

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
 Data File : BF104485.D
 Acq On : 13 Apr 2018 18:14
 Operator : JU/SJ
 Sample : J2357-01 2X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR2520258

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	4.375	384	389	395	rBV	127552	141022	9.77%	0.868%
2	5.004	492	496	504	rBV	115265	122720	8.50%	0.755%
3	5.416	562	566	569	rBV	1371211	1166136	80.76%	7.175%
4	6.434	735	739	747	rBV	1447614	1356827	93.97%	8.348%
5	6.575	759	763	766	rBV	1661874	1354105	93.78%	8.331%
6	6.810	799	803	806	rBV	976861	780395	54.05%	4.801%
7	6.863	809	812	815	rVB	23151	17672	1.22%	0.109%
8	6.963	825	829	832	rBV	1392673	1121669	77.68%	6.901%
9	7.369	894	898	901	rBV	979803	842869	58.38%	5.186%
10	8.092	1017	1021	1024	rBV	1299028	1023456	70.88%	6.297%
11	9.169	1200	1204	1207	rBV	1676435	1443870	100.00%	8.884%
12	9.563	1267	1271	1279	rBV	195866	187515	12.99%	1.154%
13	9.775	1301	1307	1310	rBV	53478	40546	2.81%	0.249%
14	9.851	1316	1320	1329	rVB	1203242	1083752	75.06%	6.668%
15	10.275	1390	1392	1395	rVB	56496	40259	2.79%	0.248%
16	10.498	1425	1430	1432	rBV	13342	16575	1.15%	0.102%
17	10.633	1450	1453	1465	rVB	537514	516666	35.78%	3.179%
18	10.751	1470	1473	1479	rVB	41685	47637	3.30%	0.293%
19	11.198	1546	1549	1551	rBV	24796	18045	1.25%	0.111%
20	11.339	1569	1573	1575	rBV	1057858	915148	63.38%	5.631%
21	11.357	1575	1576	1579	rVB	87826	64938	4.50%	0.400%
22	11.557	1606	1610	1615	rBV2	23641	29161	2.02%	0.179%
23	11.951	1674	1677	1679	rBV2	22686	22068	1.53%	0.136%
24	12.386	1747	1751	1754	rBV3	14432	20923	1.45%	0.129%
25	12.551	1776	1779	1782	rBV	214155	168338	11.66%	1.036%
26	12.780	1813	1818	1821	rBV	172932	175634	12.16%	1.081%
27	12.922	1838	1842	1846	rVV	1182137	1038854	71.95%	6.392%
