

Data Path : Z:\HPCHEM1\BNA_F\Data\BF111717\
 Data File : BF100677.D
 Acq On : 17 Nov 2017 16:06
 Operator : SJ/JU
 Sample : I6437-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DC-1

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-BF110817.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	2.204	16	20	23	rVB	21292	28038	1.24%	0.146%
2	5.110	510	514	527	rBB	266932	344572	15.28%	1.799%
3	5.504	576	581	584	rBV	2075132	2021317	89.66%	10.554%
4	6.510	746	752	767	rBV	1977307	2254438	100.00%	11.771%
5	6.651	771	776	779	rBV	2242049	2080695	92.29%	10.864%
6	6.881	811	815	819	rBV	789059	629470	27.92%	3.287%
7	7.039	837	842	845	rBV	1666986	1467902	65.11%	7.664%
8	7.445	905	911	914	rBV	1229061	1164265	51.64%	6.079%
9	8.163	1028	1033	1037	rBV	1006254	829543	36.80%	4.331%
10	8.716	1120	1127	1136	rBV	83966	75577	3.35%	0.395%
11	9.092	1183	1191	1199	rVB3	19063	37886	1.68%	0.198%
12	9.239	1210	1216	1219	rBV	2206703	1927112	85.48%	10.062%
13	9.628	1279	1282	1286	rBV	75197	55733	2.47%	0.291%
14	9.916	1327	1331	1335	rBV	916954	882468	39.14%	4.608%
