

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
 Data File : BF106316.D
 Acq On : 12 Jun 2018 00:55
 Operator : JU/SJ
 Sample : J3354-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CAS1-SB-02-03-1-27

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-BF061118.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	5.207	484	488	495	rVB	369677	423258	8.86%	0.975%
2	5.590	548	553	557	rBV	3845077	4341168	90.91%	9.999%
3	6.590	717	723	726	rBV	3971046	4513746	94.53%	10.396%
4	6.743	744	749	752	rBV	4184303	4351928	91.14%	10.024%
5	6.972	784	788	791	rVB	1633607	1275881	26.72%	2.939%
6	7.131	810	815	818	rBV	3620856	3463131	72.52%	7.976%
7	7.531	878	883	886	rBV	2948791	2906174	60.86%	6.694%
8	7.595	888	894	901	rVB	80707	96882	2.03%	0.223%
9	8.254	1002	1006	1009	rBV	1798329	1574583	32.97%	3.627%
10	9.331	1184	1189	1192	rVB	4842224	4775110	100.00%	10.998%
11	9.719	1251	1255	1258	rBV	845022	731448	15.32%	1.685%
12	9.925	1287	1290	1293	rBV	127922	101508	2.13%	0.234%
13	10.013	1301	1305	1308	rBV	1890803	1620294	33.93%	3.732%
14	10.407	1368	1372	1373	rBV	58698	51372	1.08%	0.118%
15	10.431	1373	1376	1378	rVB	172567	154267	3.23%	0.355%
16	10.648	1407	1413	1415	rBV	77178	93134	1.95%	0.215%
17	10.801	1435	1439	1442	rBV	3108685	2779518	58.21%	6.402%
18	10.901	1453	1456	1462	rBV	178088	202044	4.23%	0.465%
19	11.348	1529	1532	1535	rBV	78735	62904	1.32%	0.145%
20	11.378	1535	1537	1542	rVB	53317	51788	1.08%	0.119%
21	11.501	1554	1558	1561	rBV	1759628	1479465	30.98%	3.408%
22	12.013	1640	1645	1654	rBV2	376197	402777	8.43%	0.928%
23	12.583	1738	1742	1745	rBV2	54115	63419	1.33%	0.146%
24	12.713	1760	1764	1769	rBV	82724	89056	1.87%	0.205%
25	12.795	1775	1778	1783	rBV	140499	146144	3.06%	0.337%
