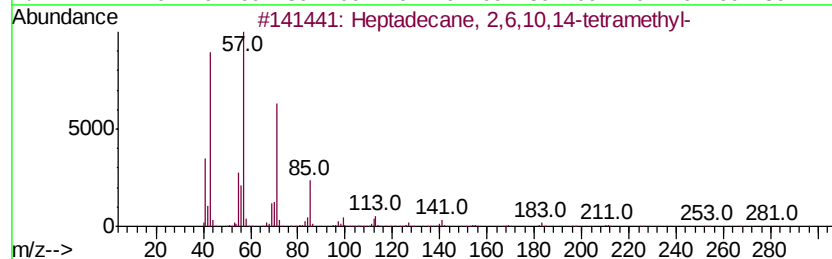
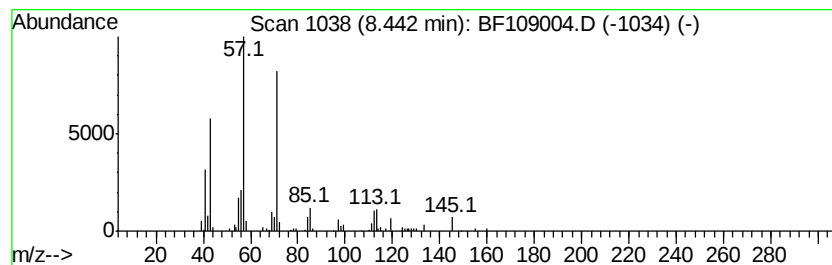
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.44	2.14 ng	126546	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	64
2		2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	59
3		Hexadecane, 7-methyl-	240	C17H36	026730-20-1	59
4		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	53
5		Heptacosane	380	C27H56	000593-49-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

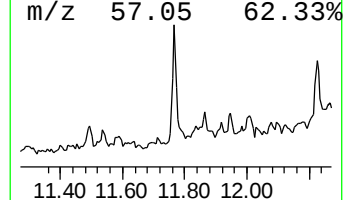
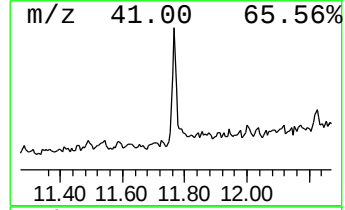
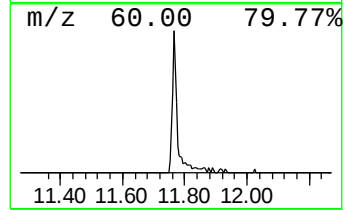
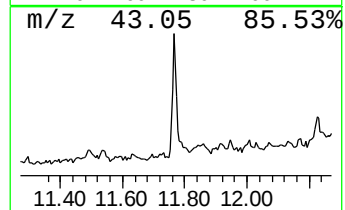
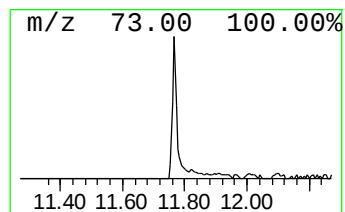
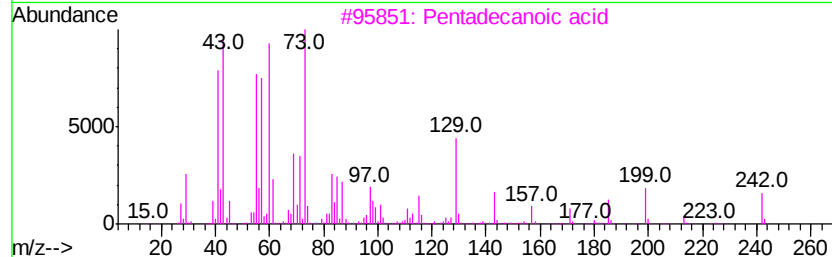
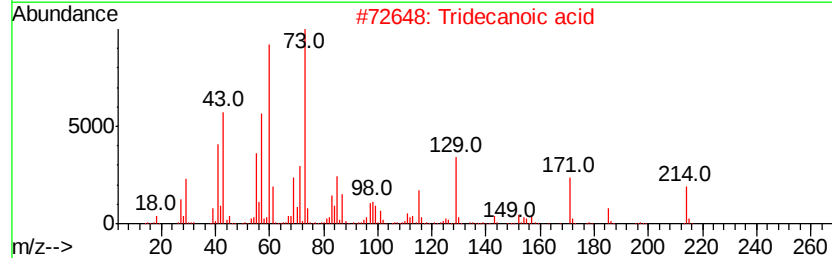
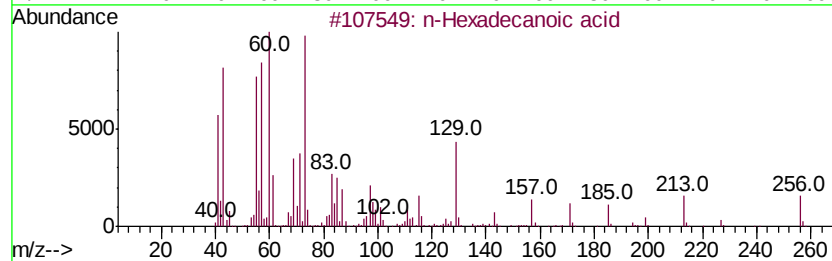
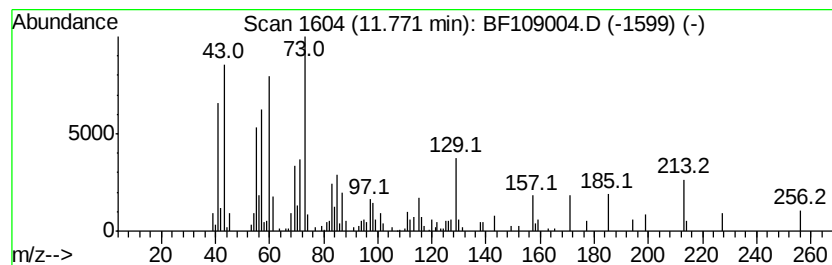
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.06 ng	141117	Phenanthrene-d10	11.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
Data File : BF109004.D
Acq On : 14 Sep 2018 19:31
Operator : JU/SJ
Sample : J4906-25
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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...	4.91	2.1	ng	93588	1	6.72	873808	20.0
unknown6.48	6.48	52.1	ng	2276220	1	6.72	873808	20.0
Dodecane, 6-methyl-	8.08	2.2	ng	127634	2	8.00	1181470	20.0
Heptadecane, 2,6,...	8.44	2.1	ng	126546	2	8.00	1181470	20.0
n-Hexadecanoic acid	11.77	2.1	ng	141117	4	11.22	1367450	20.0