15	10.192	1373	1378	1383	rBV2	19700	31168	1.38%	0.163%
16	10.627	1448	1452	1455	rBV	341498	253486	11.24%	1.324%
17	10.704	1461	1465	1469	rBV	1164882	1057001	46.89%	5.519%
18	10.992	1510	1514	1520	rVB2	63474	78608	3.49%	0.410%
19	11.404	1580	1584	1587	rBV	947794	772874	34.28%	4.035%
20	11.839	1655	1658	1662	rBV	23214	24240	1.08%	0.127%
21	11.916	1668	1671	1676	rBV2	37886	36072	1.60%	0.188%
22	12.692	1799	1803	1807	rBV6	16620	24962	1.11%	0.130%
23	12.986	1849	1853	1856	rBV	1360183	1219820	54.11%	6.369%
24	13.116	1872	1875	1877	rBV	31476	31718	1.41%	0.166%
25	13.145	1877	1880	1883	rVB	60395	62739	2.78%	0.328%
26	13.386	1918	1921	1926	rVB2	35157	38845	1.72%	0.203%
27	13.839	1994	1998	2001	rBV3	21759	32405	1.44%	0.169%
28	13.910	2007	2010	2014	rVB	207363	192408	8.53%	1.005%
29	14.039	2028	2032	2036	rBV	717051	624931	27.72%	3.263%
30	14.515	2109	2113	2119	rVB7	40146	64759	2.87%	0.338%
31	14.604	2125	2128	2131	rBV	34756	35879	1.59%	0.187%
32	15.198	2226	2229	2235	rVB3	19263	26148	1.16%	0.137%
