

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
 Data File : BF108331.D
 Acq On : 21 Aug 2018 11:43
 Operator : JU/SJ
 Sample : J4521-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT2286

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-BF080818.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	3.196	141	146	154	rVB	50106	80611	1.14%	0.165%
2	4.684	395	399	406	rBV	158750	174507	2.46%	0.357%
3	5.272	494	499	509	rVB	715305	988725	13.95%	2.025%
4	5.654	558	564	567	rBV	4445052	4630923	65.31%	9.485%
5	6.637	724	731	733	rBV	3974450	4477371	63.15%	9.171%
6	6.784	750	756	759	rBV	4770286	5144222	72.55%	10.537%
7	7.007	790	794	797	rBV	1168713	969855	13.68%	1.987%
8	7.166	816	821	824	rBV	4364451	4050229	57.12%	8.296%
9	7.572	884	890	893	rBV	3188686	3537606	49.89%	7.246%
10	8.289	1007	1012	1015	rBV	1220610	1196541	16.88%	2.451%
11	9.366	1188	1195	1198	rBV	6097485	6355312	89.64%	13.017%
12	10.048	1306	1311	1315	rBV2	1492824	1412410	19.92%	2.893%
13	10.848	1440	1447	1450	rBV	4212273	4317746	60.90%	8.844%
14	11.548	1560	1566	1569	rBV	1759154	1557483	21.97%	3.190%
15	12.930	1798	1801	1804	rBV	192944	146743	2.07%	0.301%
16	13.136	1829	1836	1840	rBV	6192510	7090157	100.00%	14.523%
17	13.636	1918	1921	1925	rBV	127830	105917	1.49%	0.217%
18	14.201	2012	2017	2020	rBV	1507831	1343928	18.95%	2.753%
19	15.324	2204	2208	2214	rVB	57161	74905	1.06%	0.153%
20	15.754	2274	2281	2288	rVB	669819	964905	13.61%	1.976%