26	12.942	1797	1803	1806	rBV	103636	101005	2.12%	0.233%
27	13.083	1823	1827	1831	rBV	4230326	4171367	87.36%	9.608%
28	13.966	1971	1977	1985	rBV	252284	266465	5.58%	0.614%
29	14.142	2003	2007	2010	rBV	1558048	1417066	29.68%	3.264%
30	14.236	2016	2023	2030	rBV9	84891	212481	4.45%	0.489%
31	14.601	2082	2085	2089	rBV2	61515	73851	1.55%	0.170%
32	14.771	2111	2114	2117	rVB	56259	53935	1.13%	0.124%
33	15.007	2151	2154	2159	rVB2	45174	48826	1.02%	0.112%
34	15.671	2261	2267	2276	rBV	902380	1165978	24.42%	2.686%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.671	2434	2437	2448	rVB8	32018	65400	1.37%	0.151%
36	17.842	2633	2636	2645	rVB8	45301	89484	1.87%	0.206%

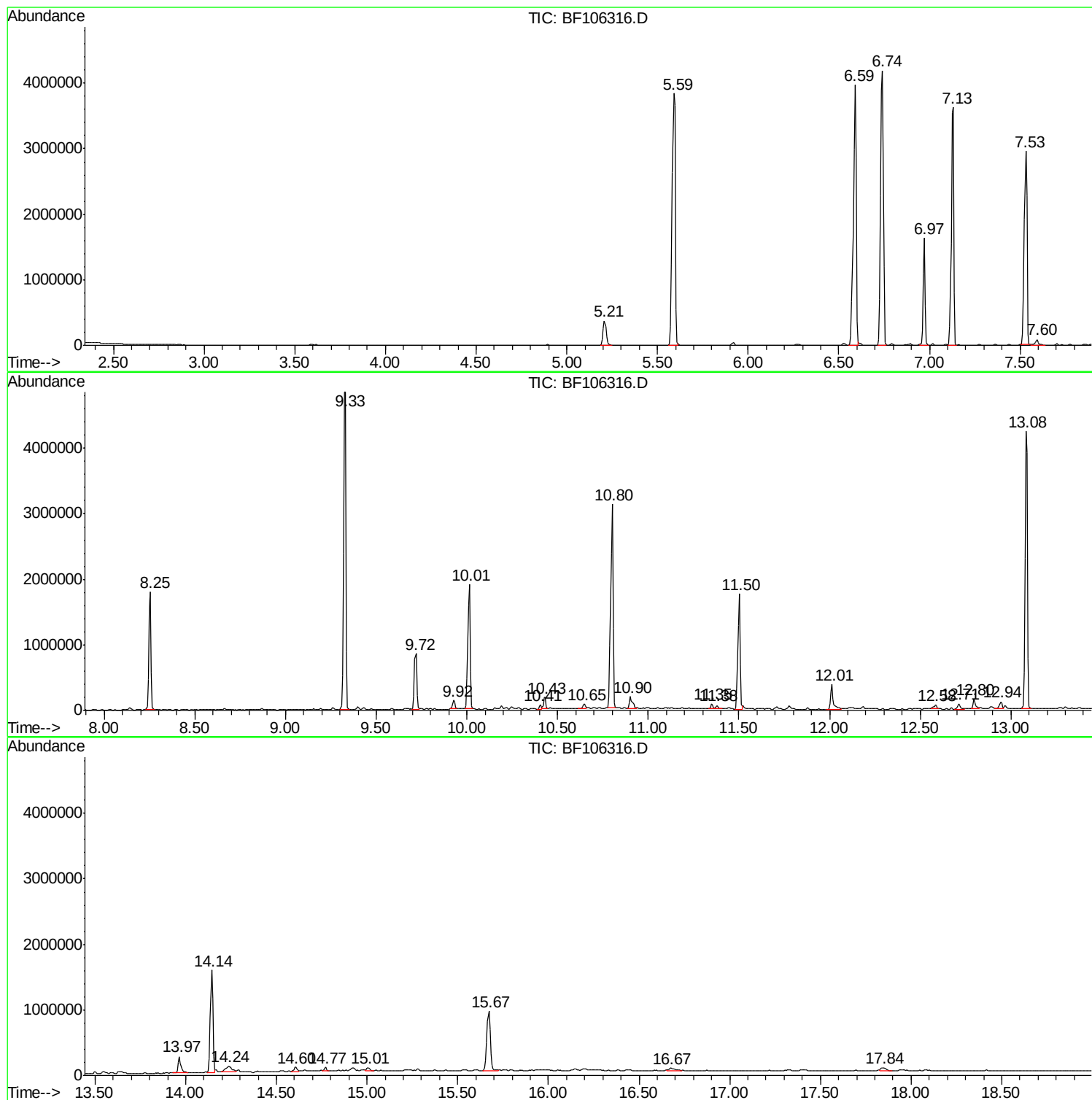
Sum of corrected areas: 43416857

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

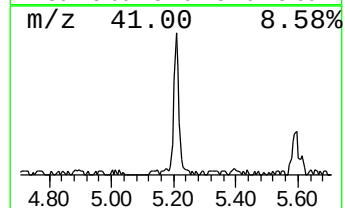