33	15.515	2278	2283	2290	rVB	491691	612639	27.17%	3.199%
34	16.104	2378	2383	2392	rVB9	55560	132752	5.89%	0.693%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

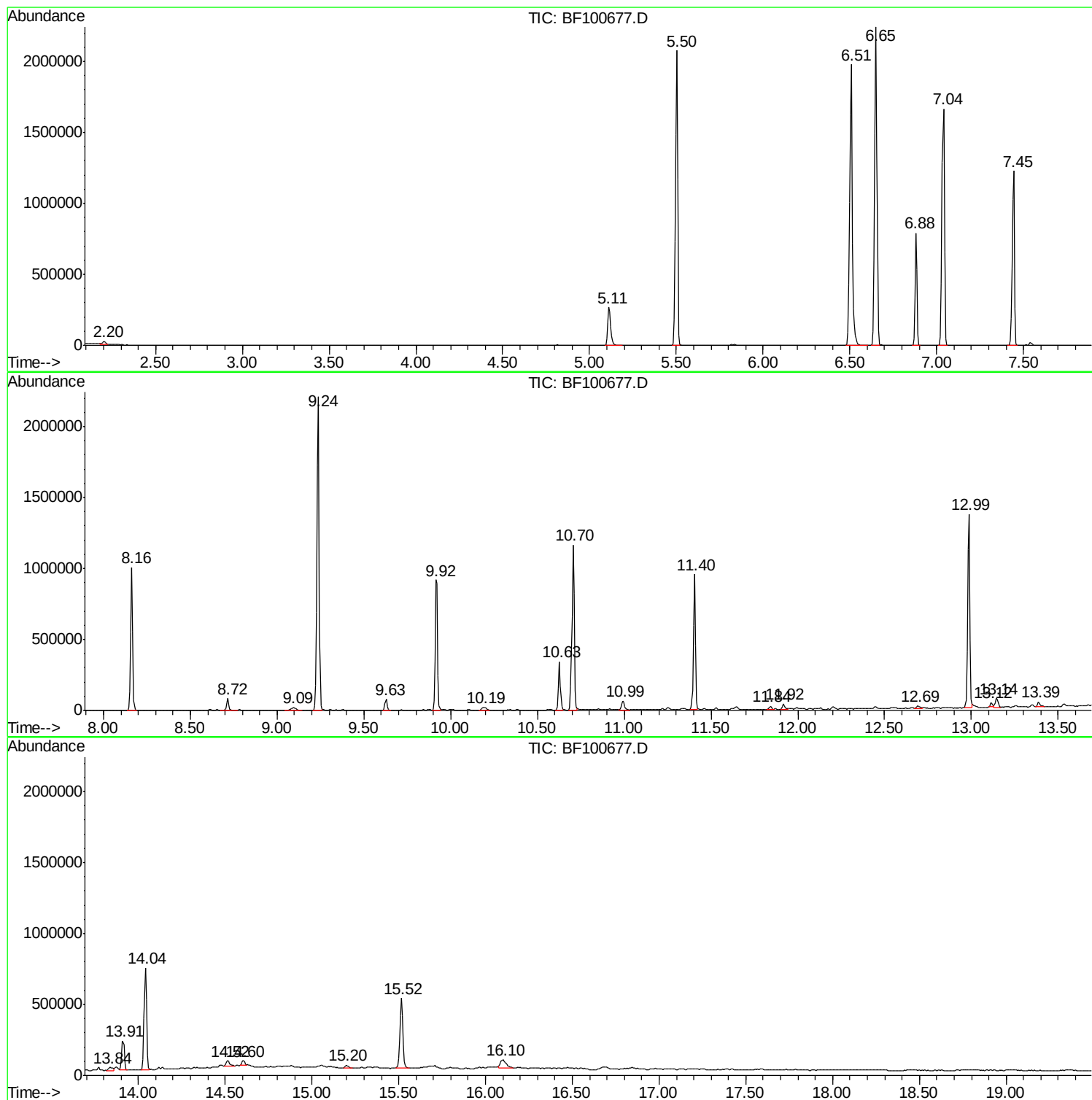
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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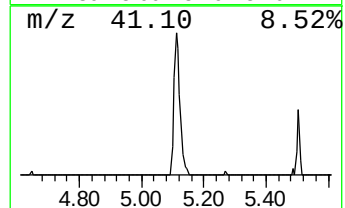
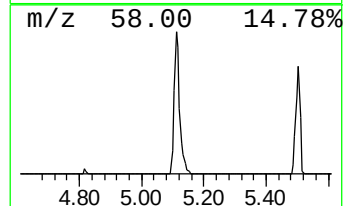
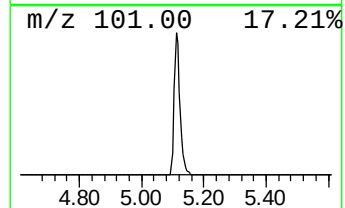
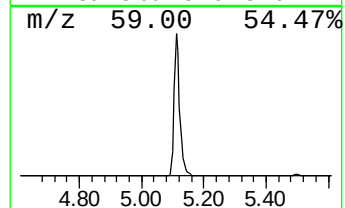
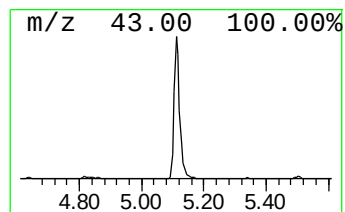
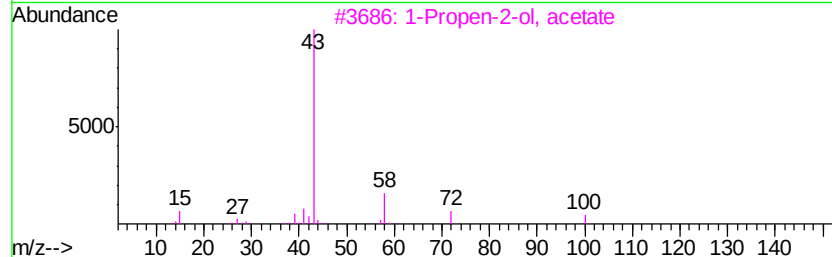
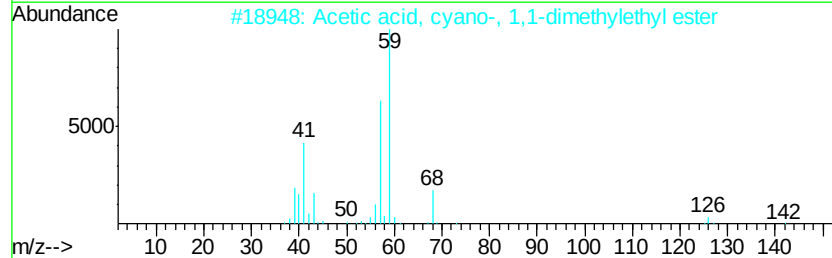
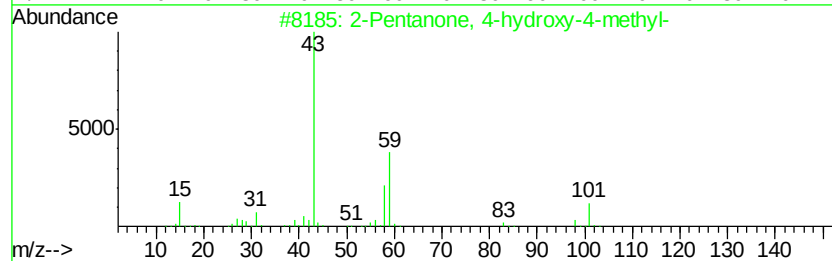
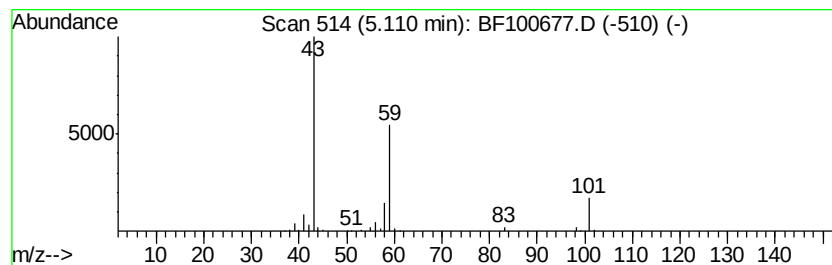
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	10.95 ng	344572	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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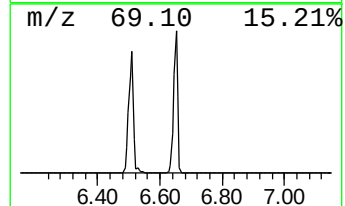
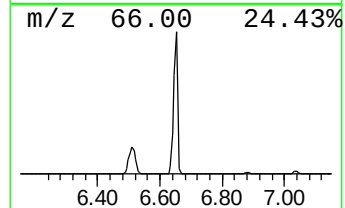
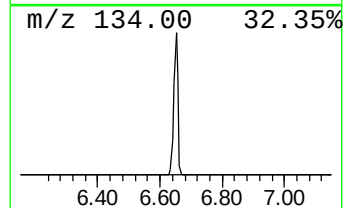
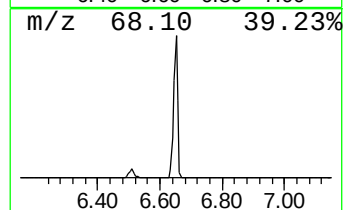
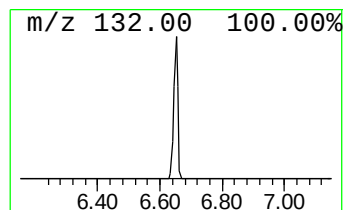
