

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
 Data File : BF107470.D
 Acq On : 18 Jul 2018 12:00
 Operator : JU/SJ
 Sample : J3906-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CB-7-8-6-ST-EW-2@2.75

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-BF071618.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	5.231	488	492	500	rVB	362611	499454	12.29%	1.310%
2	5.619	552	558	561	rBV	3644100	3716094	91.46%	9.749%
3	6.613	721	727	730	rBV	3525087	4014734	98.81%	10.532%
4	6.760	746	752	755	rBV	3956749	4042438	99.49%	10.605%
5	6.984	786	790	795	rVB	1140676	904810	22.27%	2.374%
6	7.143	812	817	820	rBV	3289681	2908256	71.58%	7.630%
7	7.548	879	886	889	rBV	2641468	2664284	65.57%	6.990%
8	8.266	1004	1008	1011	rBV	1254716	1060221	26.09%	2.781%
9	9.342	1185	1191	1194	rBV	4176613	4063221	100.00%	10.660%
10	9.442	1205	1208	1212	rVB3	57093	52790	1.30%	0.138%
11	9.731	1252	1257	1261	rBV	947919	820839	20.20%	2.153%
12	10.031	1303	1308	1311	rBV	1311607	1269939	31.25%	3.332%
13	10.819	1437	1442	1446	rBV	2578628	2778462	68.38%	7.289%
14	10.989	1468	1471	1474	rBV	41606	44859	1.10%	0.118%