21	16.212	2355	2359	2368	rVB	67569	107278	1.51%	0.220%
22	16.771	2448	2454	2459	rVB	48259	94038	1.33%	0.193%

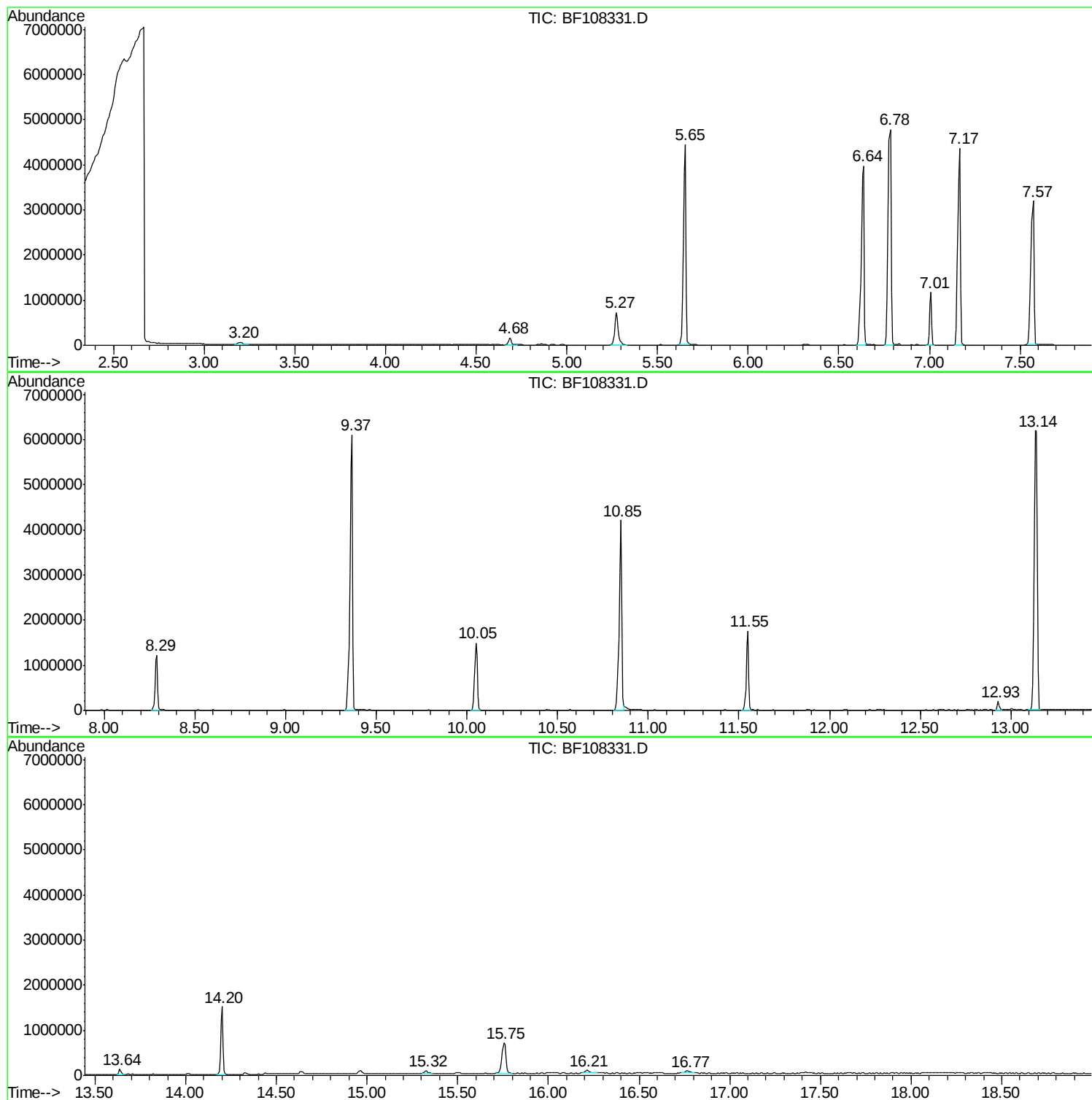
Sum of corrected areas: 48821412

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.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\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

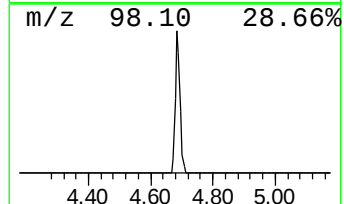
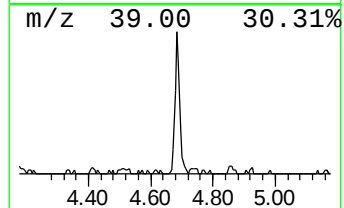
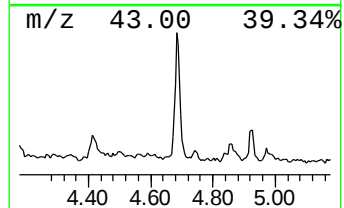
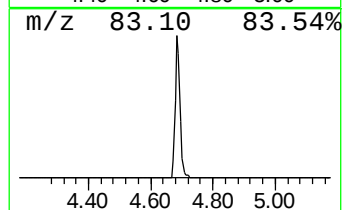
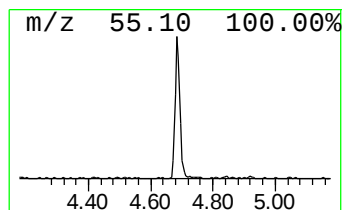
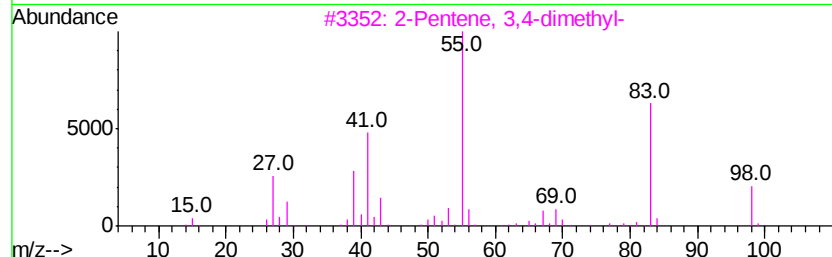
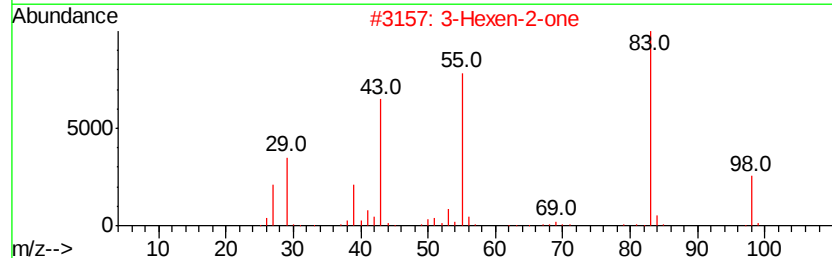
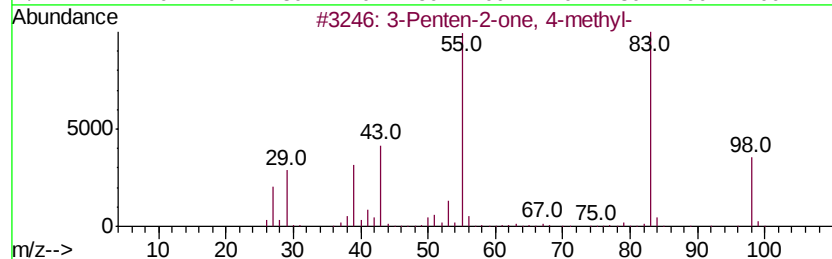
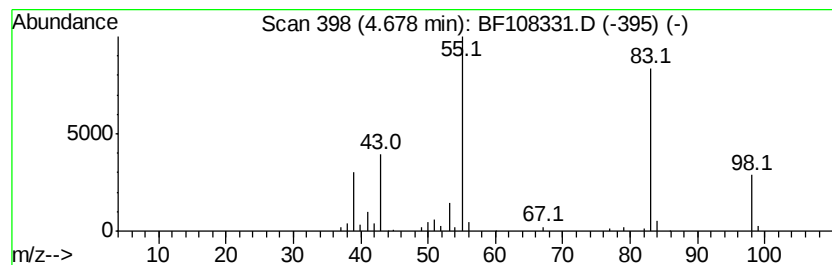