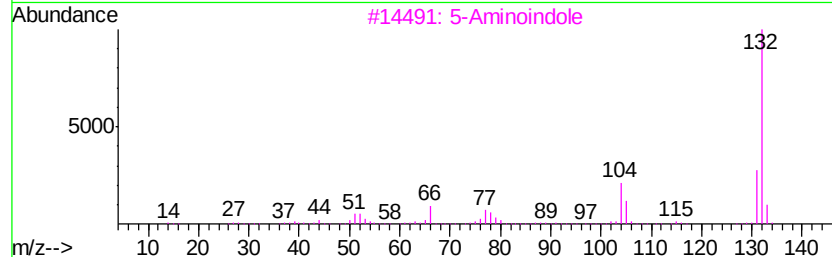
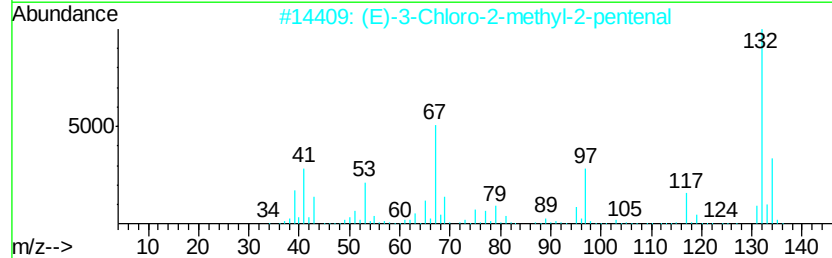
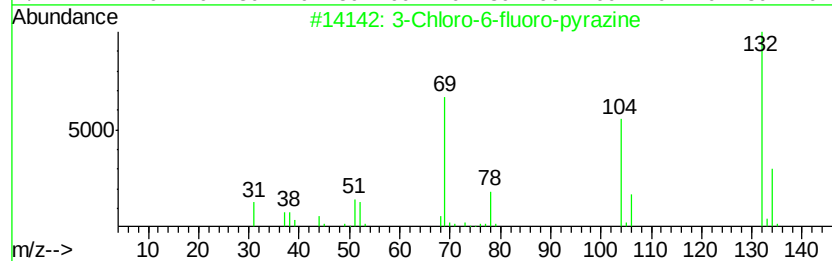
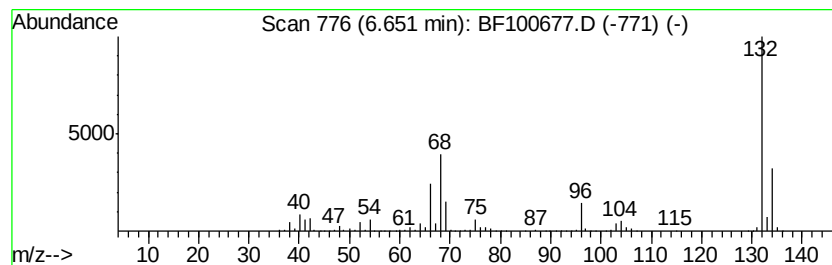
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.11 ng	2080700	1,4-Dichlorobenzene-d4	6.88

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	12
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



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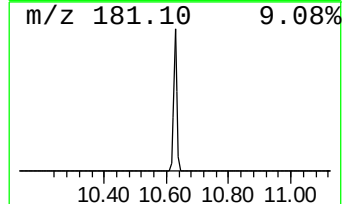
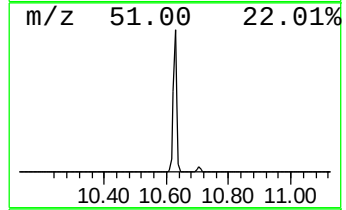
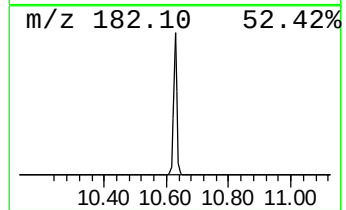
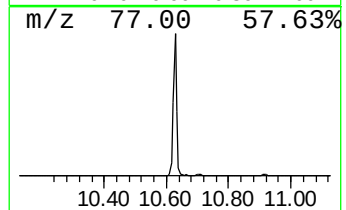
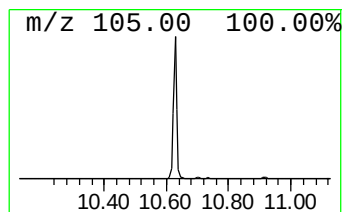
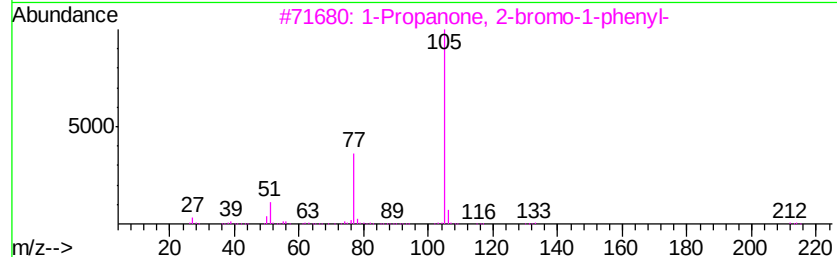
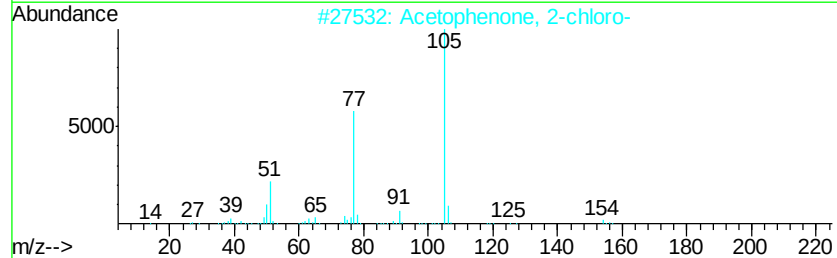
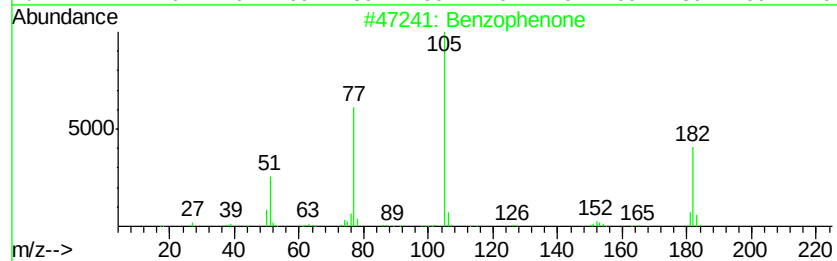
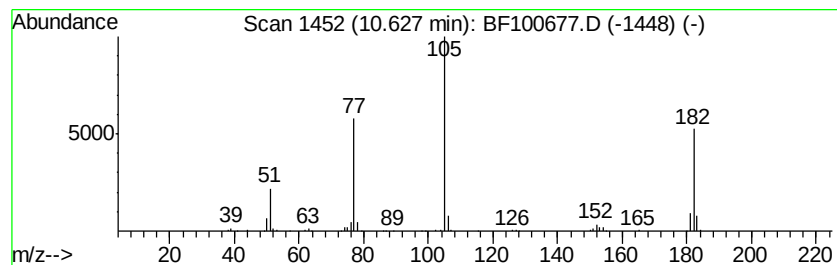
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.63	5.74 ng	253486	Acenaphthene-d10	9.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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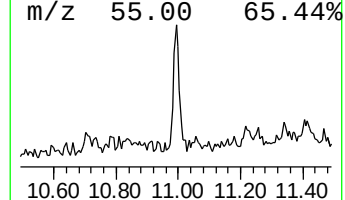