15	11.019	1474	1476	1480	rVB3	50294	43562	1.07%	0.114%
16	11.054	1480	1482	1485	rBV3	49722	47203	1.16%	0.124%
17	11.160	1498	1500	1504	rVB5	61932	54482	1.34%	0.143%
18	11.525	1557	1562	1564	rBV	1417566	1399022	34.43%	3.670%
19	11.542	1564	1565	1569	rVV	216964	160199	3.94%	0.420%
20	11.595	1570	1574	1576	rVB2	47863	60251	1.48%	0.158%
21	11.960	1633	1636	1640	rBV5	31833	47670	1.17%	0.125%
22	12.136	1662	1666	1668	rBV4	58033	55545	1.37%	0.146%
23	12.383	1705	1708	1713	rBV7	50274	67217	1.65%	0.176%
24	12.542	1732	1735	1738	rBV3	105390	107354	2.64%	0.282%
25	12.583	1738	1742	1746	rVV5	46786	76889	1.89%	0.202%
26	12.736	1765	1768	1771	rVB	282635	241449	5.94%	0.633%
27	12.966	1802	1807	1810	rBV	193255	234593	5.77%	0.615%
28	13.107	1826	1831	1835	rBV	3617257	3532579	86.94%	9.268%
29	13.266	1856	1858	1861	rBV3	37272	45472	1.12%	0.119%
30	13.319	1865	1867	1870	rVB2	72410	54605	1.34%	0.143%
31	13.660	1923	1925	1928	rBV3	91794	78091	1.92%	0.205%
32	13.983	1978	1980	1986	rVB3	240298	280082	6.89%	0.735%
33	14.166	2007	2011	2014	rBV	960515	1000739	24.63%	2.625%
34	14.313	2033	2036	2037	rBV	144826	112132	2.76%	0.294%