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	3.60 ng	174507	1,4-Dichlorobenzene-d4	7.01

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	90
3			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

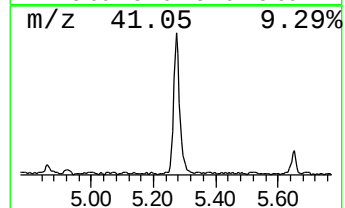
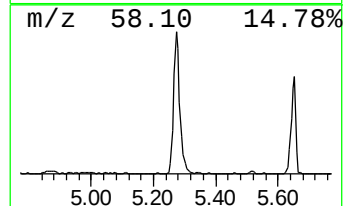
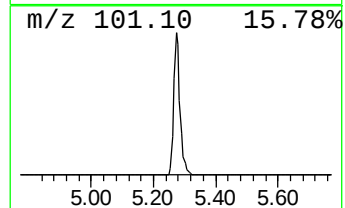
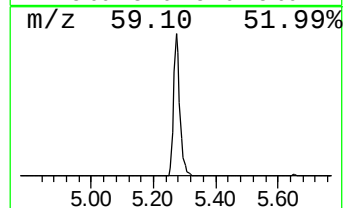
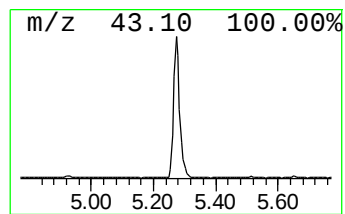
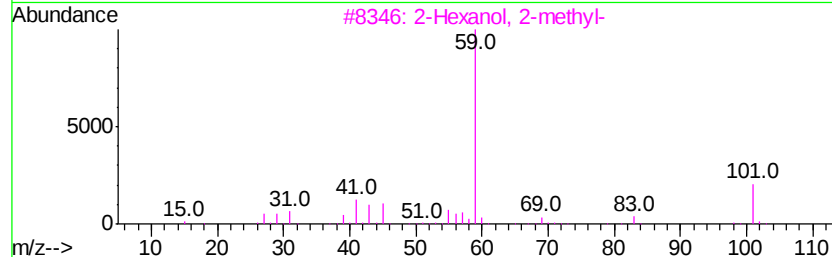
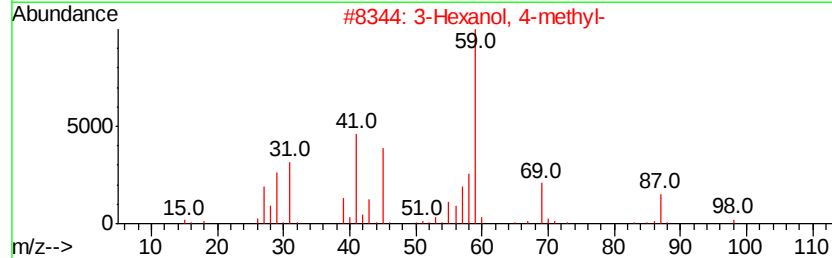
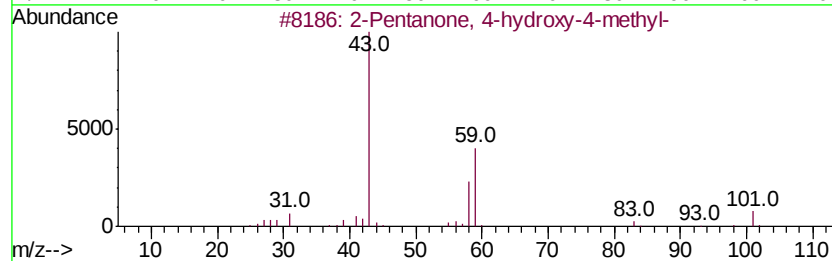
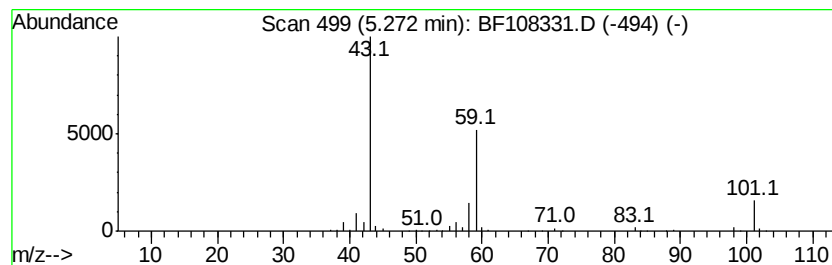
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	20.39 ng	988725	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