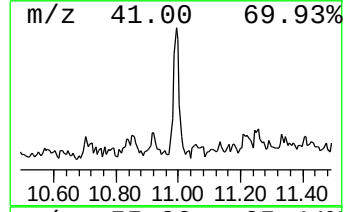
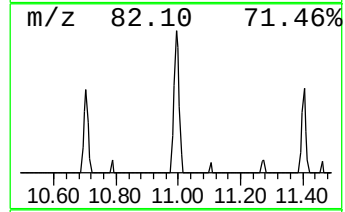
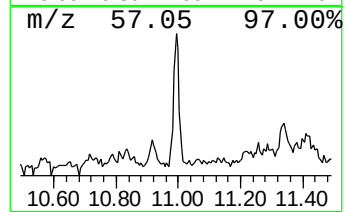
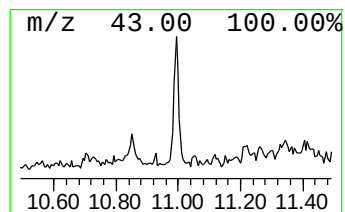
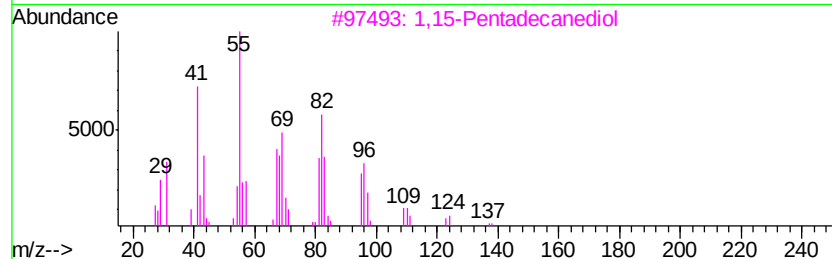
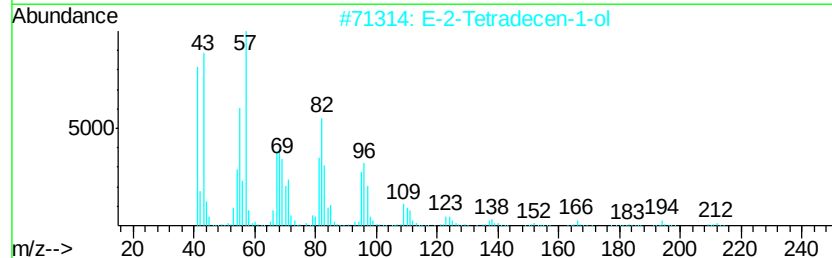
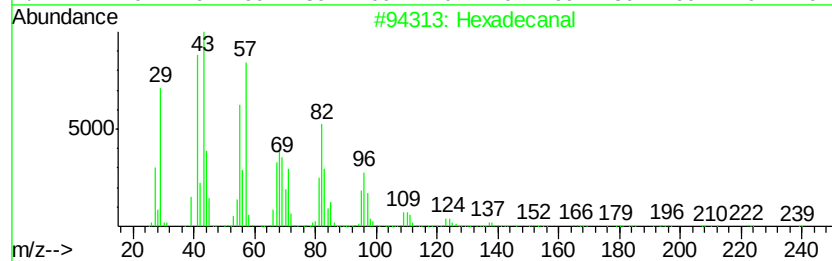
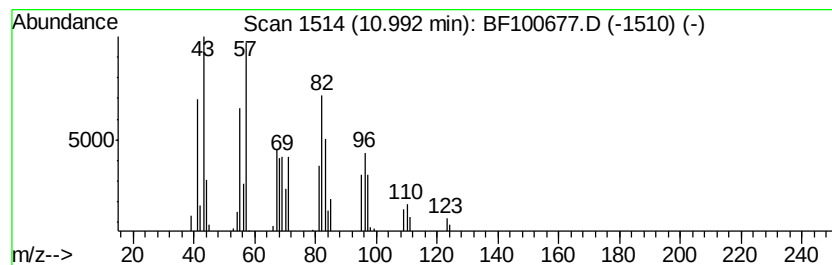
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.99	2.03 ng	78608	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	90
2	E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	72
3	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	72
4	Pentadecanal-	226	C15H30O	002765-11-9	72
5	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	68



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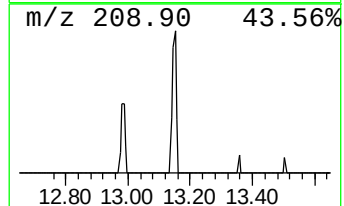
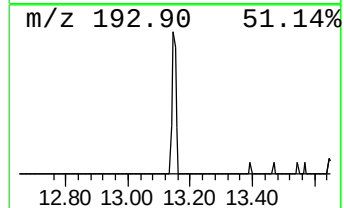
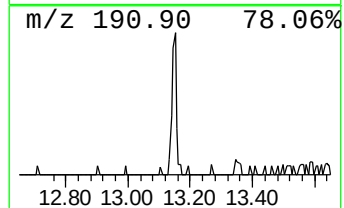
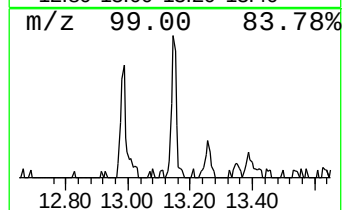
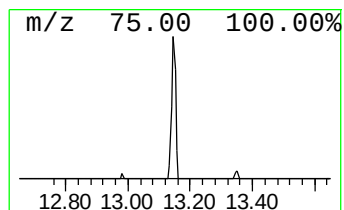
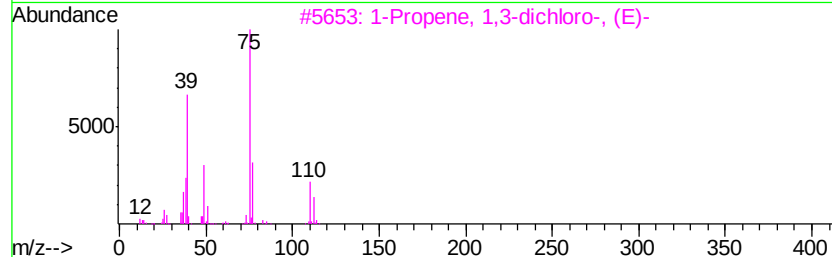
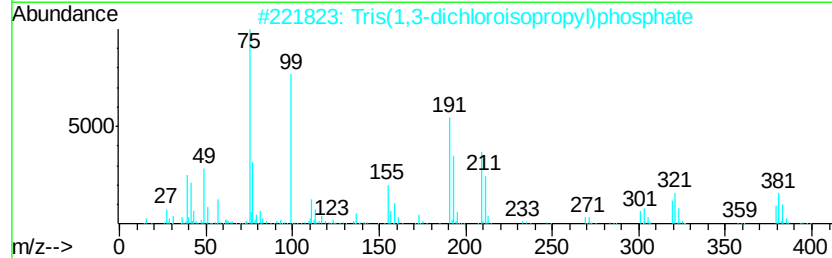