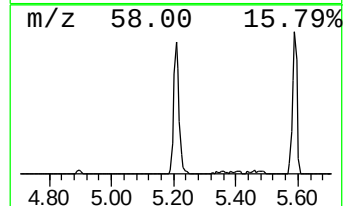
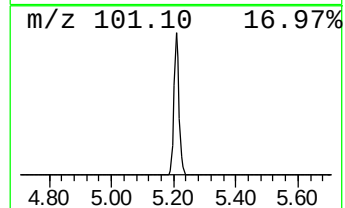
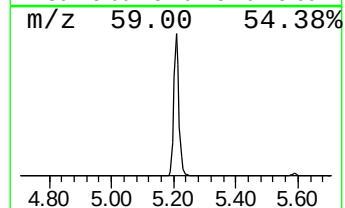
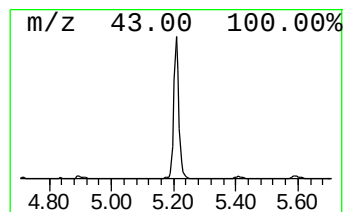
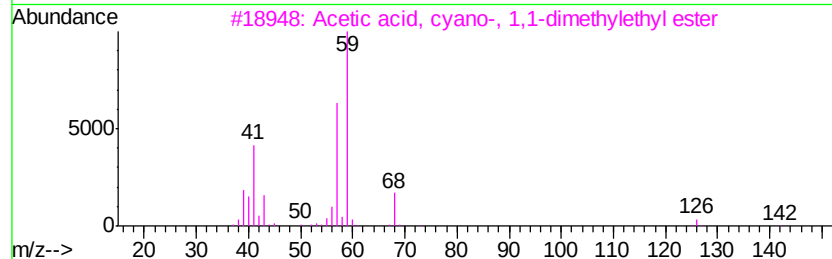
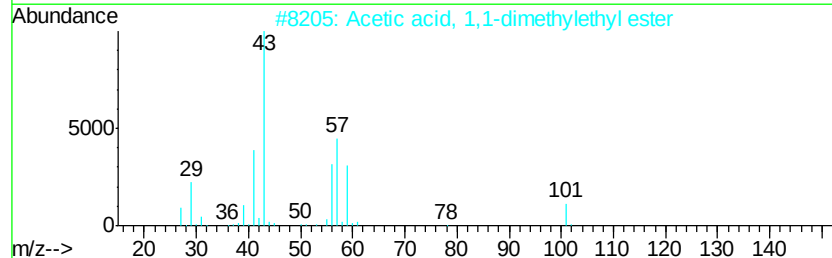
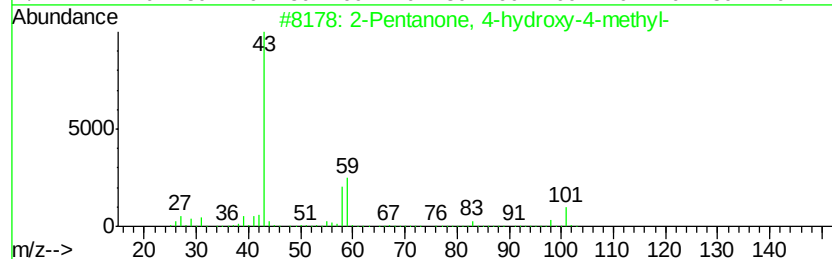
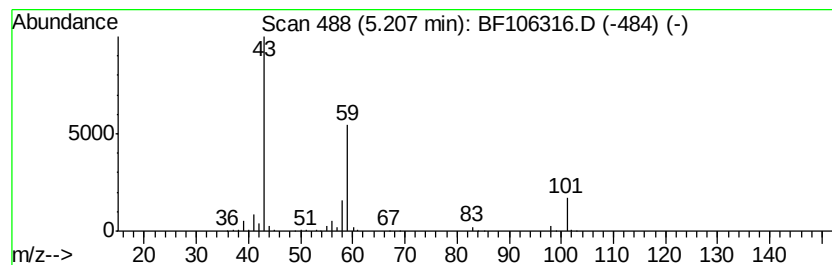
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	6.63 ng	423258	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

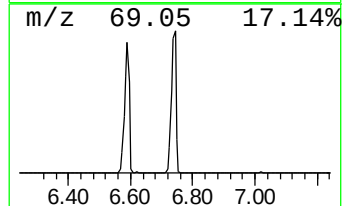
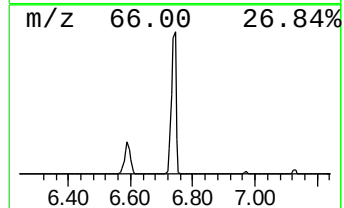
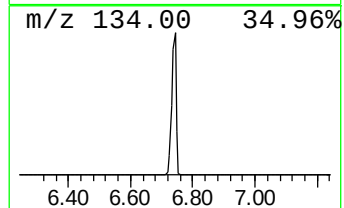
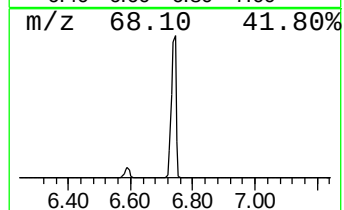
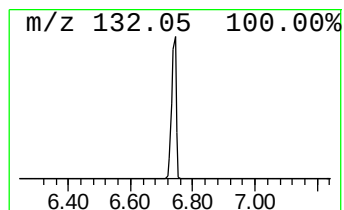
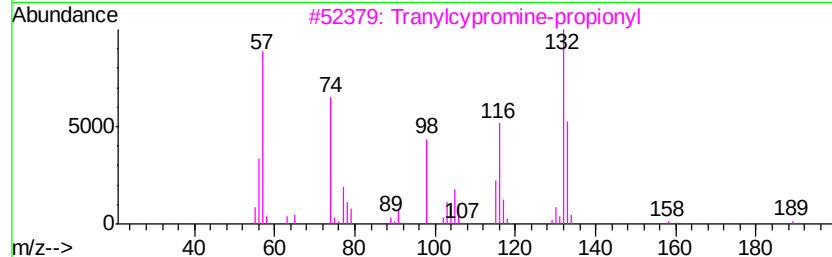
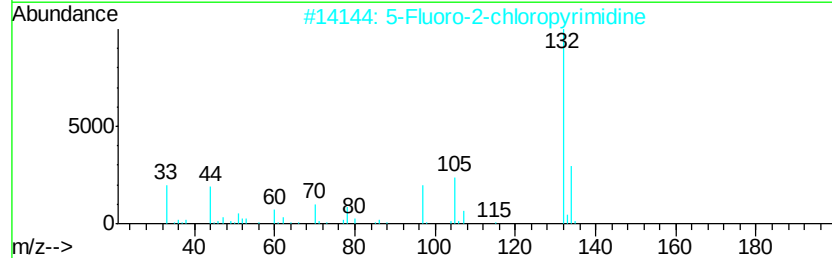
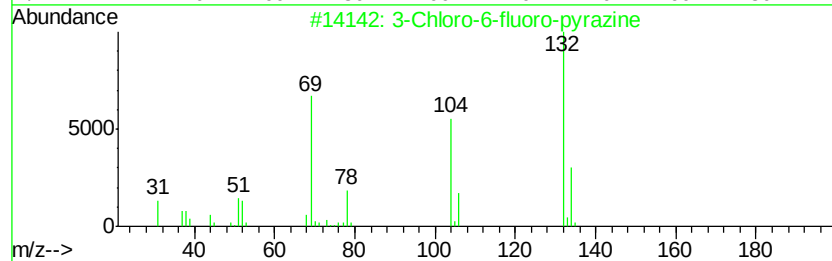
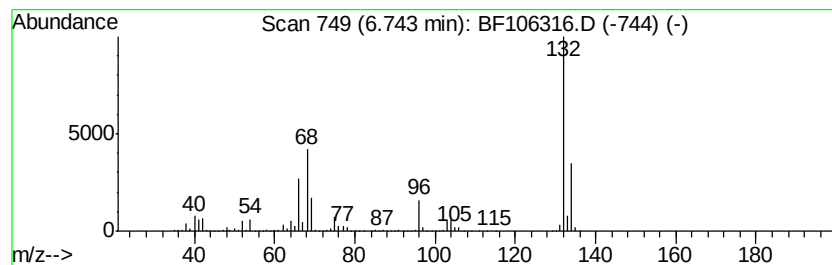
