

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
 Data File : BF106993.D
 Acq On : 30 Jun 2018 00:40
 Operator : JU/SJ
 Sample : J3693-05
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-41

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-BF061918.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	2.401	8	11	20	rVB2	9951	22683	1.07%	0.140%
2	5.184	481	484	493	rBV	60908	70176	3.31%	0.434%
3	5.589	550	553	566	rBV	876606	892341	42.14%	5.514%
4	6.589	720	723	734	rVB	523939	563695	26.62%	3.483%
5	6.731	742	747	750	rBV	1705441	1572148	74.25%	9.715%
6	6.948	781	784	790	rBB	507526	470783	22.23%	2.909%
7	7.107	807	811	815	rBV	1534055	1425023	67.30%	8.806%
8	7.519	876	881	884	rBV	1244383	1257149	59.37%	7.769%
9	7.672	903	907	910	rVB	38659	33911	1.60%	0.210%
10	8.236	999	1003	1013	rBV	589102	565674	26.72%	3.496%
11	8.719	1081	1085	1088	rVB	27521	26338	1.24%	0.163%
12	8.825	1100	1103	1106	rVB	27871	22407	1.06%	0.138%
13	9.307	1181	1185	1189	rBV	2132967	2117392	100.00%	13.085%
14	9.701	1246	1252	1262	rBV	195912	208208	9.83%	1.287%
15	9.901	1283	1286	1289	rBV	48329	42425	2.00%	0.262%
16	9.995	1298	1302	1308	rVB	640672	599812	28.33%	3.707%
17	10.154	1326	1329	1332	rBV2	24342	22461	1.06%	0.139%
18	10.377	1364	1367	1369	rBV	23464	23598	1.11%	0.146%
19	10.401	1369	1371	1374	rVB	78876	54688	2.58%	0.338%
20	10.507	1384	1389	1392	rBV	19585	23208	1.10%	0.143%
21	10.619	1404	1408	1410	rBV2	22236	27615	1.30%	0.171%
22	10.654	1410	1414	1417	rBV	429920	402781	19.02%	2.489%
23	10.789	1433	1437	1440	rBV	1437450	1346877	63.61%	8.323%
24	10.848	1443	1447	1450	rVV	240581	229229	10.83%	1.417%
25	10.871	1450	1451	1456	rVB	68292	57155	2.70%	0.353%
26	11.324	1525	1528	1530	rBV	36452	33301	1.57%	0.206%
27	11.483	1552	1555	1559	rBV	626142	566512	26.76%	3.501%
28	11.748	1597	1600	1607	rVB2	24788	33106	1.56%	0.205%
29	12.495	1724	1727	1731	rBV	28757	27019	1.28%	0.167%
30	12.701	1760	1762	1766	rVB	28752	27756	1.31%	0.172%
31	12.871	1788	1791	1795	rVB	71377	65254	3.08%	0.403%
32	12.936	1800	1802	1804	rVV	25675	30375	1.43%	0.188%
33	12.960	1804	1806	1809	rVB	32190	27847	1.32%	0.172%
34	13.071	1820	1825	1828	rBV	2124852	2019200	95.36%	12.478%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.571	1908	1910	1914	rBV	47452	46205	2.18%	0.286%
36	13.948	1971	1974	1979	rVB	114571	103747	4.90%	0.641%
37	14.142	2002	2007	2015	rBV	610415	623376	29.44%	3.852%
38	15.248	2193	2195	2199	rVB2	18029	21356	1.01%	0.132%
39	15.677	2264	2268	2278	rVB	353729	479219	22.63%	2.961%