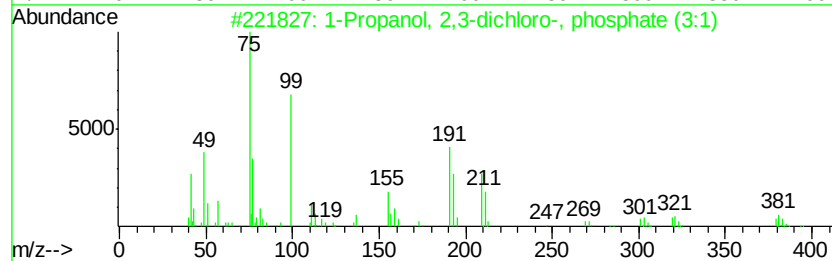
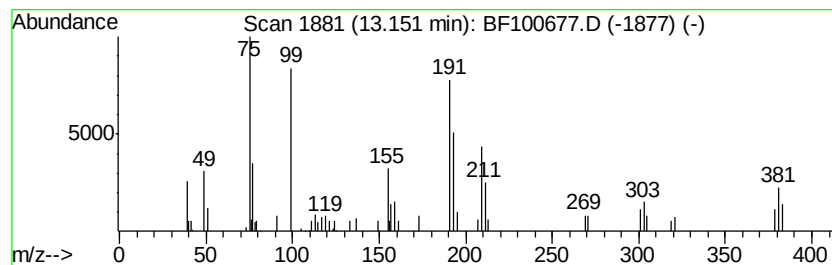
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Propanol, 2,3-dichloro-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	2.01 ng	62739	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol, 2,3-dichloro-, phosph...	428	C9H15Cl6O4P	000078-43-3	91
2		Tris(1,3-dichloroisopropyl)phosp...	428	C9H15Cl6O4P	013674-87-8	72
3		1-Propene, 1,3-dichloro-, (E)-	110	C3H4Cl2	010061-02-6	25
4		Propane, 1,2,3-trichloro-	146	C3H5Cl3	000096-18-4	23
5		Propane, 2,2'-oxybis[1,3-dichloro-	238	C6H10Cl4O	059440-89-0	23



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Misc :
ALS Vial : 15 Sample Multiplier: 1

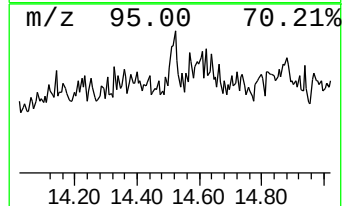
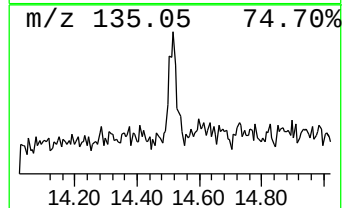
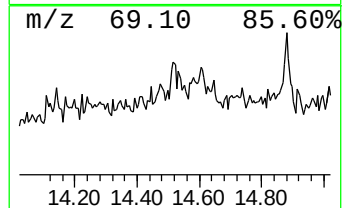
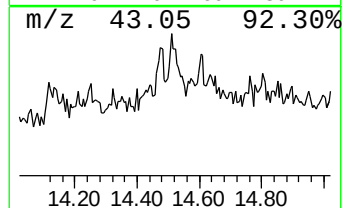
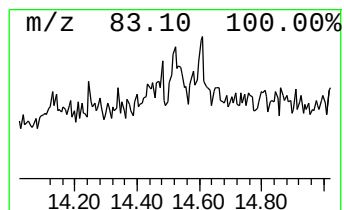
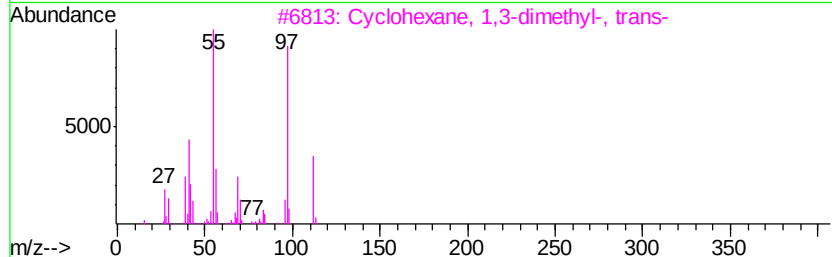
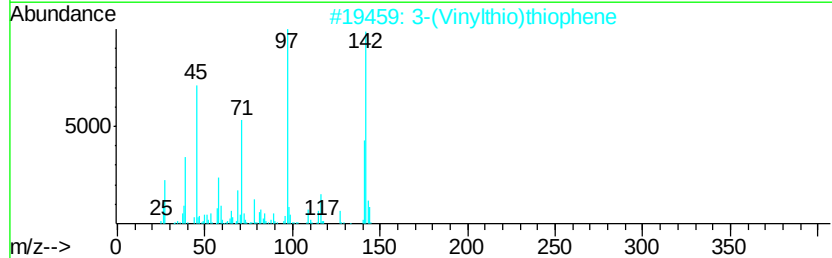
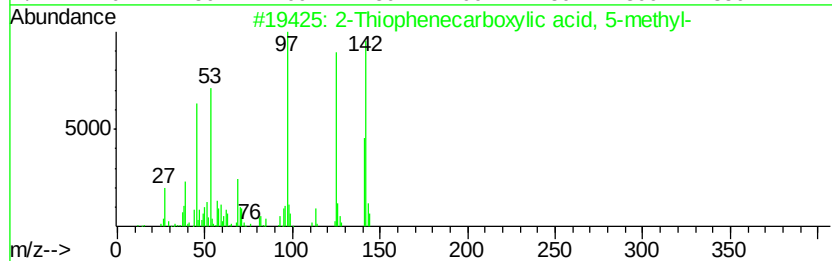
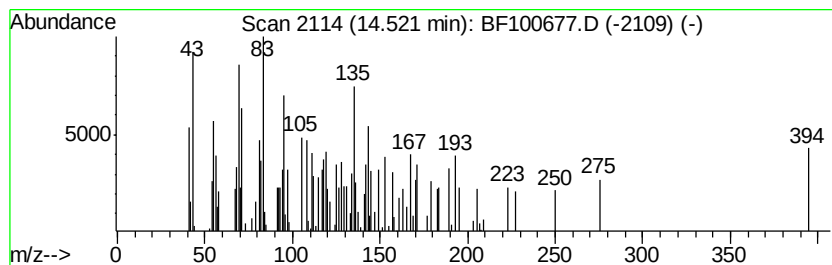