28	12.998	1850	1855	1858	rBV3	12883	19097	1.32%	0.117%
29	13.110	1871	1874	1876	rVB	24555	23266	1.61%	0.143%
30	13.216	1888	1892	1895	rBV3	24517	32628	2.26%	0.201%
31	13.616	1955	1960	1964	rBV	22849	28558	1.98%	0.176%
32	13.727	1975	1979	1982	rBV3	19037	25574	1.77%	0.157%
33	13.816	1991	1994	2004	rVB3	133078	164703	11.41%	1.013%
34	13.980	2014	2022	2025	rBV	832171	943182	65.32%	5.803%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

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	14.004	2025	2026	2032	rVB	110830	98324	6.81%	0.605%
36	14.368	2084	2088	2092	rVB2	27182	40953	2.84%	0.252%
37	14.404	2092	2094	2097	rBV3	17222	21138	1.46%	0.130%
38	14.457	2101	2103	2107	rVV4	17870	23780	1.65%	0.146%
39	14.839	2165	2168	2171	rBV2	49545	47069	3.26%	0.290%
40	15.021	2195	2199	2202	rBV	102873	152560	10.57%	0.939%
41	15.321	2248	2250	2257	rVB	56408	64294	4.45%	0.396%
42	15.380	2257	2260	2266	rBV	70448	99176	6.87%	0.610%
43	15.451	2267	2272	2285	rVB	508069	712219	49.33%	4.382%

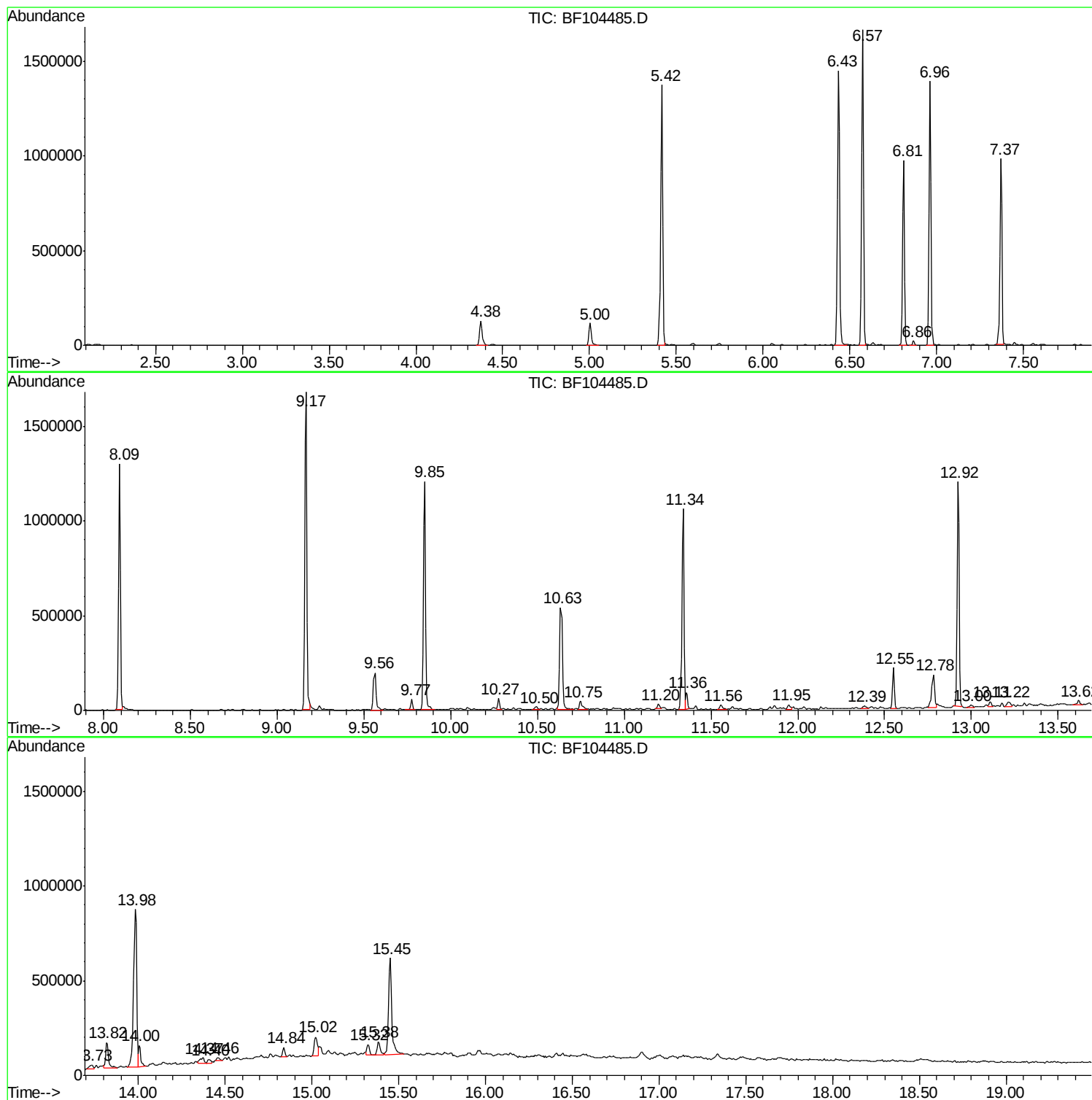
Sum of corrected areas: 16253321

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

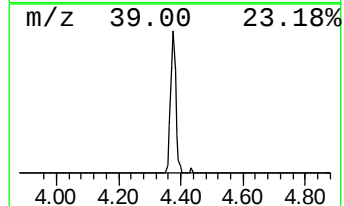
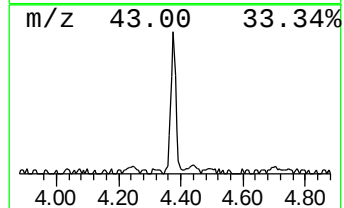
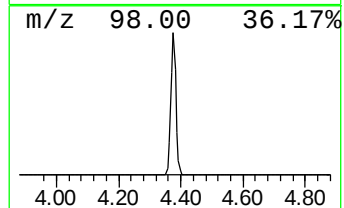
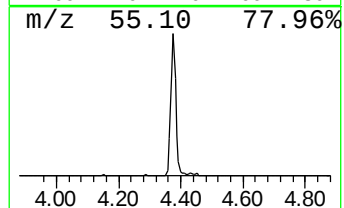
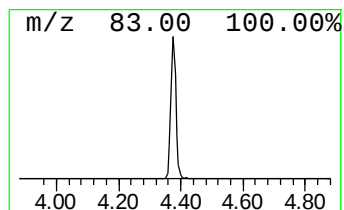
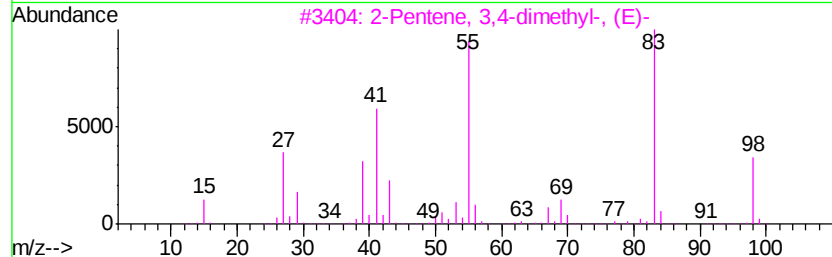
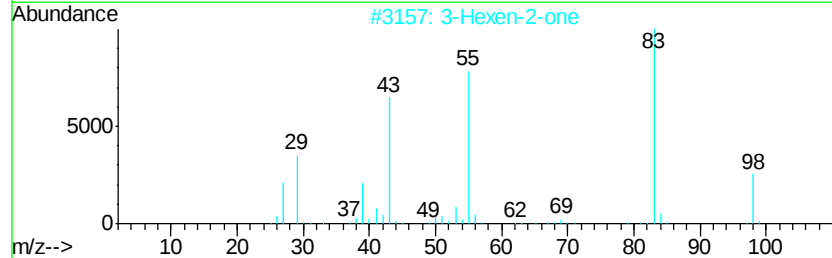
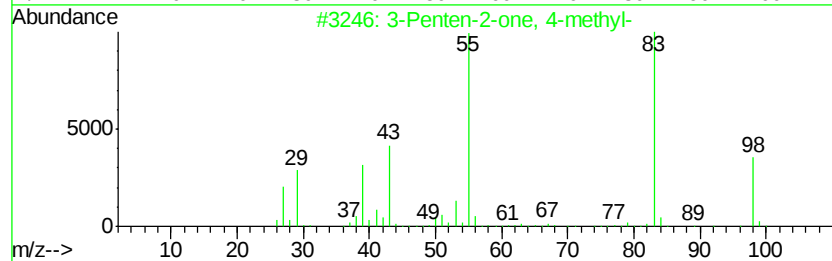
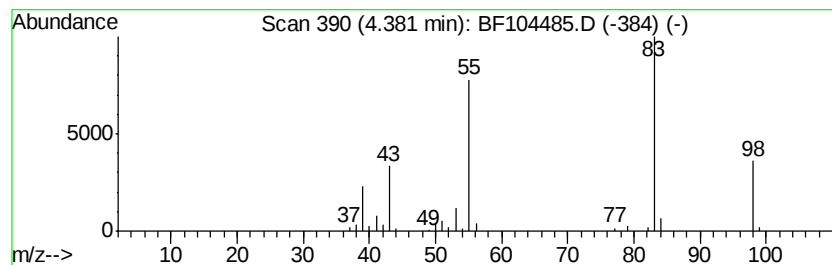
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	3.61 ng	141022	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

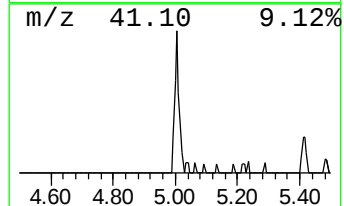
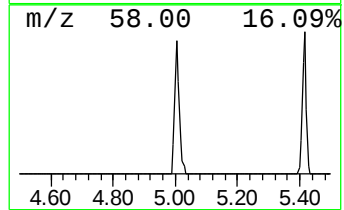
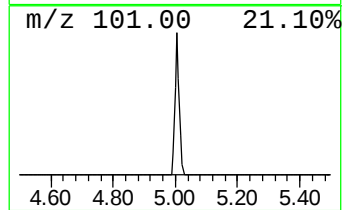
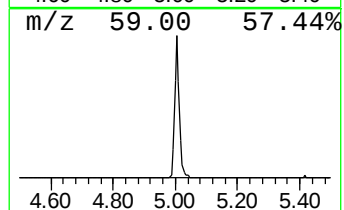