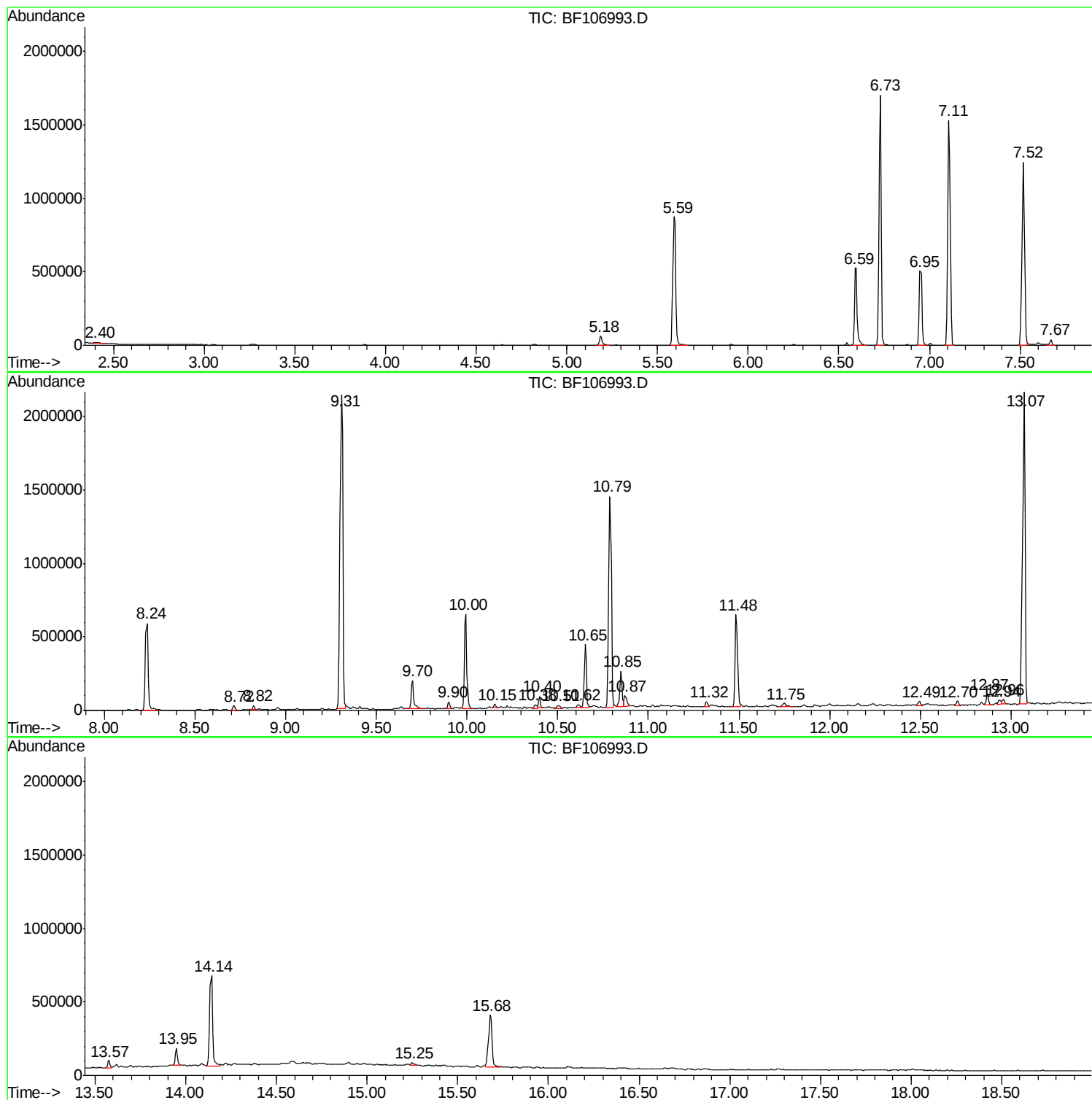
Sum of corrected areas: 16182050

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
W-41

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.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\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

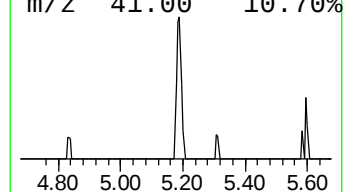
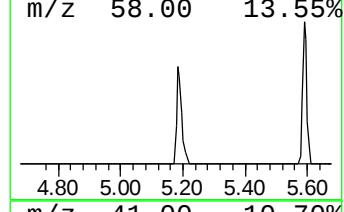
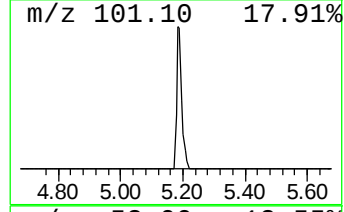
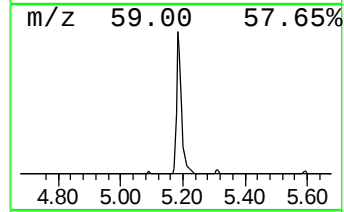
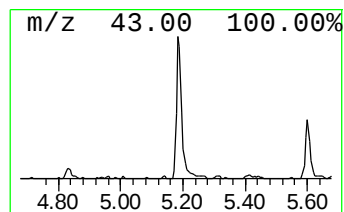
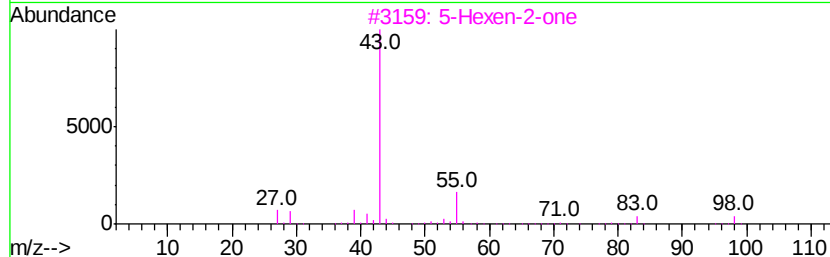
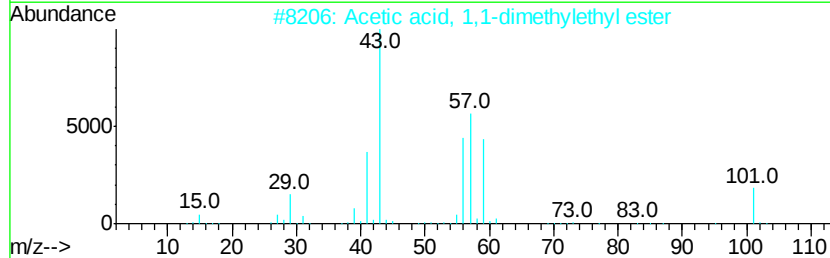
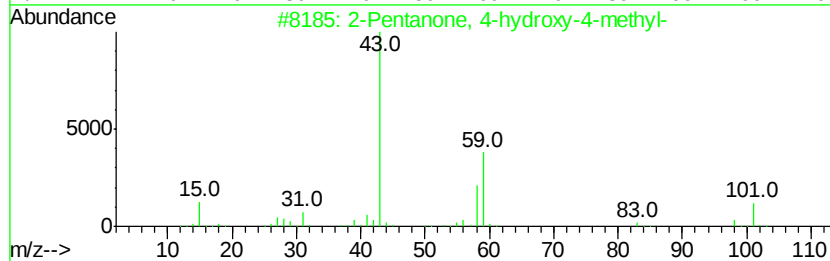
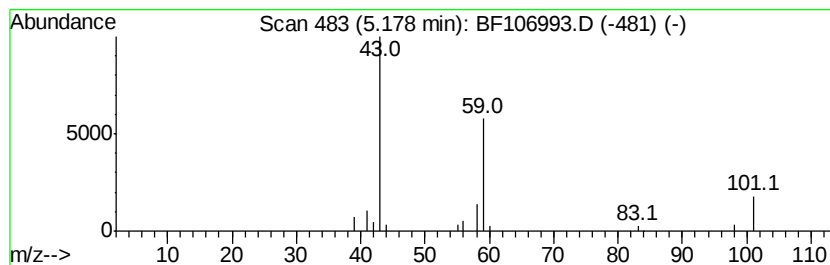
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.98 ng	70176	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
5			2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