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	68.22 ng	4351930	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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

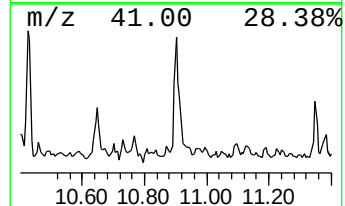
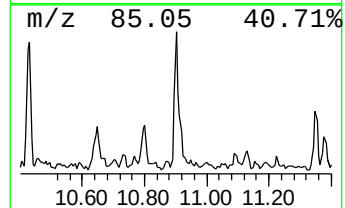
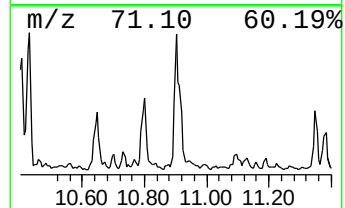
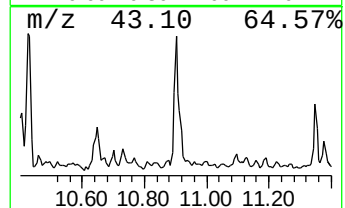
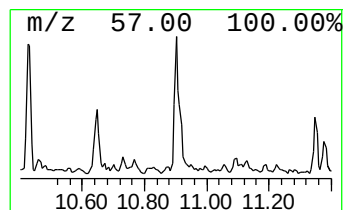
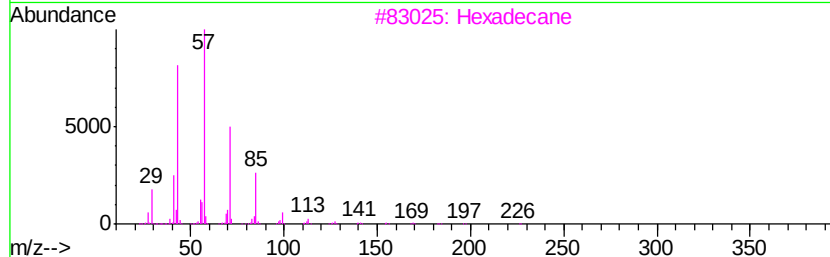
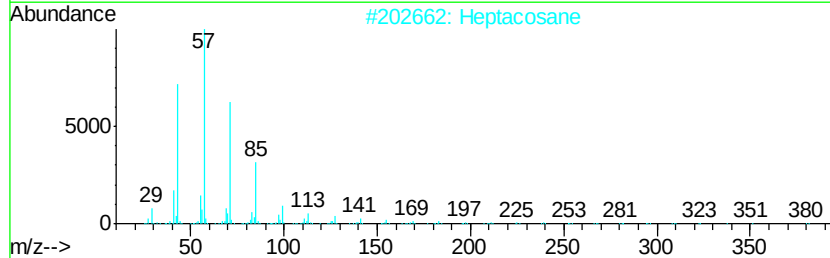
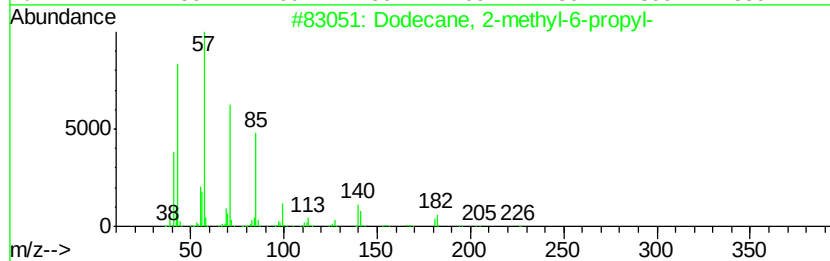
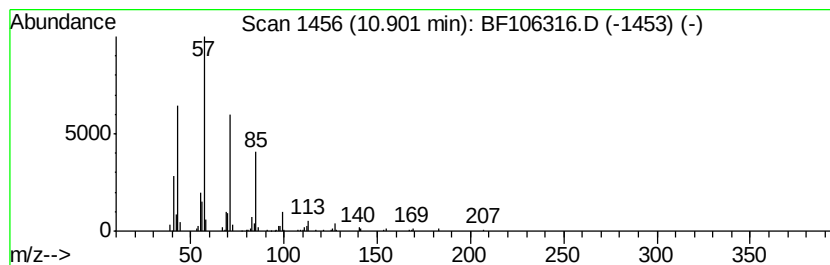
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecane, 2-methyl-6-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.73 ng	202044	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
2		Heptacosane	380	C27H56	000593-49-7	86
3		Hexadecane	226	C16H34	000544-76-3	80