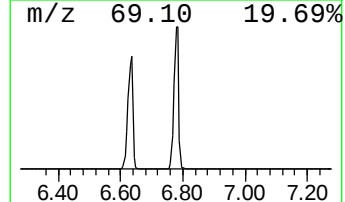
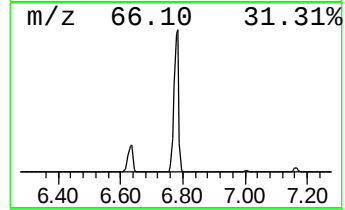
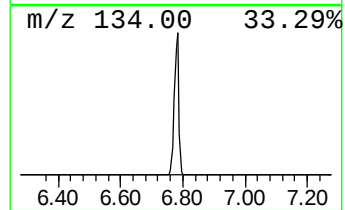
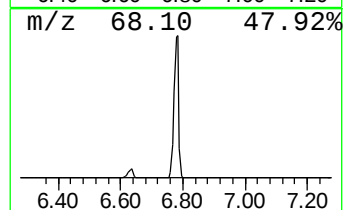
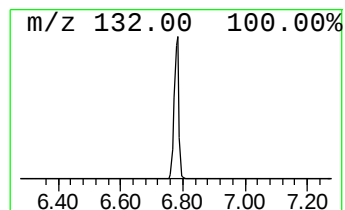
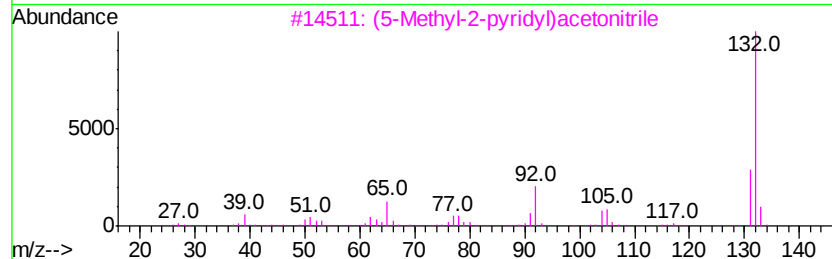
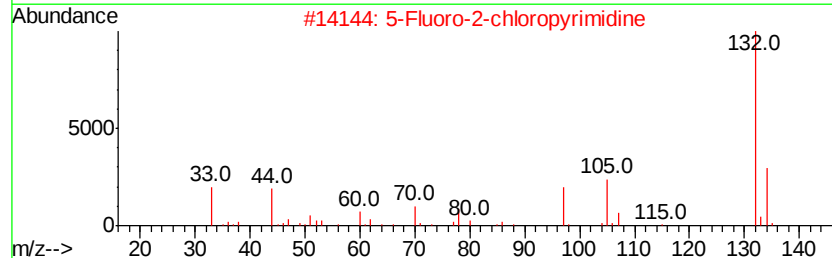
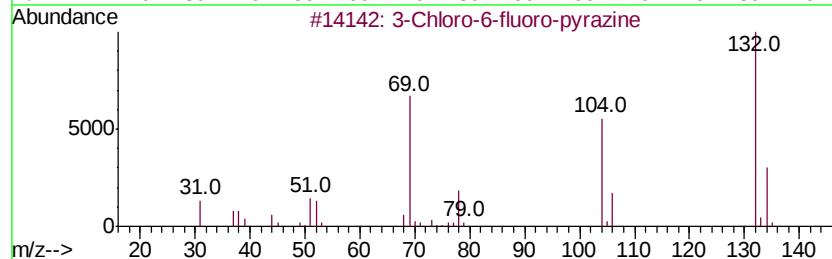
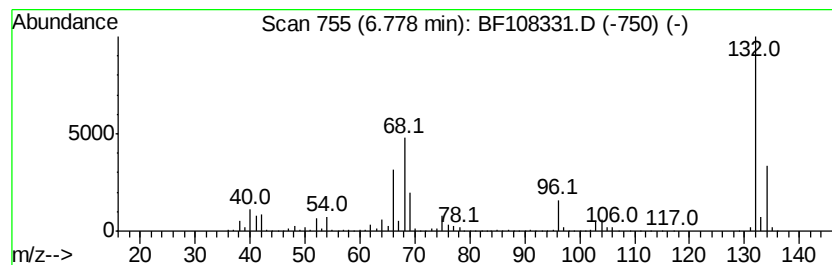
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	106.08 ng	5144220	1,4-Dichlorobenzene-d4	7.01

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		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

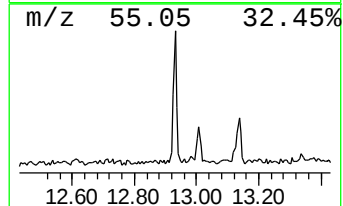
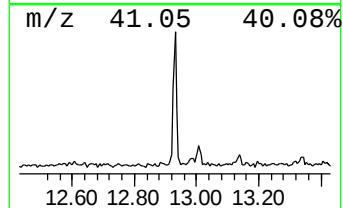
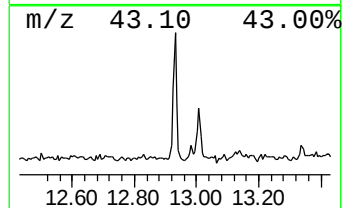