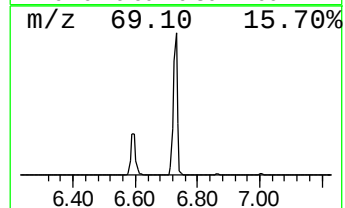
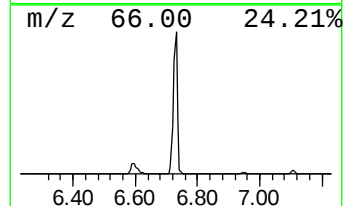
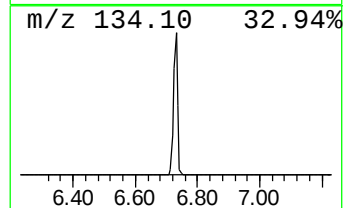
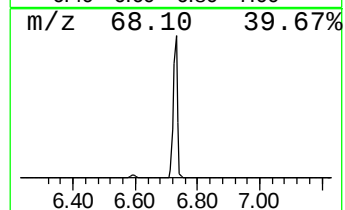
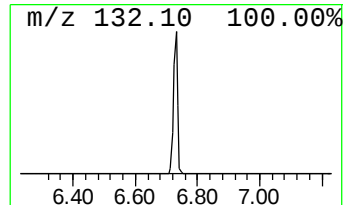
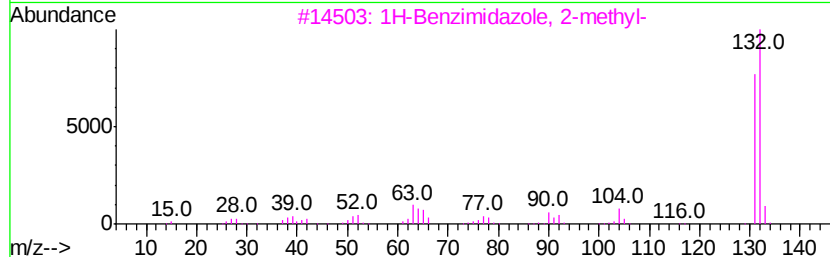
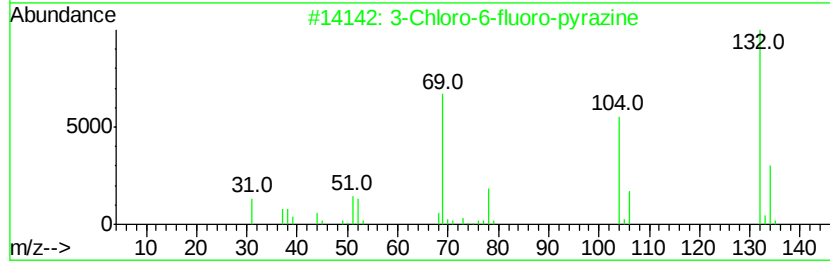
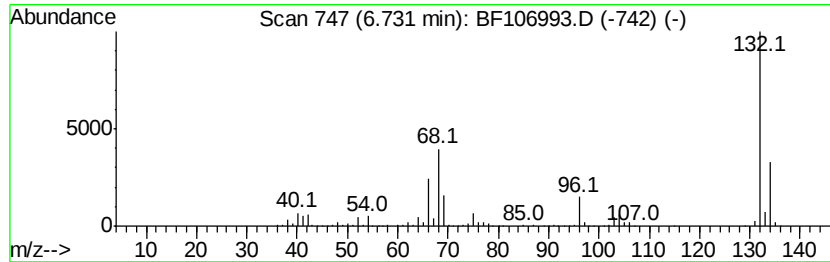
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	66.79 ng	1572150	1,4-Dichlorobenzene-d4	6.95