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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

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35	14.618	2085	2088	2090	rVB2	177019	153245	3.77%	0.402%
36	14.942	2140	2143	2147	rVB	159198	151197	3.72%	0.397%
37	15.301	2201	2204	2208	rVB3	156746	177107	4.36%	0.465%
38	15.707	2269	2273	2281	rVB2	741181	1096788	26.99%	2.877%

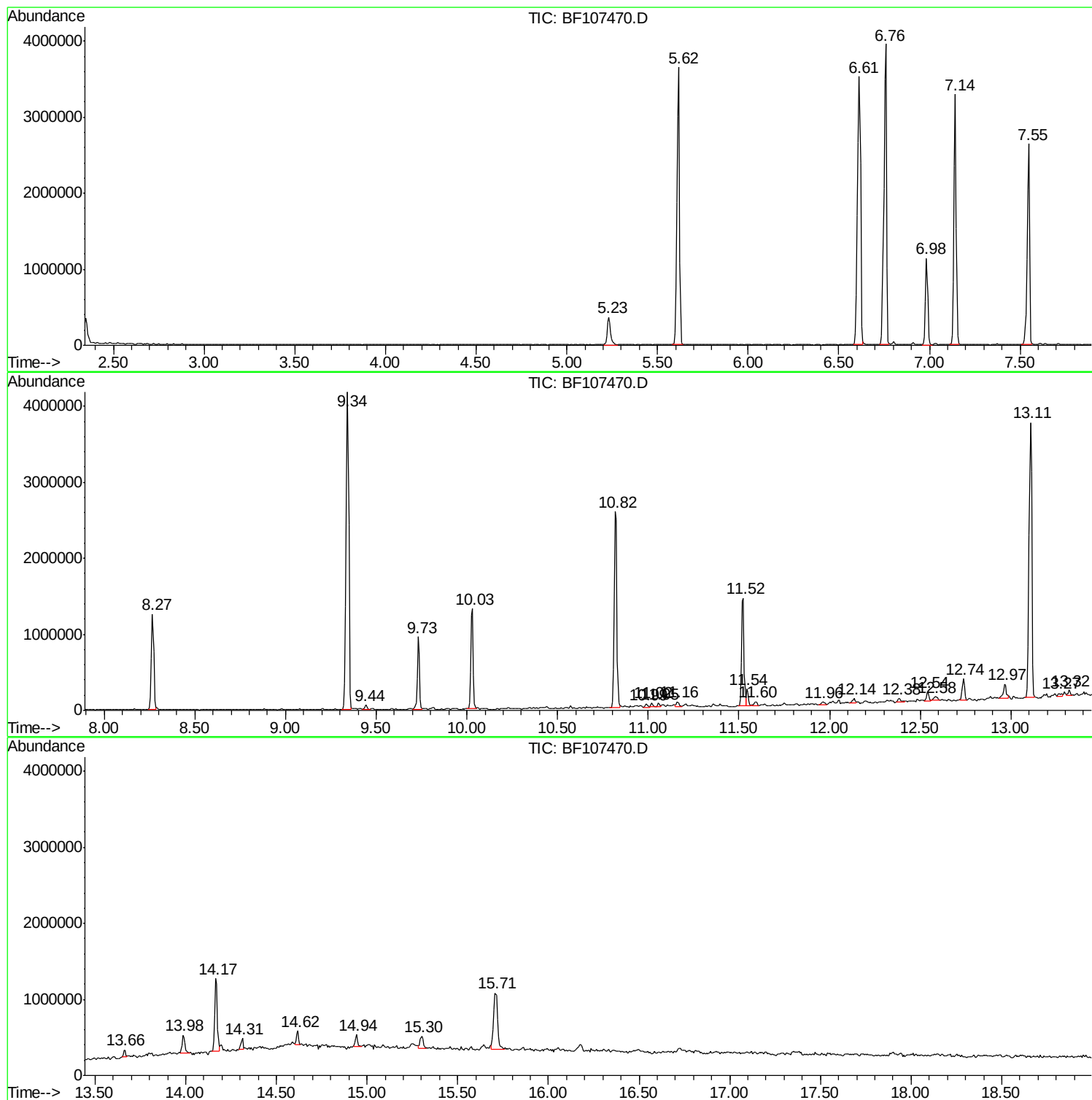
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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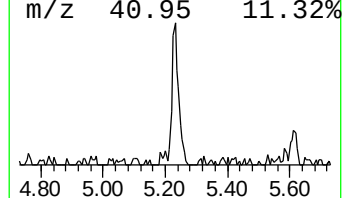
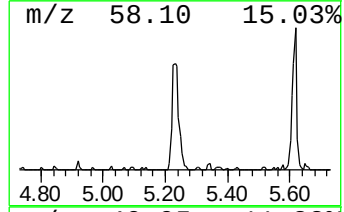
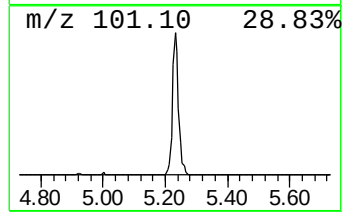
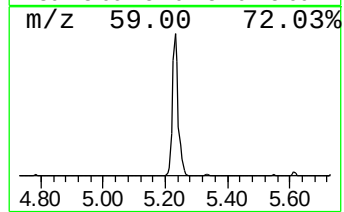
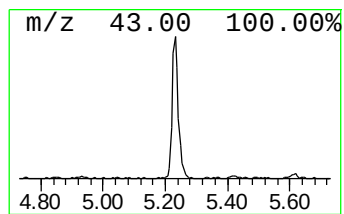
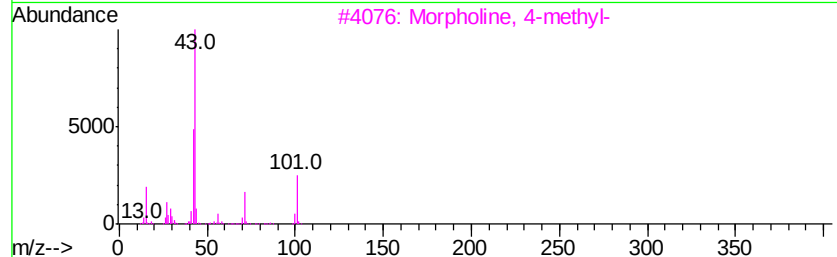
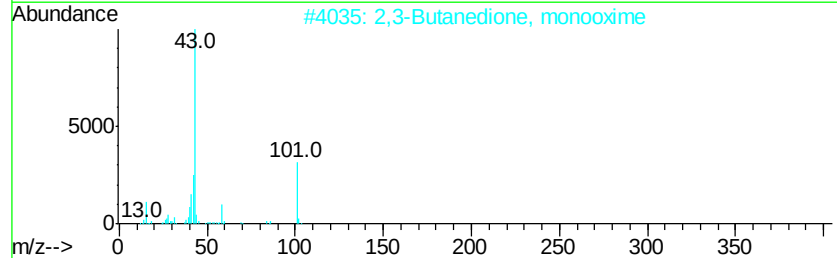
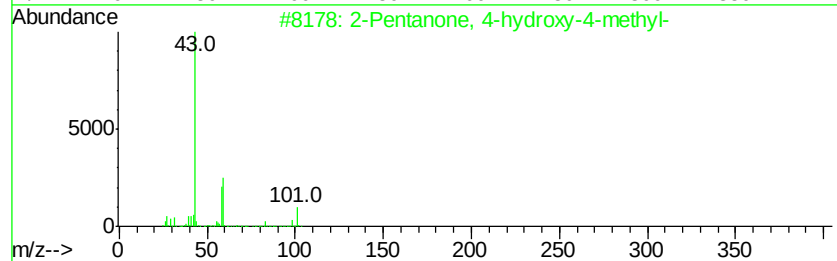
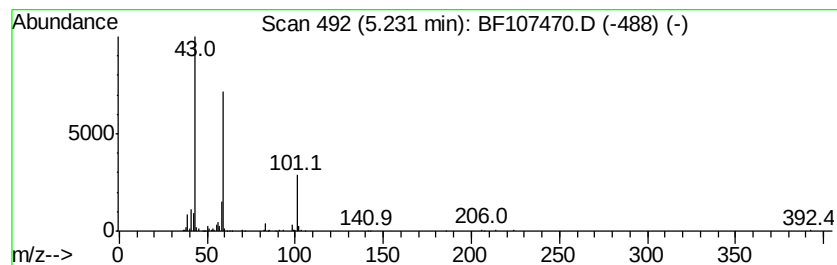
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	11.04 ng	499454	1,4-Dichlorobenzene-d4	6.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9



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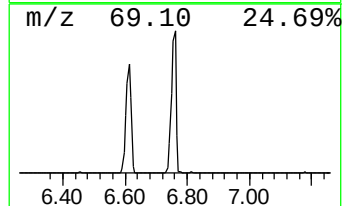