Instrument :
BNA_F
ClientSampleId :
DC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.52 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.52	2.07 ng	64759	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxylic acid, 5-me...	142	C6H6O2S	001918-79-2	18
2	3-(Vinylthio)thiophene	142	C6H6S2	1000249-93-3	14
3	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	11
4	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	11
5	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	11



Data Path : Z:\HPCHEM1\BNA_F\Data\BF111717\
Data File : BF100677.D
Acq On : 17 Nov 2017 16:06
Operator : SJ/JU
Sample : I6437-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
DC-1

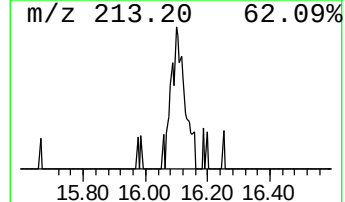
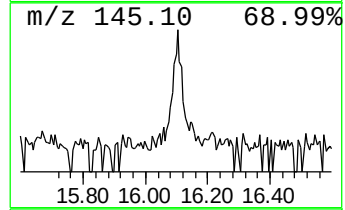
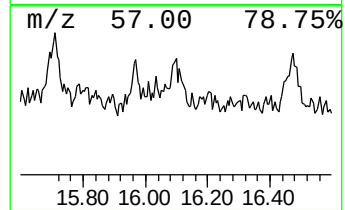
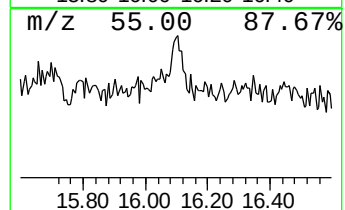
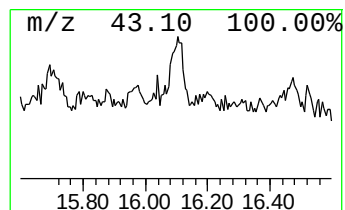
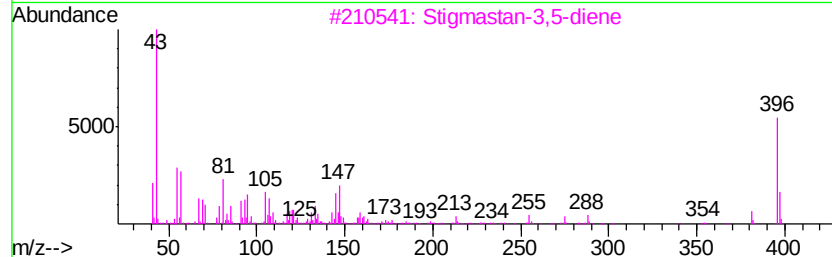
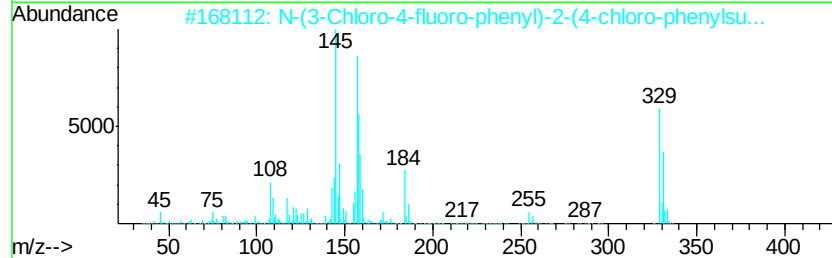
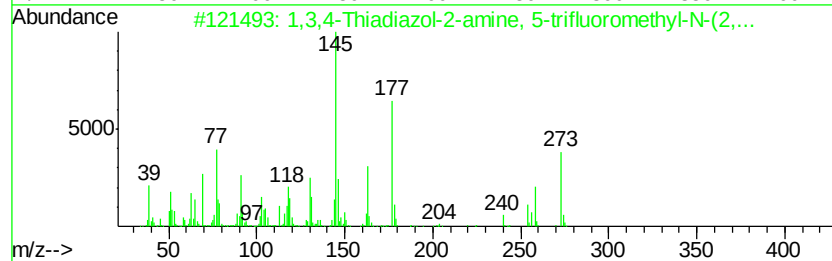