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

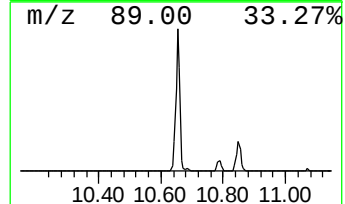
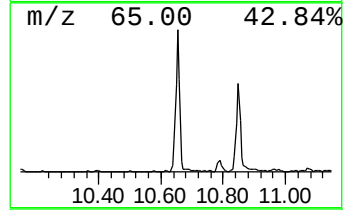
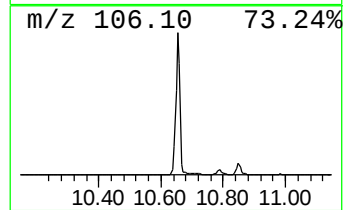
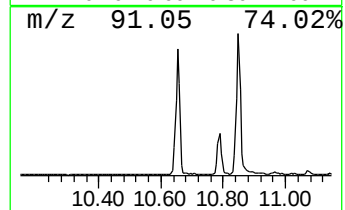
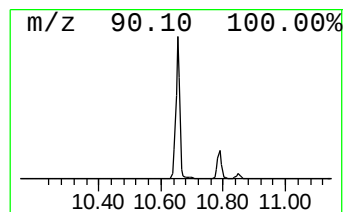
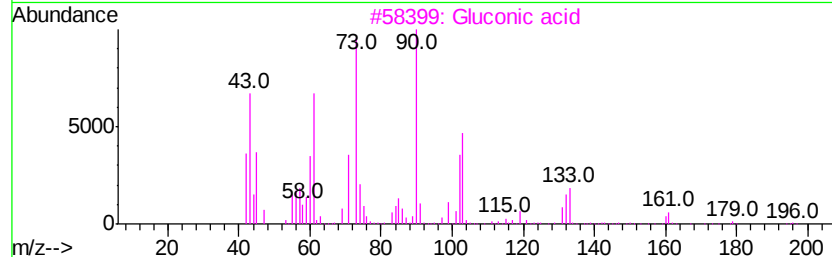
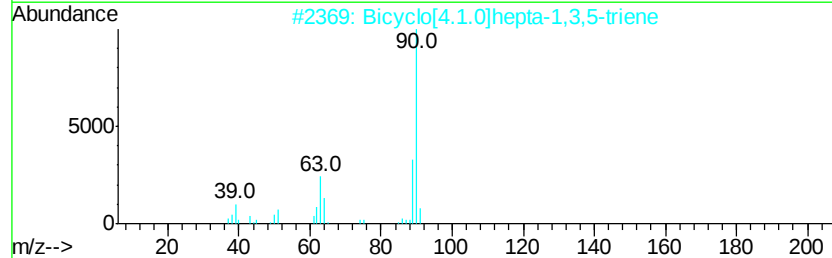
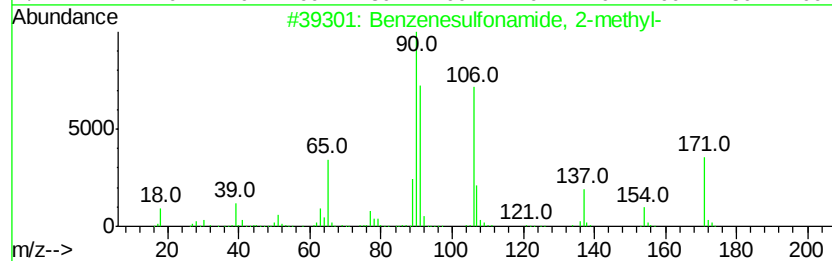
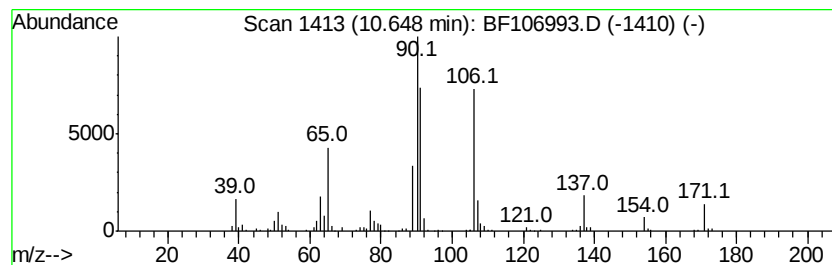
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	13.43 ng	402781	Acenaphthene-d10	10.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	96
2		Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	43
3		Gluconic acid	196	C6H12O7	000526-95-4	43
4		4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	38
5		Thiourea, methyl-	90	C2H6N2S	000598-52-7	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