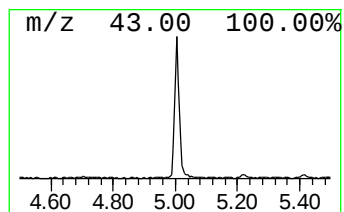
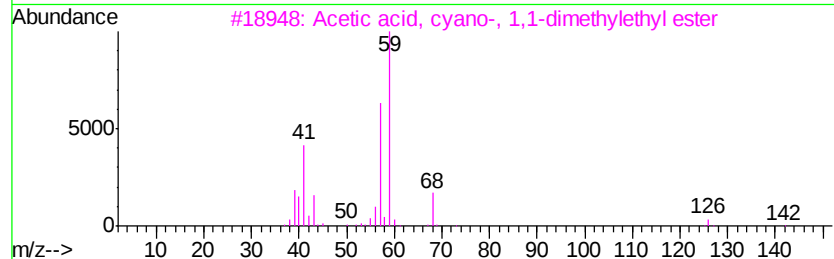
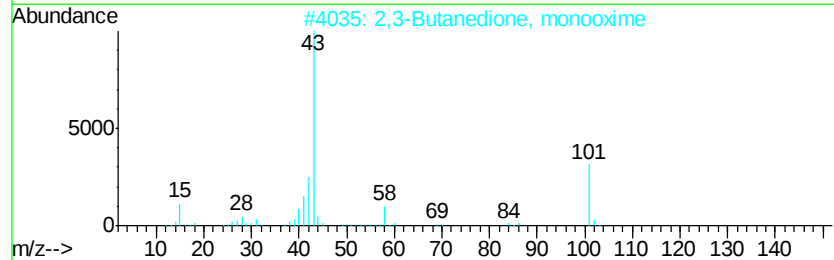
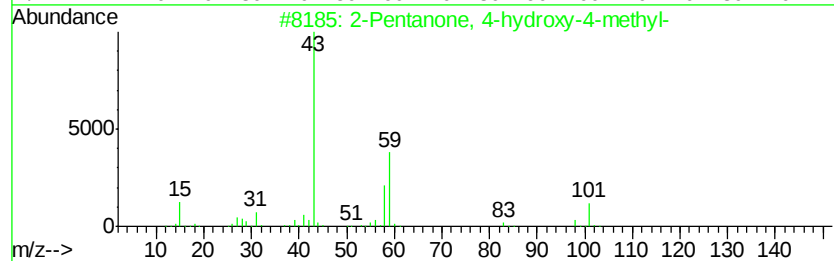
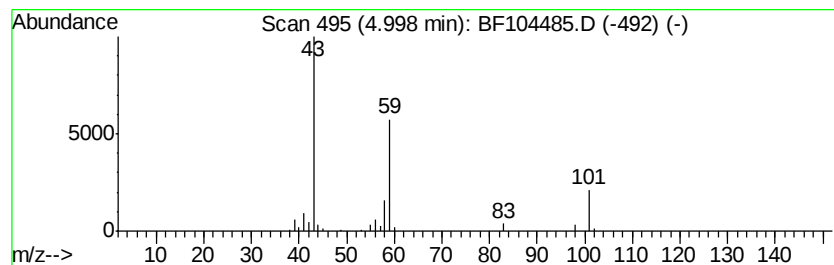
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.15 ng	122720	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

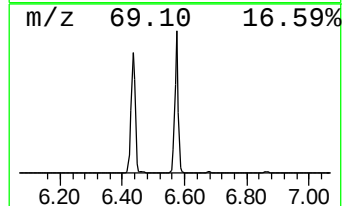
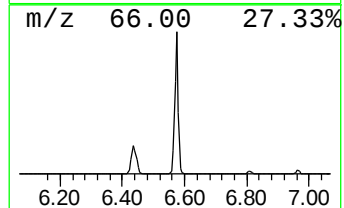
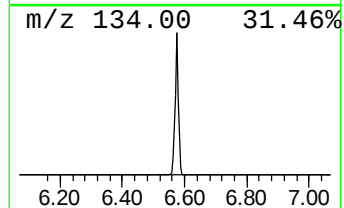
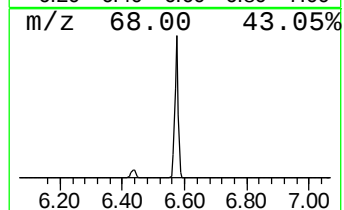
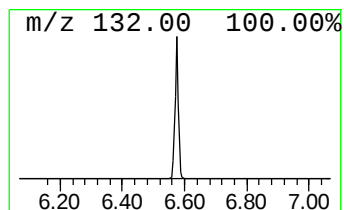
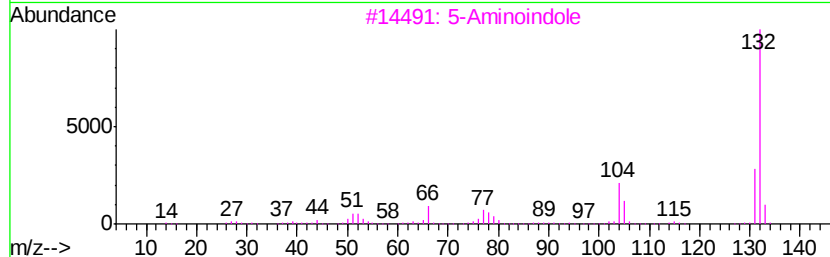
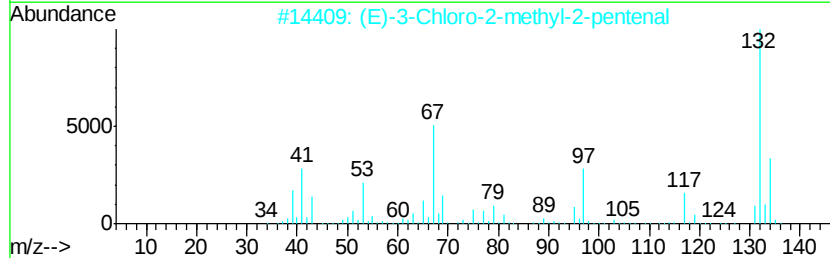
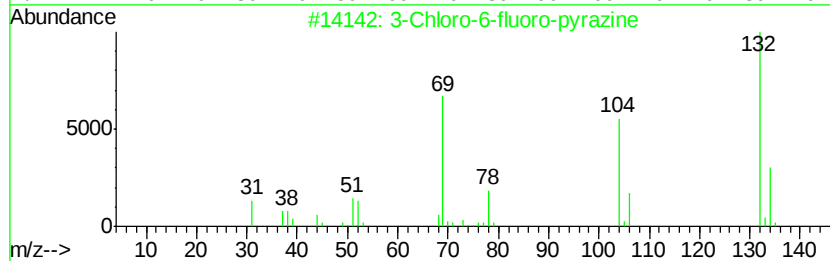
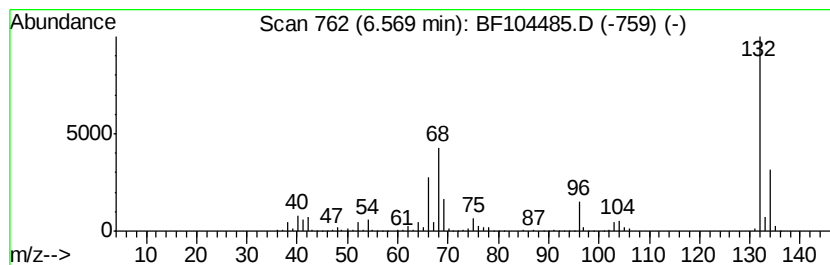
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	34.70 ng	1354110	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

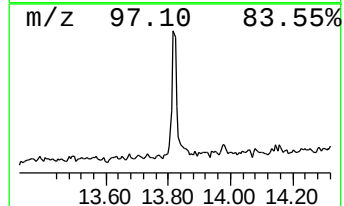