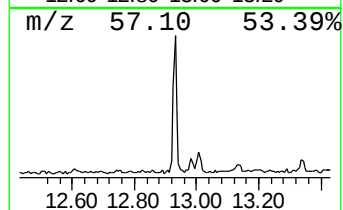
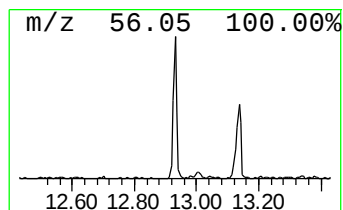
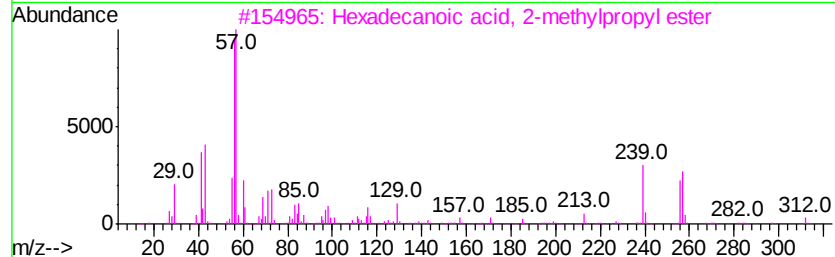
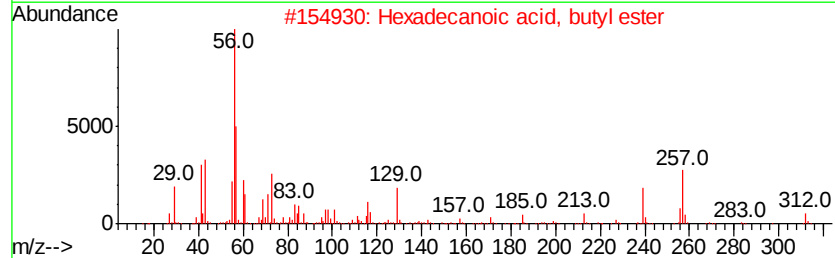
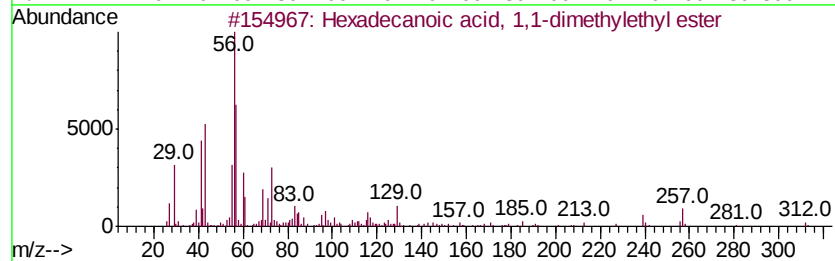
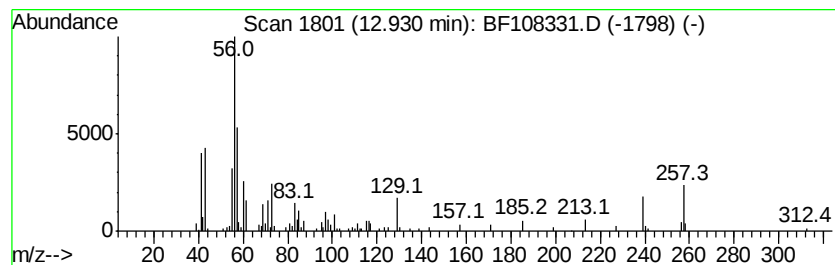
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	2.18 ng	146743	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

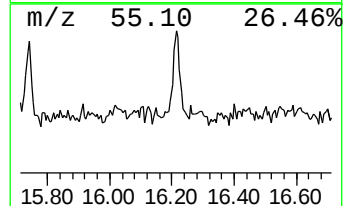
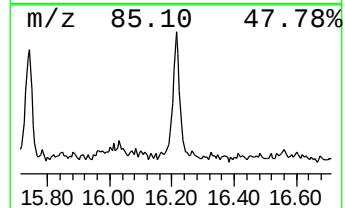
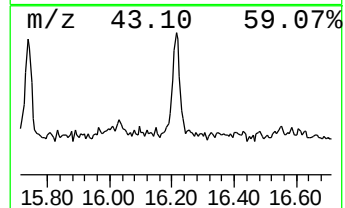
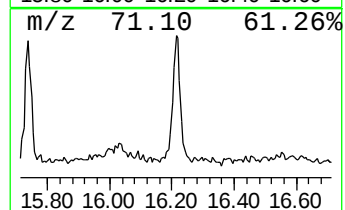
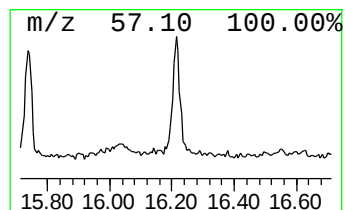
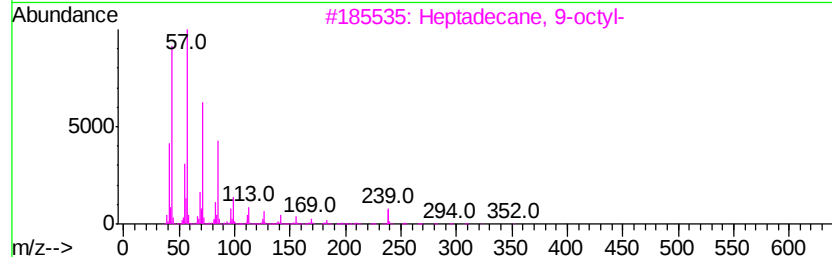
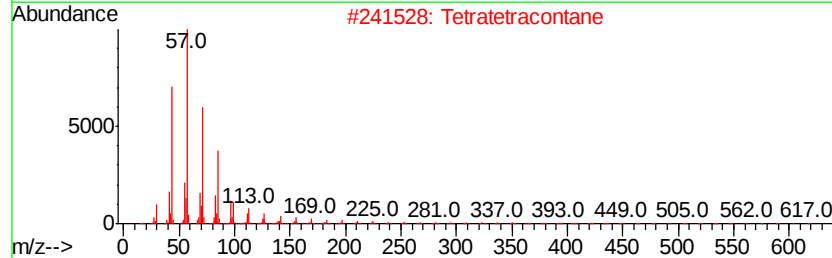
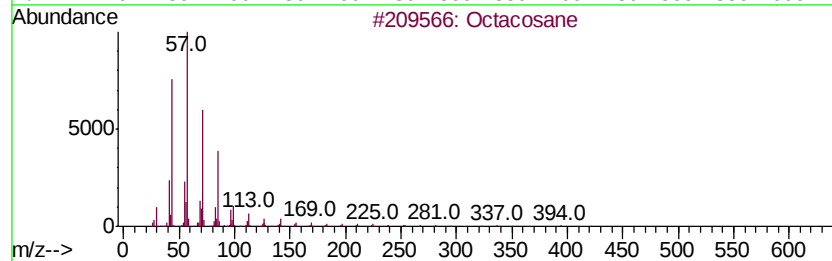