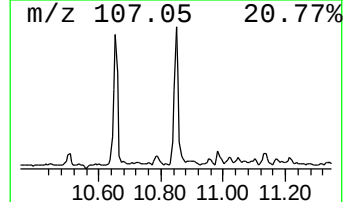
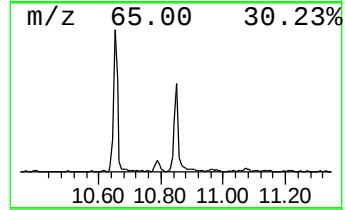
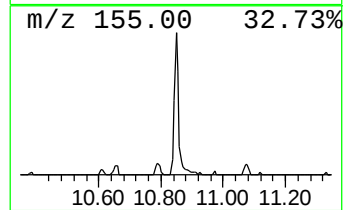
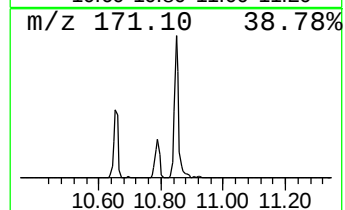
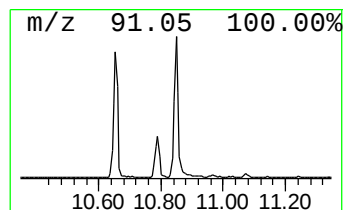
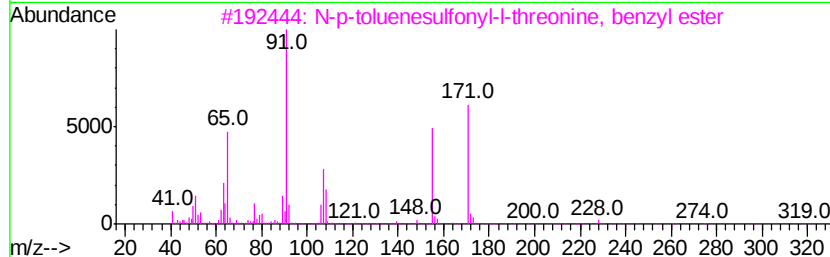
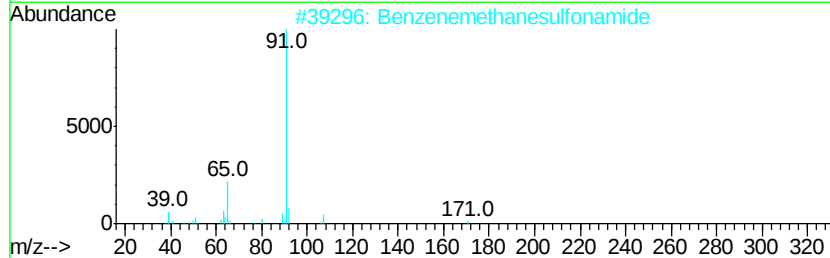
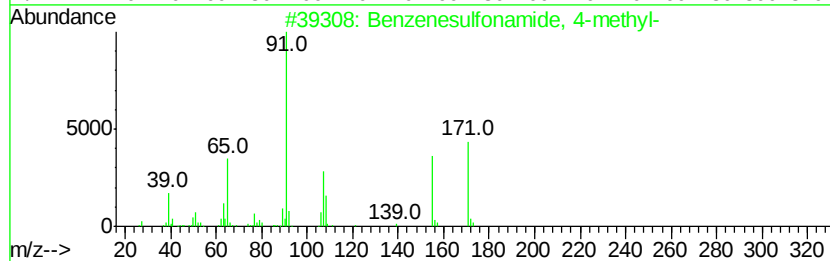
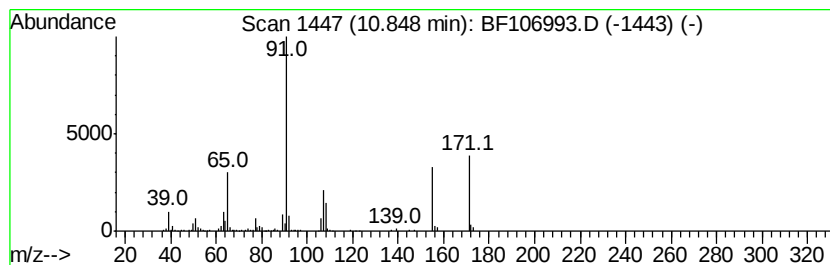
Instrument :
BNA_F
ClientSampleId :
W-41