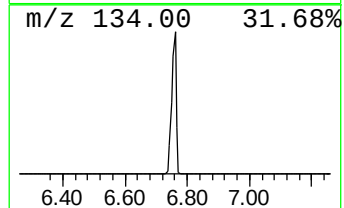
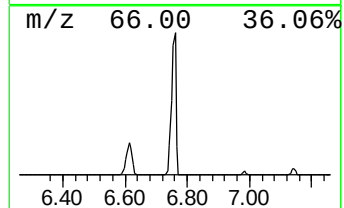
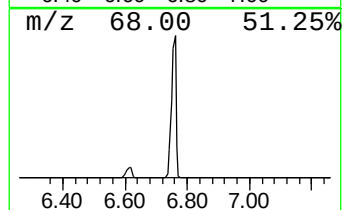
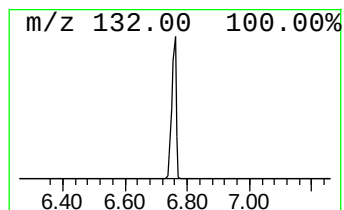
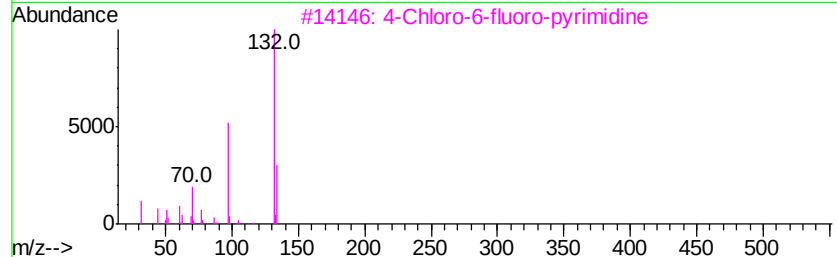
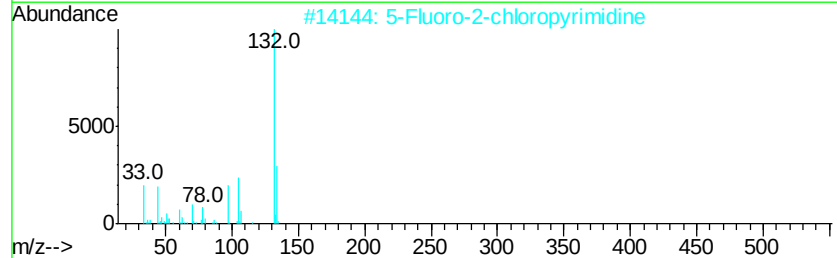
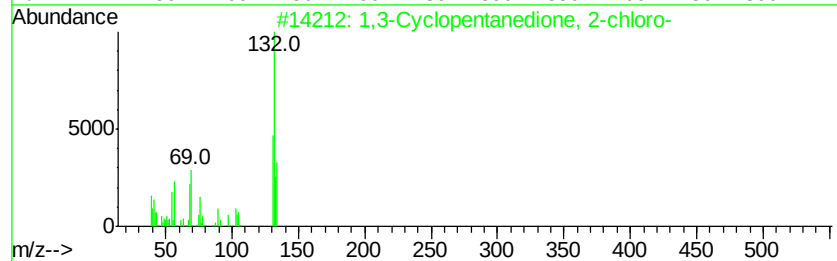
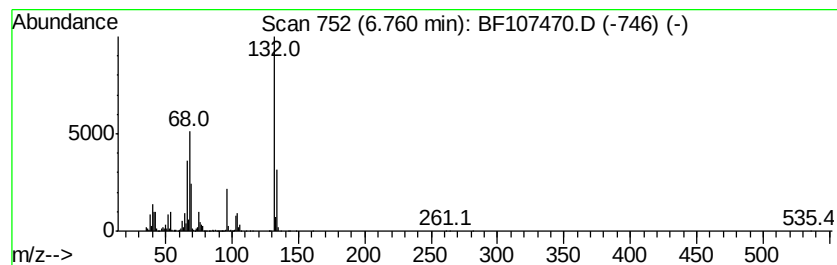
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Peak Number 2 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	89.35 ng	4042440	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	22



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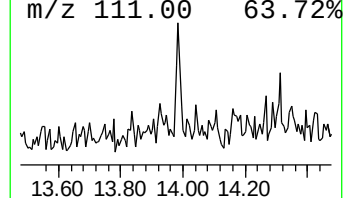
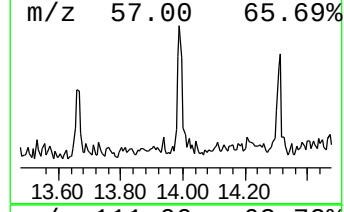
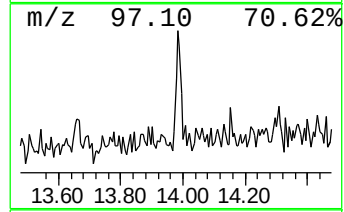
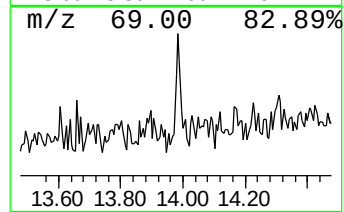
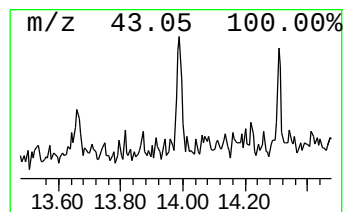
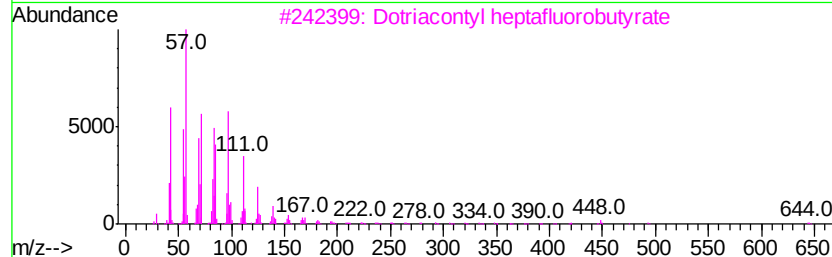
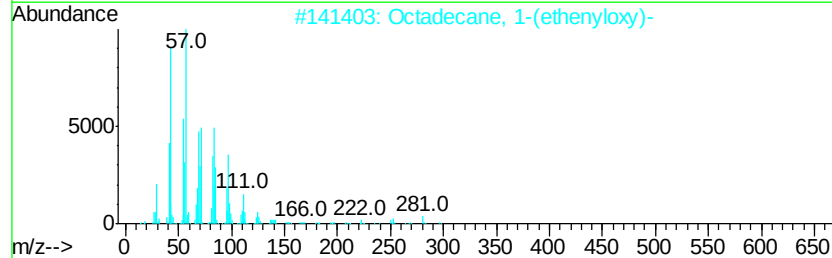
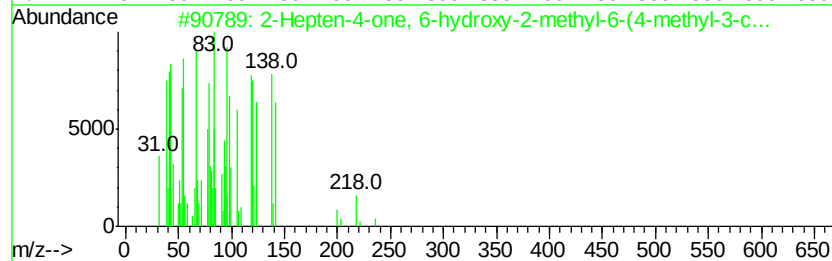
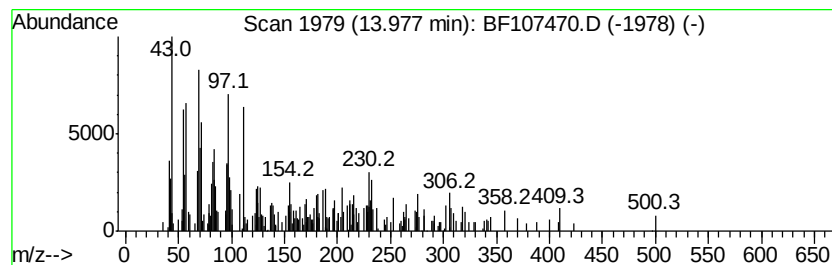
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hepten-4-one, 6-hydroxy-2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.98	5.60 ng	280082	Chrysene-d12	14.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	92