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5		Eicosane	282	C20H42	000112-95-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

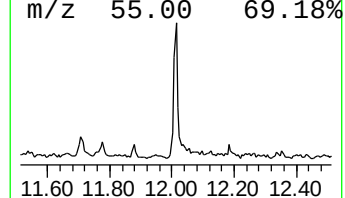
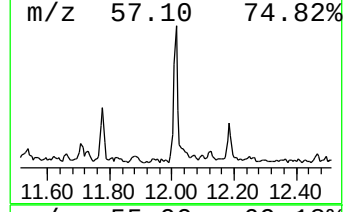
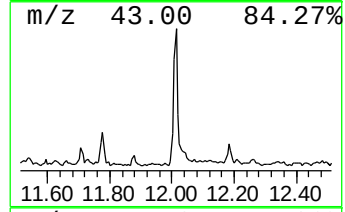
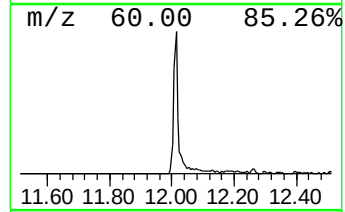
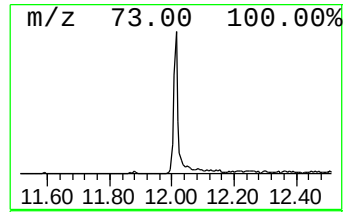
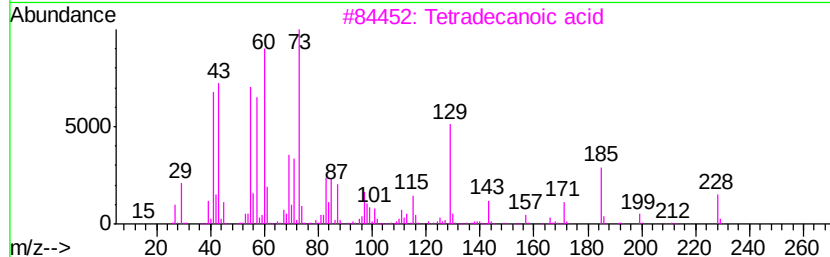
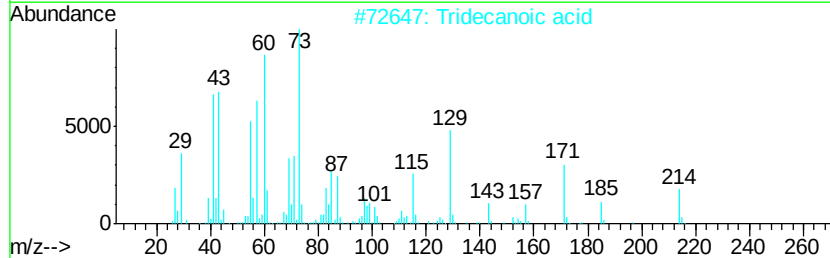
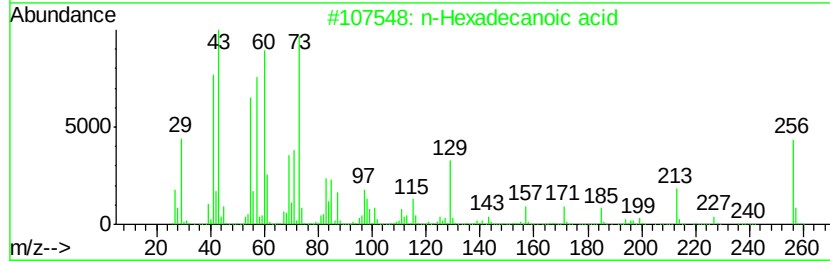
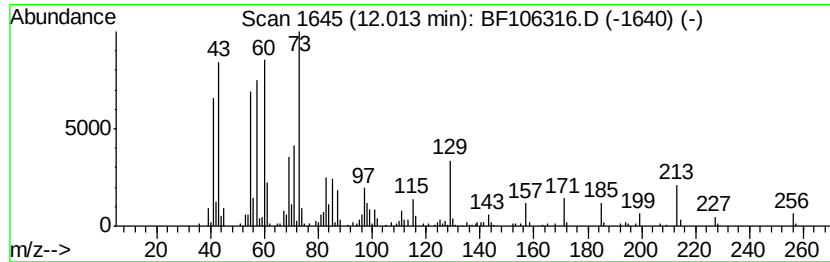
Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.01	5.44 ng	402777	Phenanthrene-d10	11.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

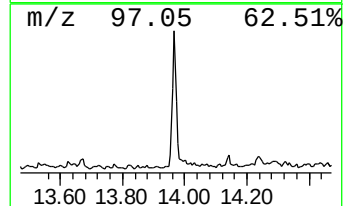
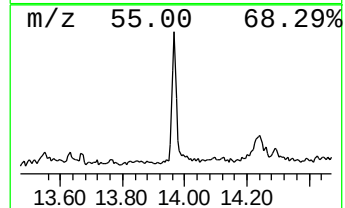
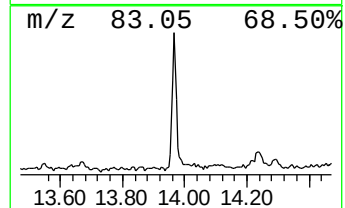
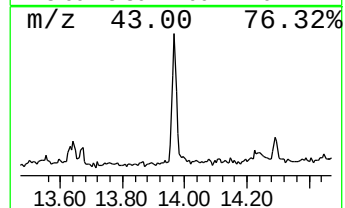
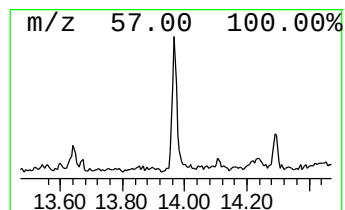
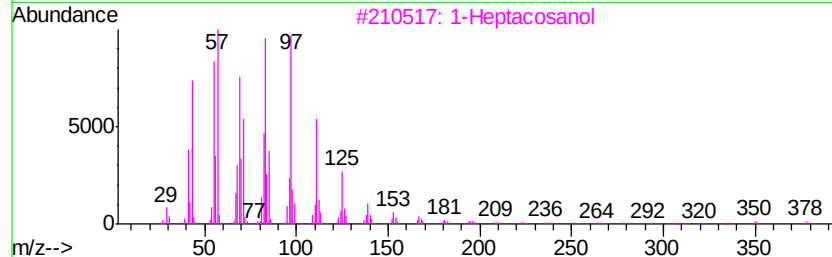