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.85	8.09 ng	229229	Phenanthrene-d10	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2	Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	50
3	N-p-toluenesulfonyl-L-threonine, ...	363	C18H21NO5S	1000130-34-4	47
4	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	35
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

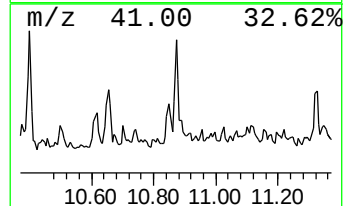
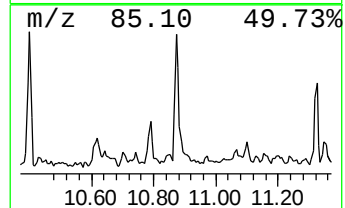
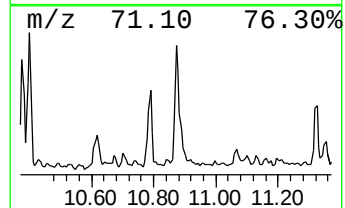
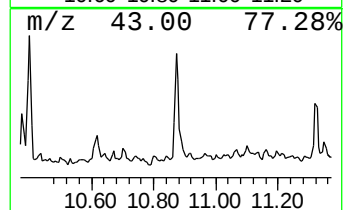
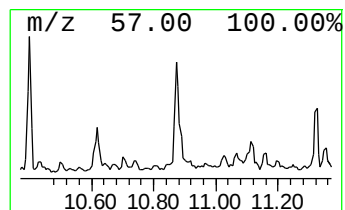
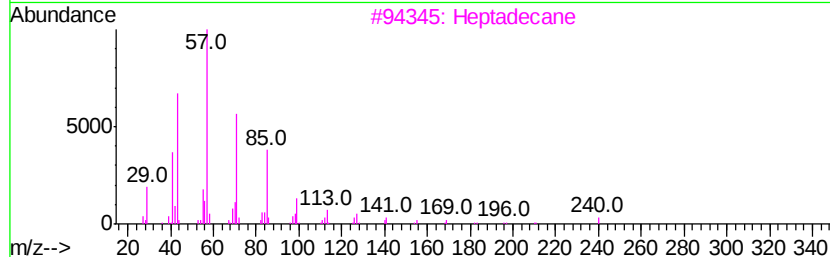
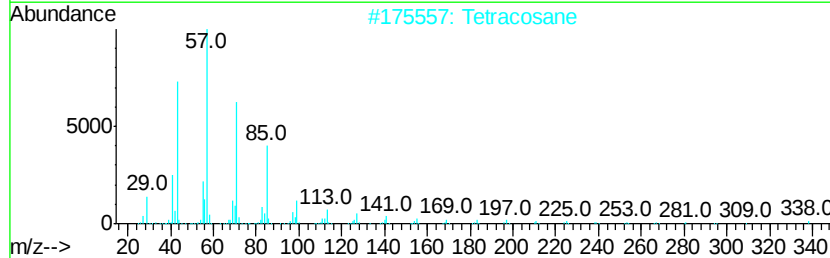
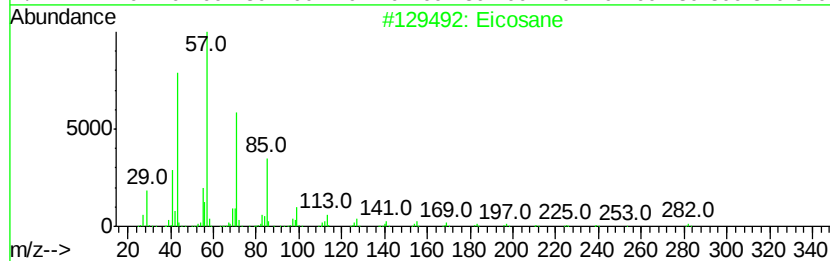
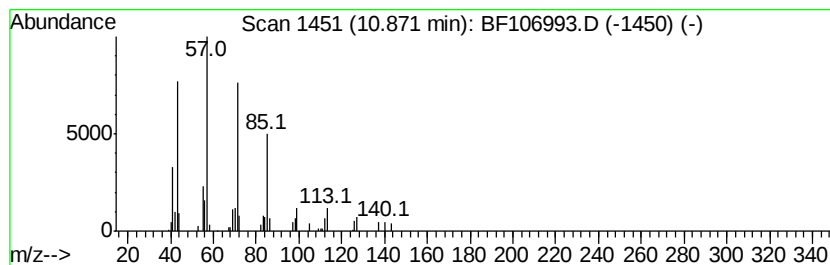
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.02 ng	57155	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	86
2	Tetracosane		338	C24H50	000646-31-1	86
3	Heptadecane		240	C17H36	000629-78-7	86
4	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	86
5	Octacosane		394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