2	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	76
3	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	74
4	Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	68
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	64



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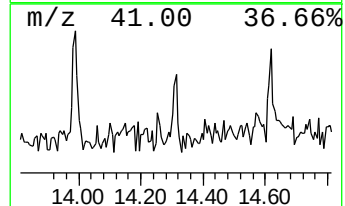
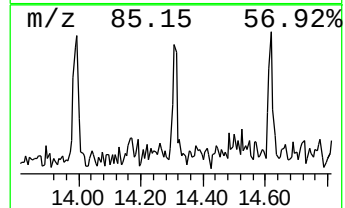
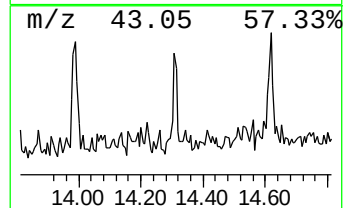
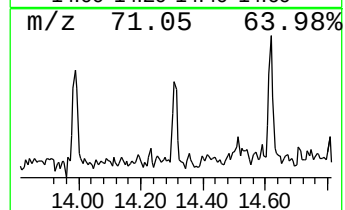
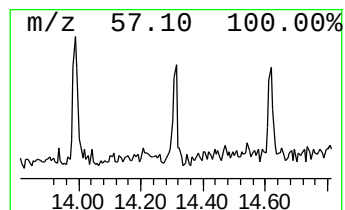
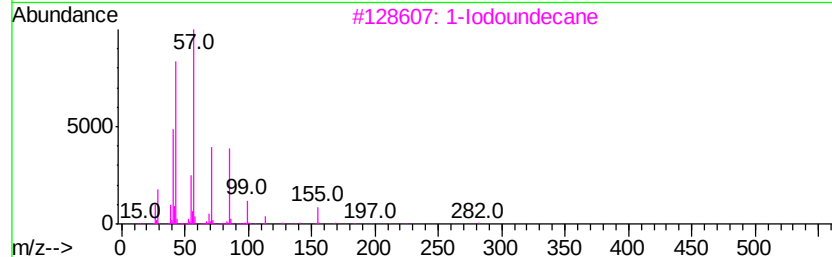
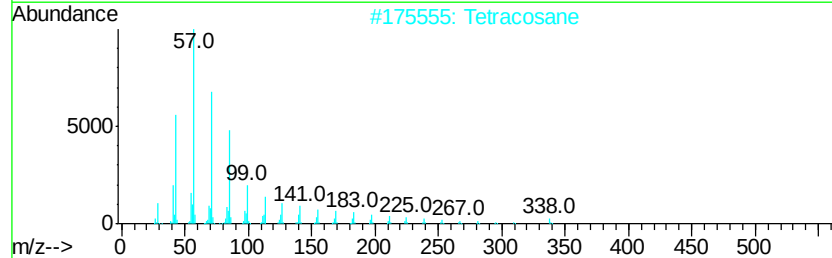
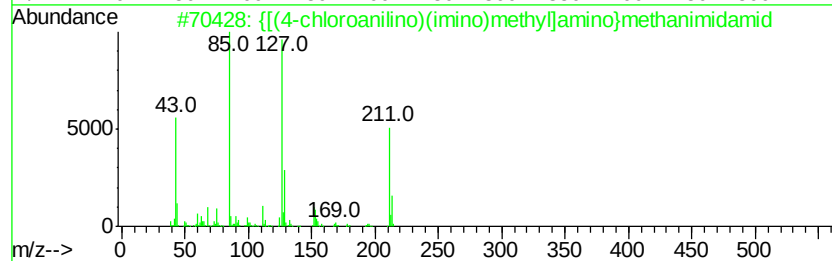
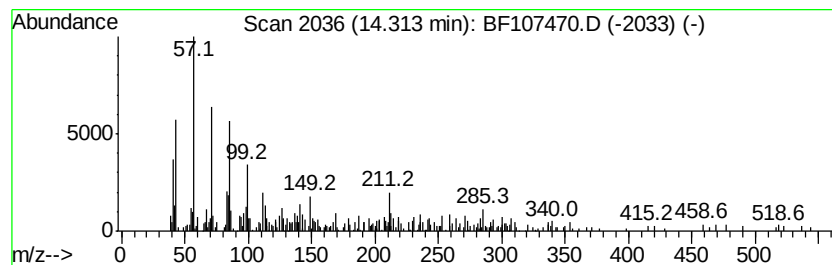
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Peak Number 5 unknown14.31 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	2.24 ng	112132	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	{[(4-chloroanilino)(imino)methyl...}	211	C8H10ClN5	1000297-60-3	46
2		Tetracosane	338	C24H50	000646-31-1	46
3		1-Iodoundecane	282	C11H23I	004282-44-4	38
4		Docosane	310	C22H46	000629-97-0	38