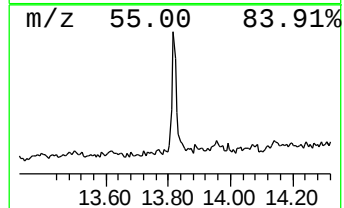
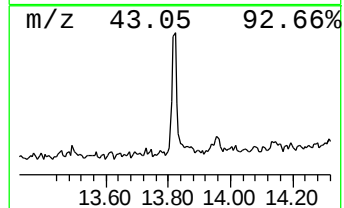
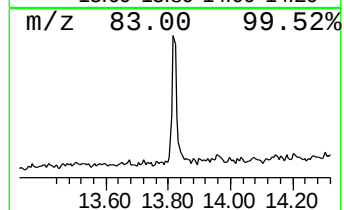
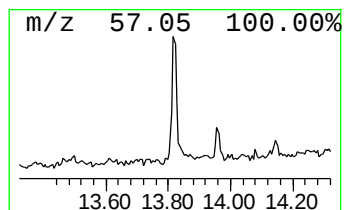
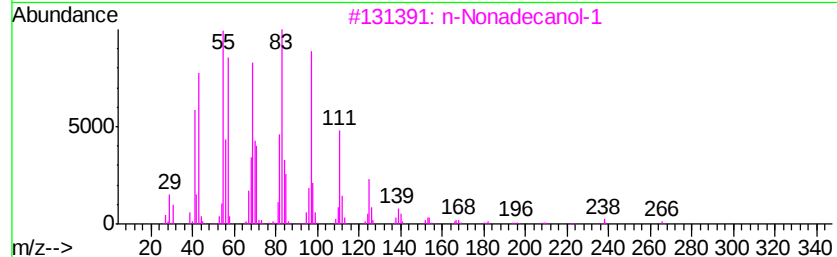
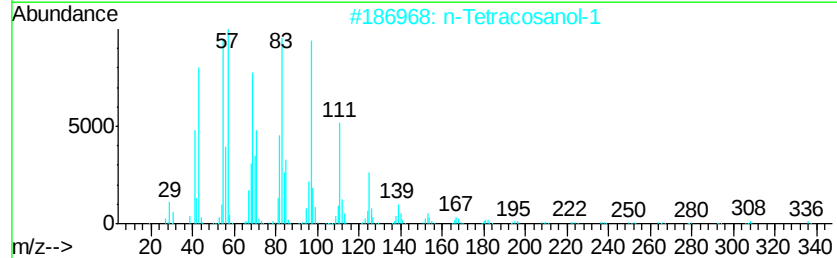
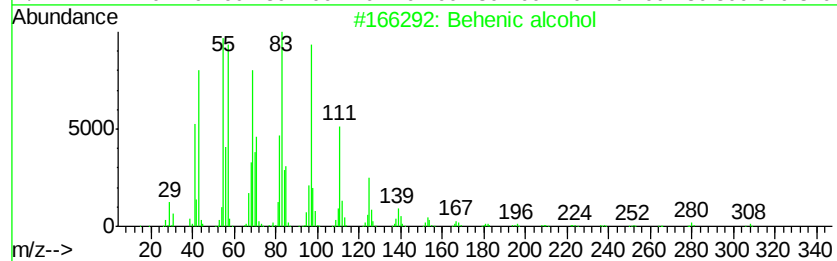
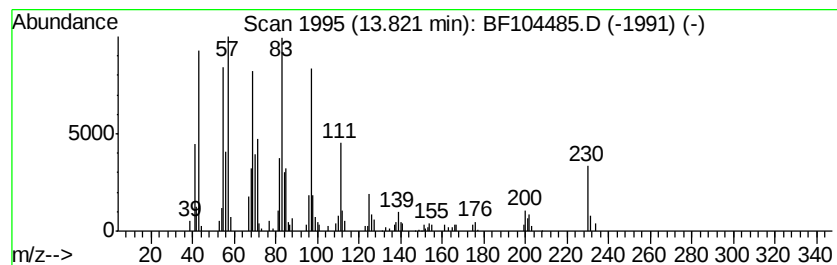
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.49 ng	164703	Chrysene-d12	13.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
Data File : BF104485.D
Acq On : 13 Apr 2018 18:14
Operator : JU/SJ
Sample : J2357-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

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
3-Penten-2-one, 4...	4.38	3.6	ng	141022	1	6.81	780395	20.0
2-Pentanone, 4-hy...	5.00	3.1	ng	122720	1	6.81	780395	20.0
unknown6.57	6.57	34.7	ng	1354110	1	6.81	780395	20.0
Behenic alcohol	13.82	3.5	ng	164703	5	13.98	943182	20.0