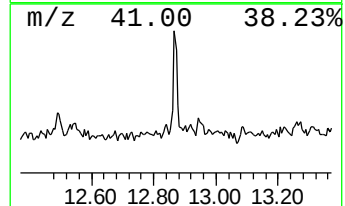
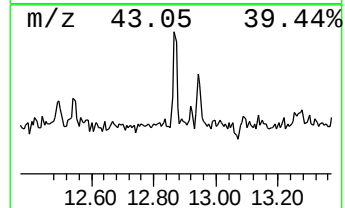
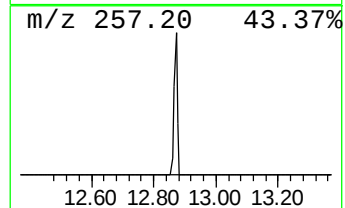
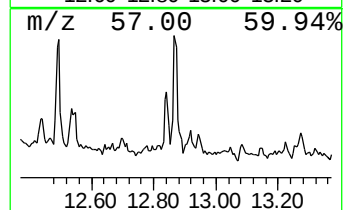
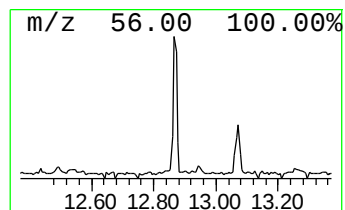
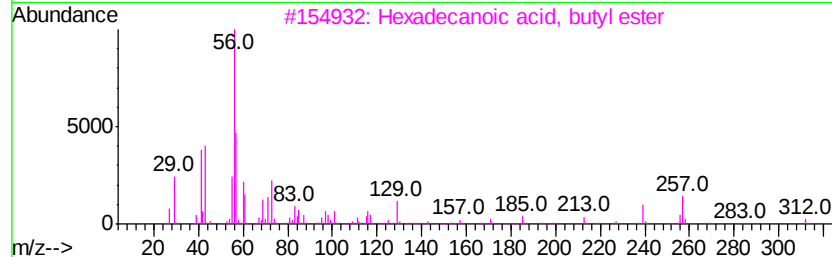
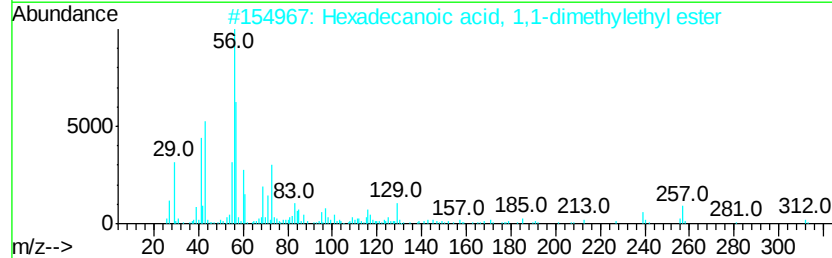
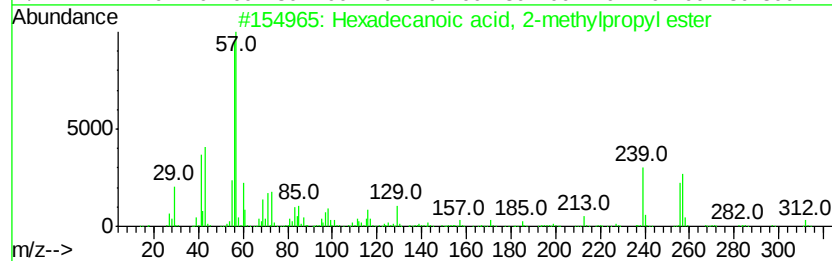
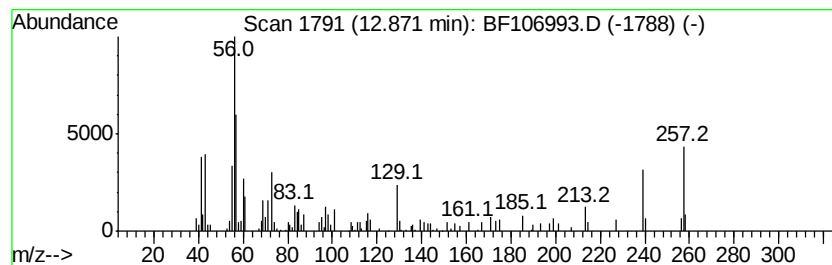
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 2-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.09 ng	65254	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	68
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
4		n-Butyl laurate	256	C16H32O2	000106-18-3	47
5		Isobutyl laurate	256	C16H32O2	037811-72-6	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