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	38



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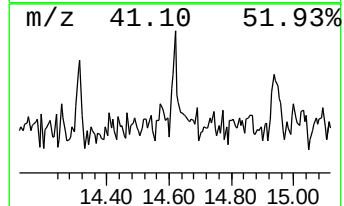
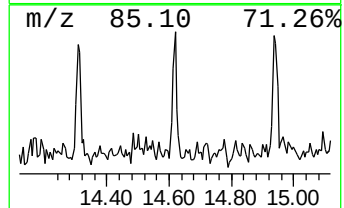
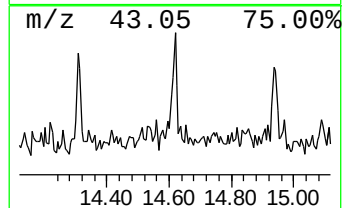
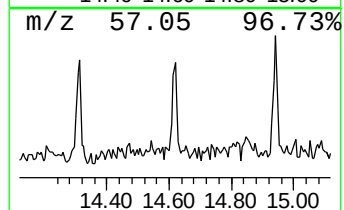
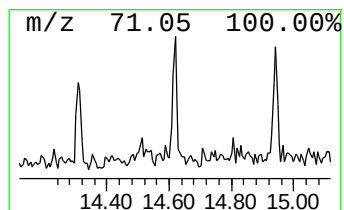
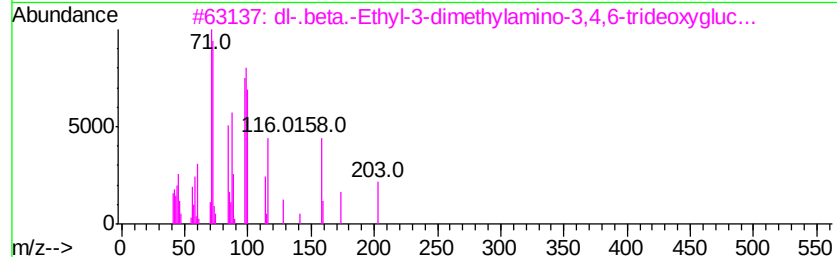
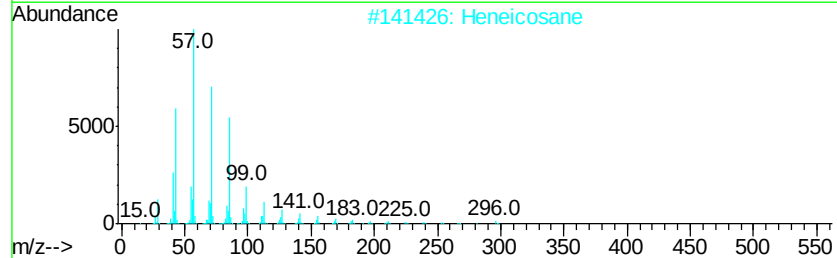
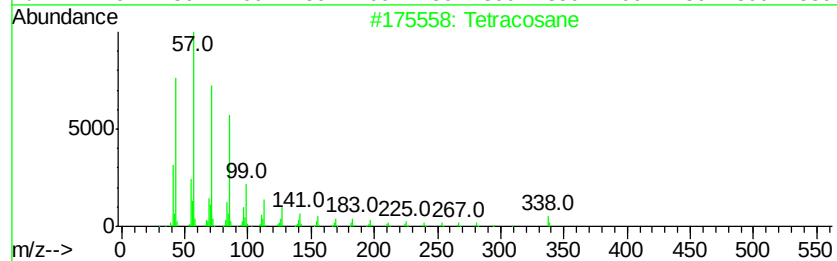
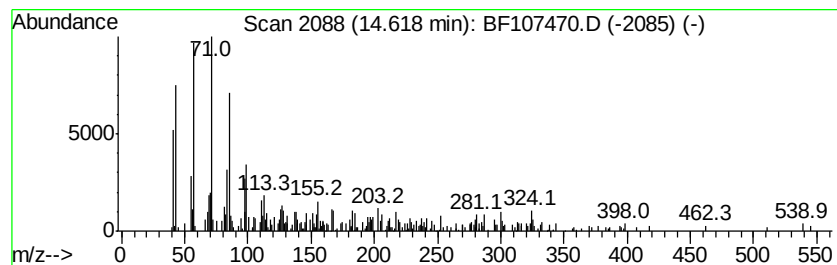
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.06 ng	153245	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	93
2		Heneicosane	296	C21H44	000629-94-7	89
3		dl-.beta.-Ethyl-3-dimethylamino-...	203	C10H21N03	1000298-96-2	86
4		Octadecane	254	C18H38	000593-45-3	86
5		Heptadecane	240	C17H36	000629-78-7	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
Data File : BF107470.D
Acq On : 18 Jul 2018 12:00
Operator : JU/SJ
Sample : J3906-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CB-7-8-6-ST-EW-2@2.75

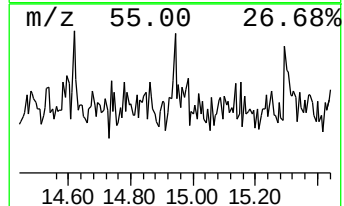
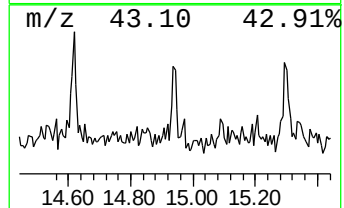
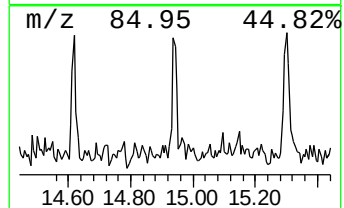
