

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
 Data File : BG023162.D
 Acq On : 18 Jul 2016 17:14
 Operator : UM/SJ
 Sample : H4044-29
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 H10-B1(6-12)C

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_G\METHODS\8270-BG070816.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	3.015	25	30	49	rVV	5131891	8435200	70.41%	7.851%
2	3.156	49	54	66	rVB	336161	694392	5.80%	0.646%
3	5.183	394	399	404	rVB	177706	262744	2.19%	0.245%
4	5.653	473	479	496	rBV	2397342	4108269	34.29%	3.824%
5	6.176	552	568	569	rBV4	109753	353584	2.95%	0.329%
6	7.274	745	755	769	rBV	2328599	5046514	42.12%	4.697%
7	7.633	809	816	821	rBV	2549409	4720481	39.40%	4.394%
8	7.709	821	829	840	rVB	5616211	11980162	100.00%	11.151%
9	8.103	889	896	905	rBV	569902	994973	8.31%	0.926%
10	8.432	944	952	961	rVB	1747131	3133818	26.16%	2.917%
11	9.278	1088	1096	1106	rBV	1677840	3121316	26.05%	2.905%
12	10.929	1369	1377	1385	rBV	870348	1577979	13.17%	1.469%
13	11.088	1392	1404	1414	rBV2	282955	1003544	8.38%	0.934%
14	12.298	1598	1610	1624	rBV3	635647	2188240	18.27%	2.037%
15	13.297	1767	1780	1781	rBV3	63076	158897	1.33%	0.148%
16	13.361	1784	1791	1804	rVB	4240755	6812301	56.86%	6.341%
17	14.184	1925	1931	1937	rBV	821696	1174693	9.81%	1.093%
18	14.742	2019	2026	2036	rVB2	1430510	2340889	19.54%	2.179%
19	15.230	2101	2109	2121	rBV	2852793	5332942	44.51%	4.964%
20	15.806	2200	2207	2210	rBV3	73287	126885	1.06%	0.118%
21	16.229	2272	2279	2291	rBV	3620870	5811990	48.51%	5.410%
22	16.417	2306	2311	2318	rBV3	112901	204254	1.70%	0.190%
23	16.975	2399	2406	2414	rBV2	1470562	2517134	21.01%	2.343%
24	17.480	2486	2492	2499	rBV2	1705659	2664893	22.24%	2.480%
25	18.179	2607	2611	2618	rBV3	118590	222912	1.86%	0.207%
26	18.338	2633	2638	2644	rBV2	242719	381678	3.19%	0.355%
27	20.001	2915	2921	2927	rBV	5393297	7116503	59.40%	6.624%
28	20.071	2927	2933	2939	rVB	5753592	7700266	64.28%	7.167%
29	20.453	2982	2998	3005	rBV2	751912	3199887	26.71%	2.978%