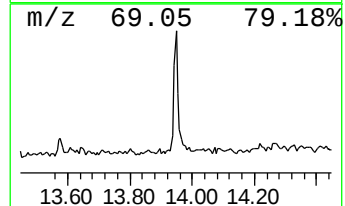
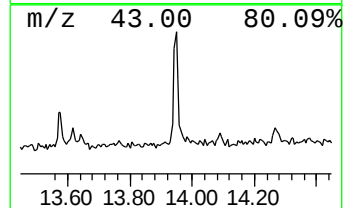
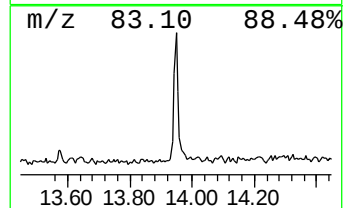
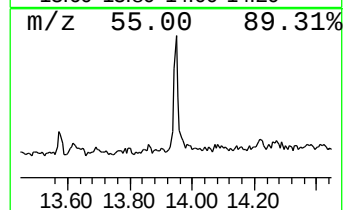
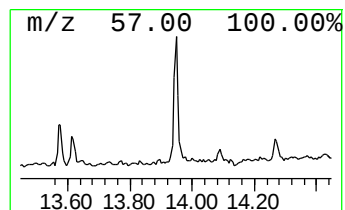
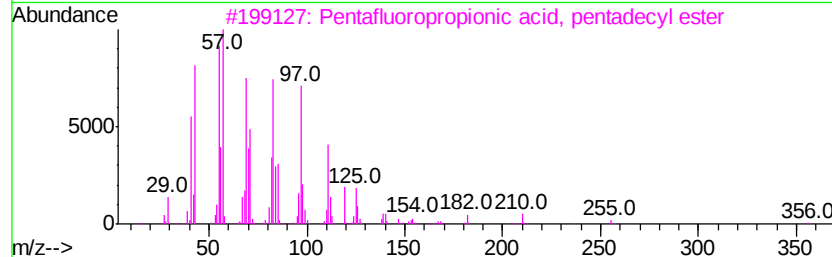
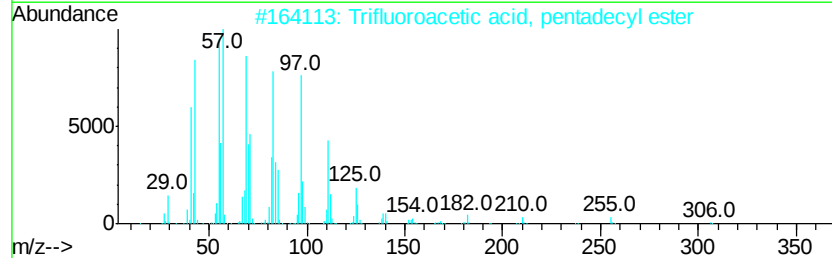
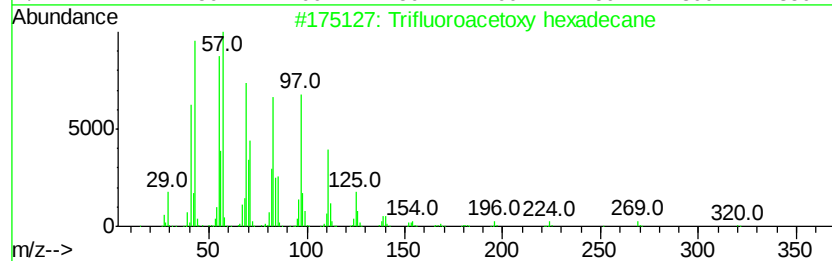
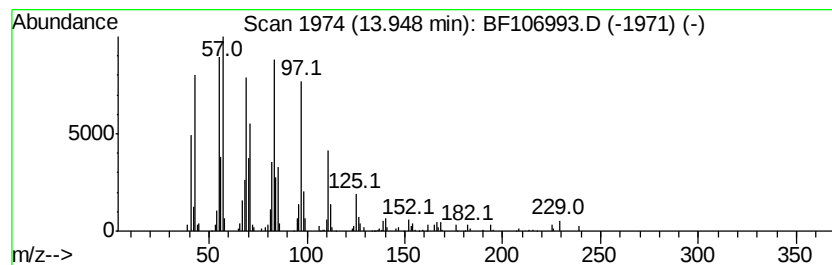
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.33 ng	103747	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	93
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062918\
Data File : BF106993.D
Acq On : 30 Jun 2018 00:40
Operator : JU/SJ
Sample : J3693-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-41

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.18	3.0	ng	70176	1	6.95	470783	20.0
unknown6.73	6.73	66.8	ng	1572150	1	6.95	470783	20.0
Benzenesulfonamid...	10.65	13.4	ng	402781	3	10.00	599812	20.0
Benzenesulfonamid...	10.85	8.1	ng	229229	4	11.48	566512	20.0
Eicosane	10.87	2.0	ng	57155	4	11.48	566512	20.0
Hexadecanoic acid...	12.87	2.1	ng	65254	5	14.14	623376	20.0
Trifluoroacetoxy ...	13.95	3.3	ng	103747	5	14.14	623376	20.0