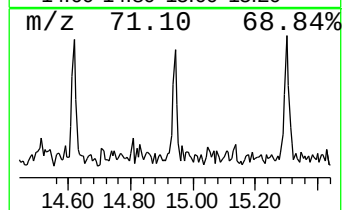
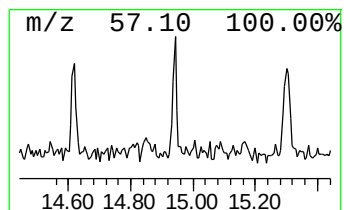
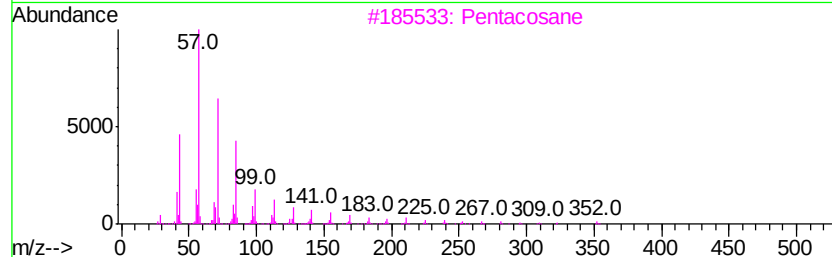
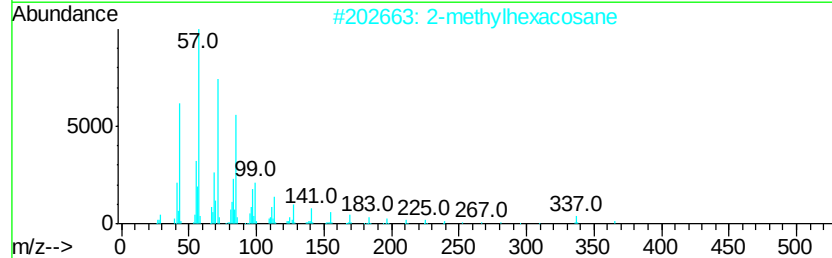
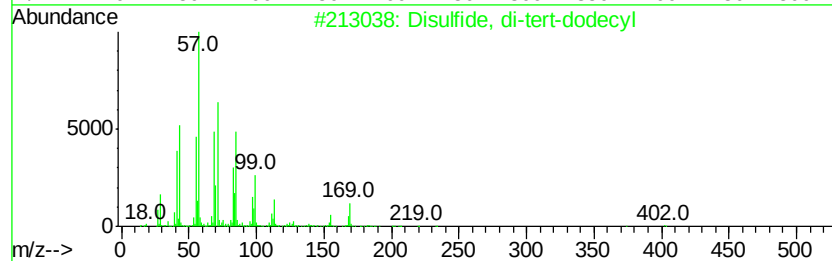
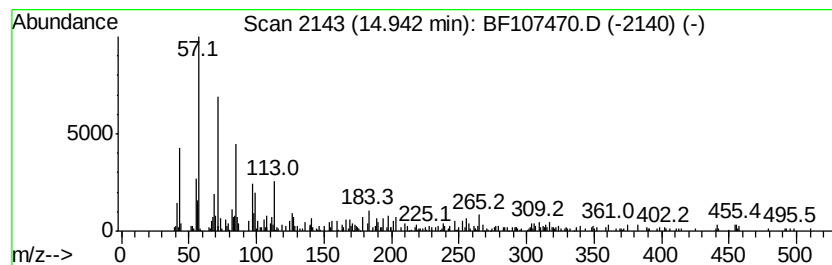
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Disulfide, di-tert-dodecyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.76 ng	151197	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	68
2		2-methylhexacosane	380	C27H56	1000376-72-7	64
3		Pentacosane	352	C25H52	000629-99-2	64
4		Heptadecane	240	C17H36	000629-78-7	60
5		Nonadecane	268	C19H40	000629-92-5	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
Data File : BF107470.D
Acq On : 18 Jul 2018 12:00
Operator : JU/SJ
Sample : J3906-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

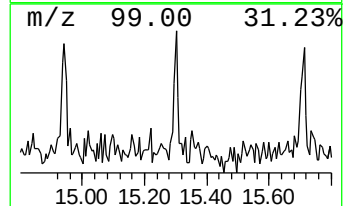
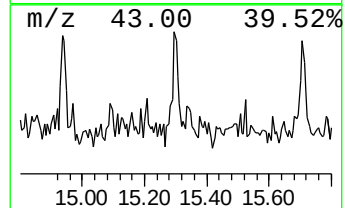
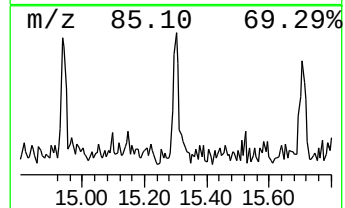
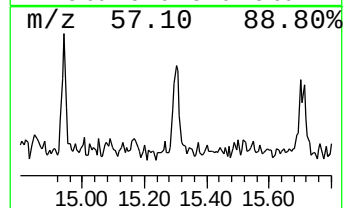
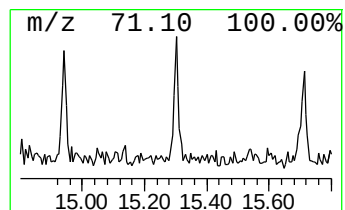
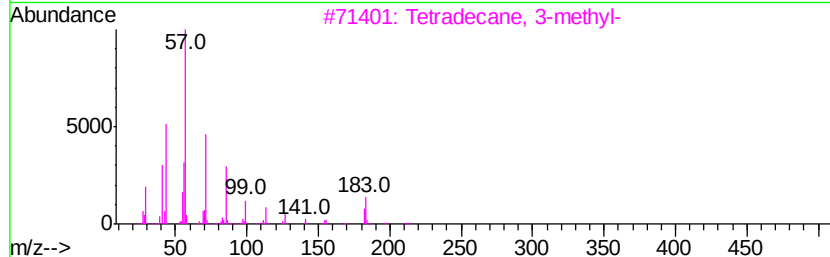
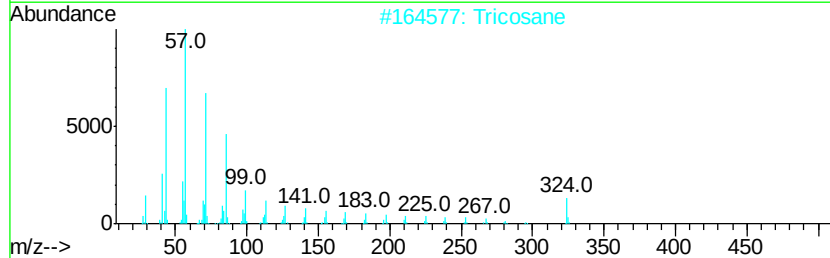