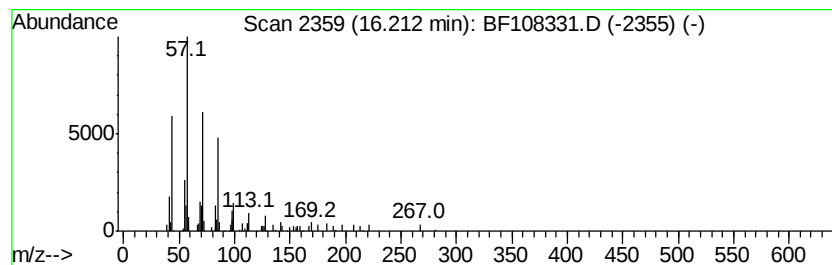
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.22 ng	107278	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Tetratetracontane		619	C44H90	007098-22-8	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Heptadecane		240	C17H36	000629-78-7	90
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
Data File : BF108331.D
Acq On : 21 Aug 2018 11:43
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	4.68	3.6	ng	174507	1	7.01	969855	20.0
2-Pentanone, 4-hy...	5.27	20.4	ng	988725	1	7.01	969855	20.0
unknown6.78	6.78	106.1	ng	5144220	1	7.01	969855	20.0
Hexadecanoic acid...	12.93	2.2	ng	146743	5	14.20	1343930	20.0
Octacosane	16.21	2.2	ng	107278	6	15.75	964905	20.0