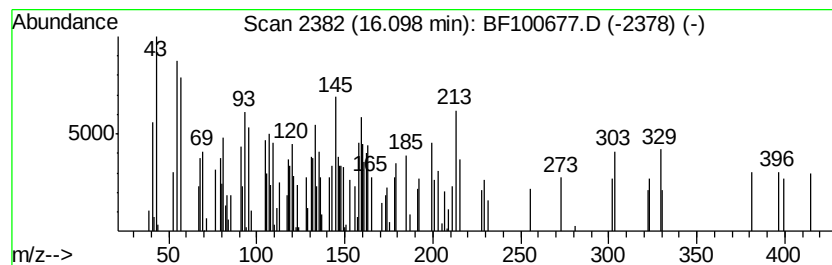
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.10 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	4.33 ng	132752	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	284488-18-2	47
2		N-(3-Chloro-4-fluoro-phenyl)-2-(...	329	C14H10Cl2FNOS	1000295-12-7	30
3		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	27
4		1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	1000267-89-8	18
5		Benzofuran-2-carboxylic acid, (2...	303	C16H11F2N03	1000311-07-8	14



Data Path : Z:\HPCHEM1\BNA_F\Data\BF111717\
Data File : BF100677.D
Acq On : 17 Nov 2017 16:06
Operator : SJ/JU
Sample : I6437-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.11	10.9	ng	344572	1	6.88	629470	20.0
unknown6.65	6.65	66.1	ng	2080700	1	6.88	629470	20.0
Benzophenone	10.63	5.7	ng	253486	3	9.92	882468	20.0
Hexadecanal	10.99	2.0	ng	78608	4	11.40	772874	20.0
1-Propanol, 2,3-d...	13.15	2.0	ng	62739	5	14.04	624931	20.0
unknown14.52	14.52	2.1	ng	64759	5	14.04	624931	20.0
unknown16.10	16.10	4.3	ng	132752	6	15.52	612639	20.0