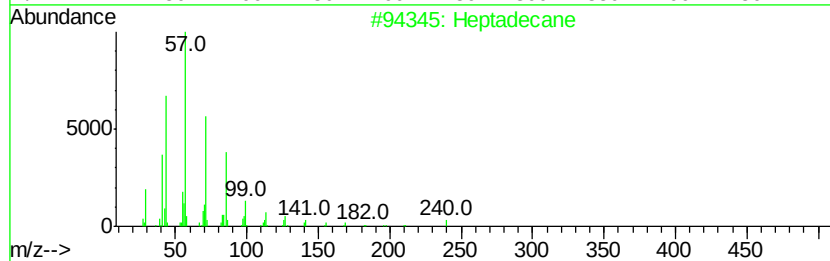
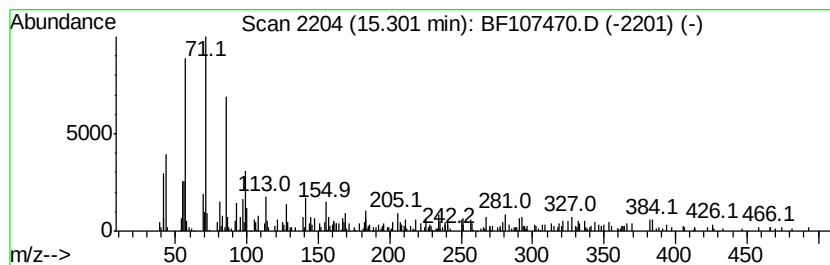
Instrument :
BNA_F
ClientSampleId :
CB-7-8-6-ST-EW-2@2.75

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.30	3.23 ng	177107	Perylene-d12	15.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	81
2	Tricosane	324	C23H48	000638-67-5	74
3	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	72
4	Nonacosane	408	C29H60	000630-03-5	72
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071818\
Data File : BF107470.D
Acq On : 18 Jul 2018 12:00
Operator : JU/SJ
Sample : J3906-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CB-7-8-6-ST-EW-2@2.75

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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...	5.23	11.0	ng	499454	1	6.98	904810	20.0
unknown6.76	6.76	89.3	ng	4042440	1	6.98	904810	20.0
2-Hepten-4-one, 6...	13.98	5.6	ng	280082	5	14.17	1000740	20.0
unknown14.31	14.31	2.2	ng	112132	5	14.17	1000740	20.0
Tetracosane	14.62	3.1	ng	153245	5	14.17	1000740	20.0
Disulfide, di-ter...	14.94	2.8	ng	151197	6	15.71	1096790	20.0
Heptadecane	15.30	3.2	ng	177107	6	15.71	1096790	20.0