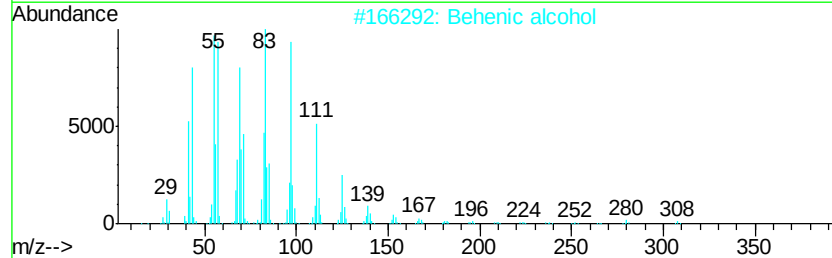
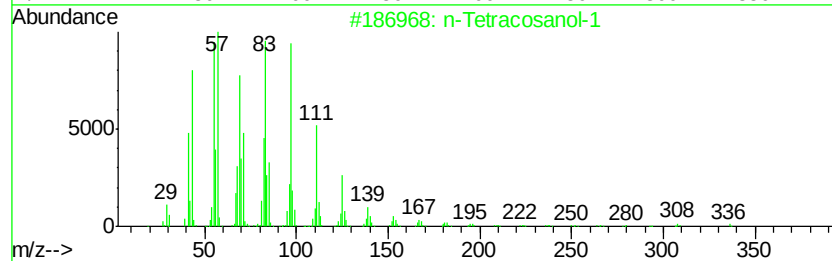
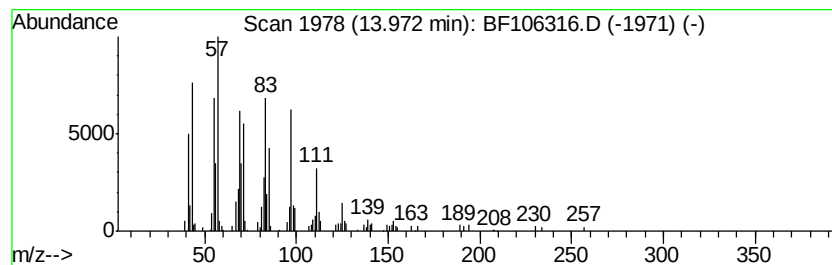
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.76 ng	266465	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

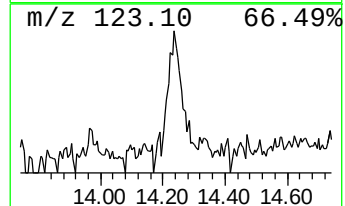
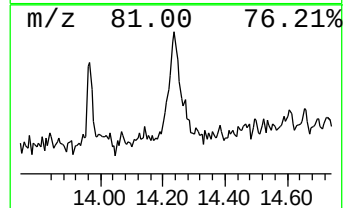
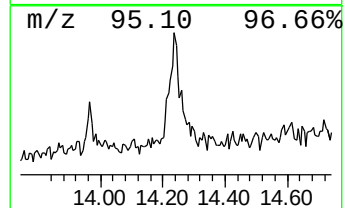
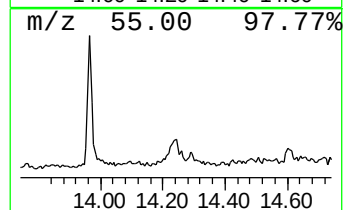
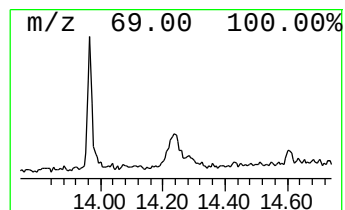
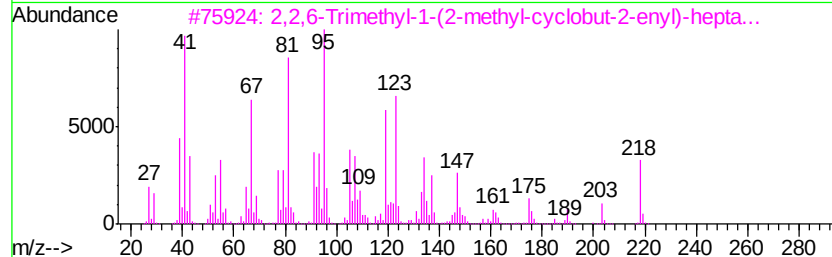
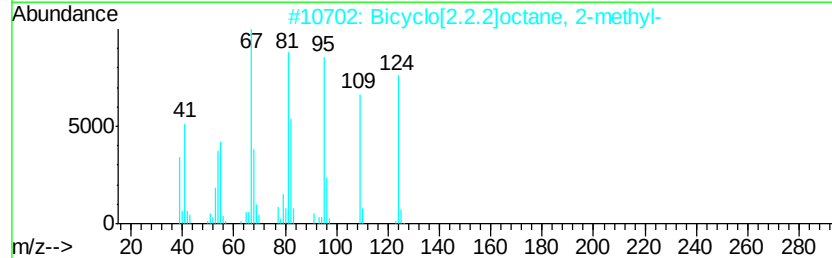
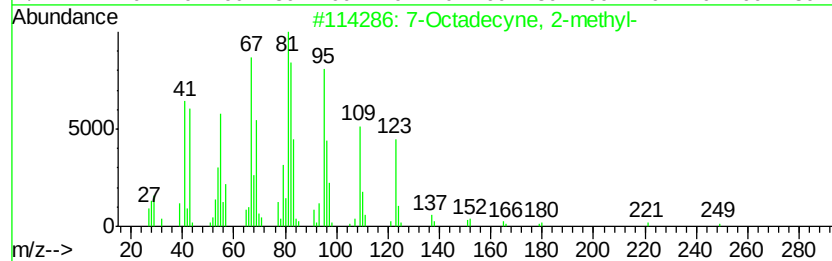
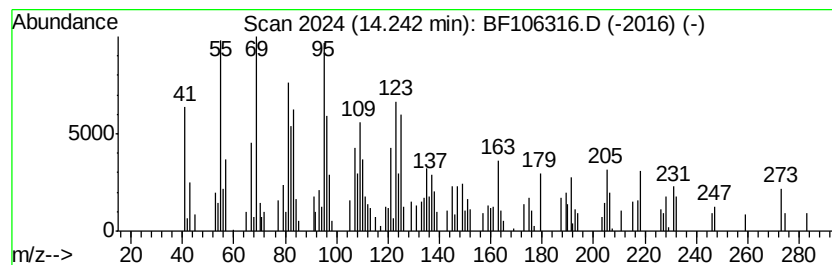
Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7-Octadecyne, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	3.00 ng	212481	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	7-Octadecyne, 2-methyl-	264 C19H36	035354-38-2	52
2	Bicyclo[2.2.2]octane, 2-methyl-	124 C9H16	000766-53-0	49
3	2,2,6-Trimethyl-1-(2-methyl-cycl...	218 C15H22O	1000188-72-8	46
4	6-Isopropenyl-4,8a-dimethyl-4a,5...	218 C15H22O	086917-79-5	45
5	Bicyclo[3.3.1]nonane	124 C9H16	000280-65-9	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061118\
Data File : BF106316.D
Acq On : 12 Jun 2018 00:55
Operator : JU/SJ
Sample : J3354-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS1-SB-02-03-1-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.21	6.6	ng	423258	1	6.97	1275880	20.0
unknown6.74	6.74	68.2	ng	4351930	1	6.97	1275880	20.0
Dodecane, 2-methy...	10.90	2.7	ng	202044	4	11.50	1479470	20.0
n-Hexadecanoic acid	12.01	5.4	ng	402777	4	11.50	1479470	20.0
n-Tetracosanol-1	13.97	3.8	ng	266465	5	14.14	1417070	20.0
7-Octadecyne, 2-m...	14.24	3.0	ng	212481	5	14.14	1417070	20.0