30	21.358	3148	3152	3159	rBV5	156398	332180	2.77%	0.309%
31	21.710	3199	3212	3215	rBV2	2062750	4623195	38.59%	4.303%
32	21.746	3215	3218	3228	rVB2	1994015	3480858	29.06%	3.240%
33	23.408	3495	3501	3507	rVB	294283	619696	5.17%	0.577%
34	25.024	3765	3776	3795	rVB2	1561901	4993398	41.68%	4.648%

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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_G\METHODS\8270-BG070816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

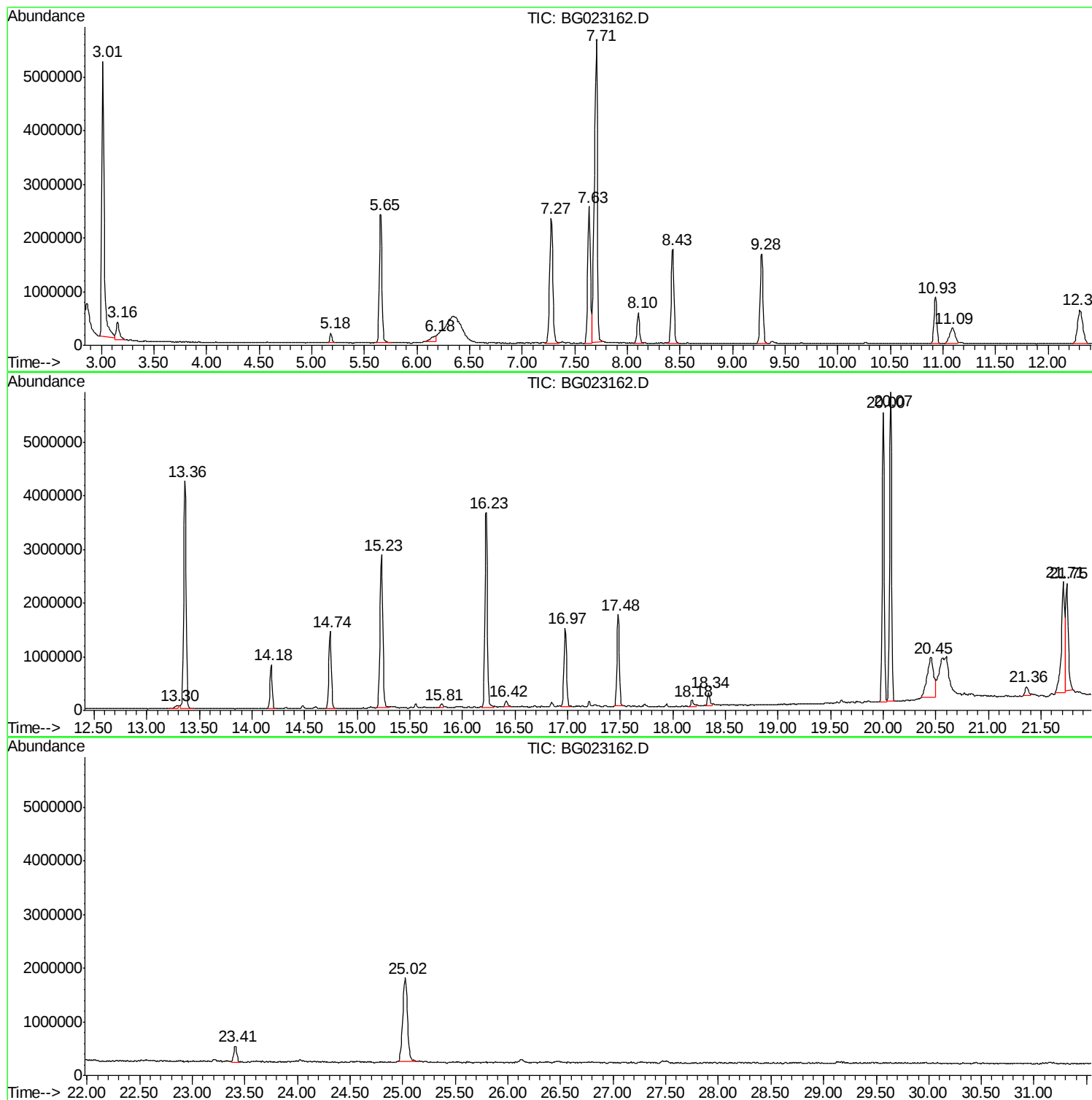
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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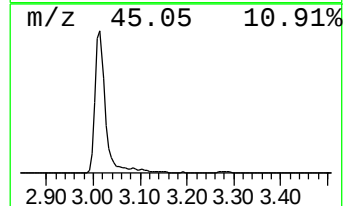
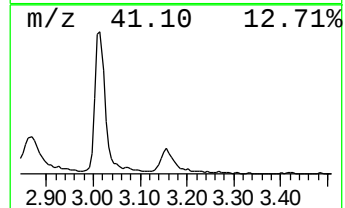
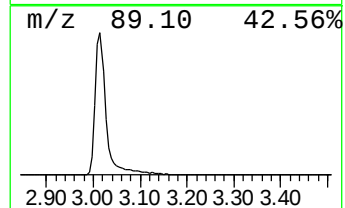
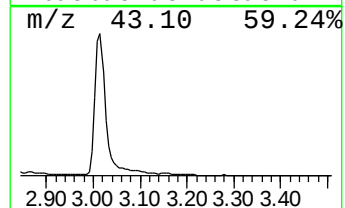
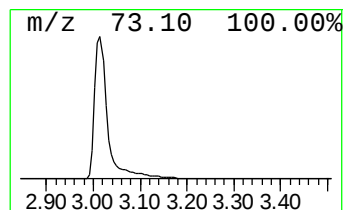
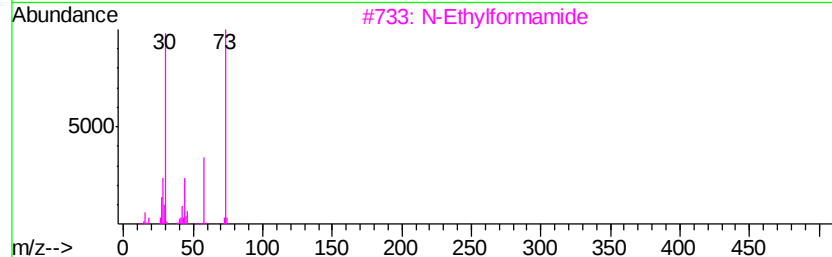
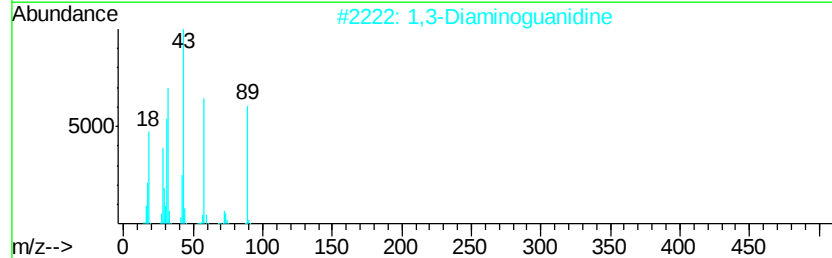
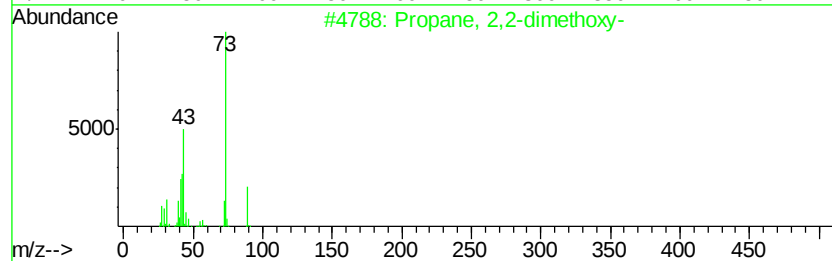
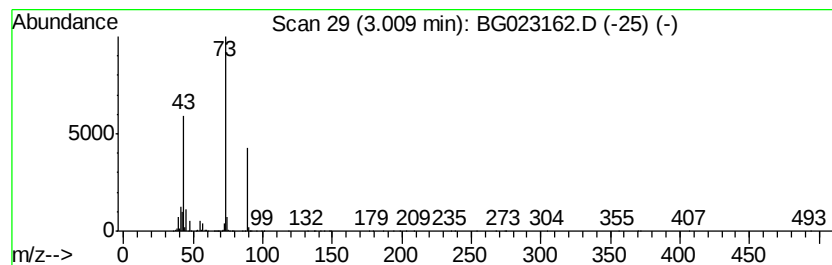
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	169.56 ng	8435200	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Butyric acid, 2-hydroxy-3-methyl...	132	C6H12O3	017417-00-4	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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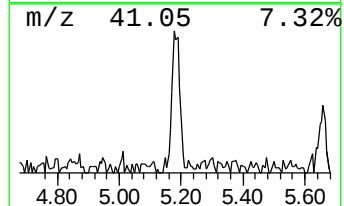
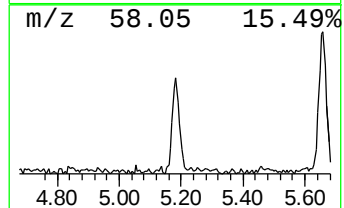
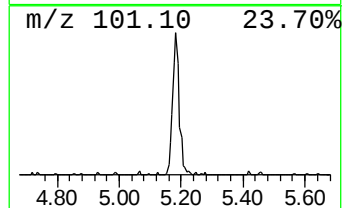
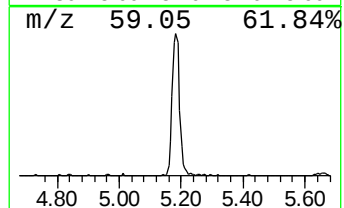
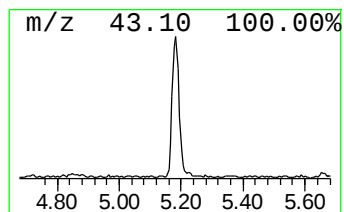
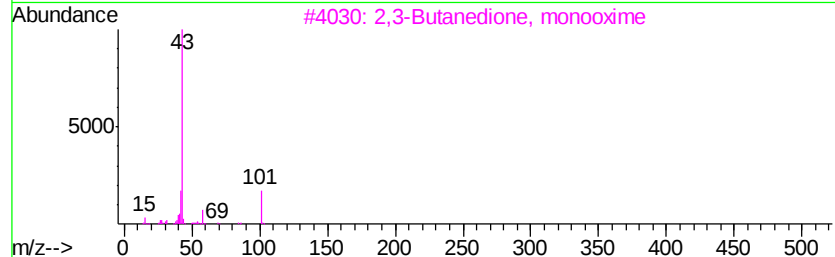
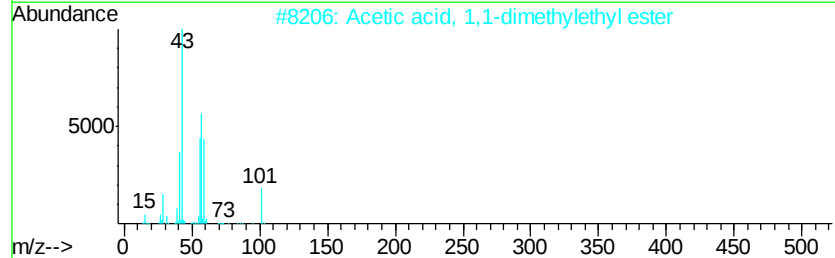
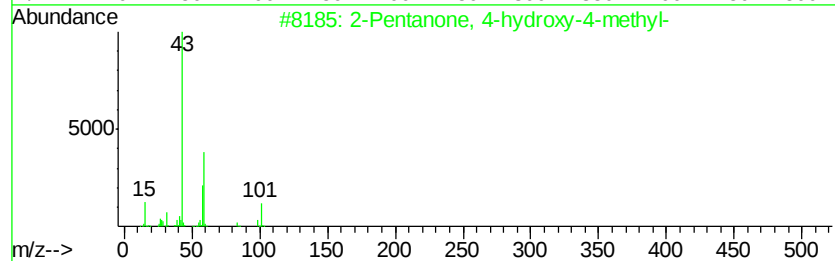
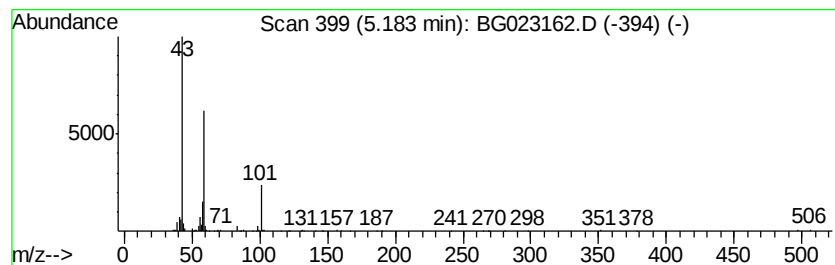
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.18 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	5.28 ng	262744	1,4-Dichlorobenzene-d4	8.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
4	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	17		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12		



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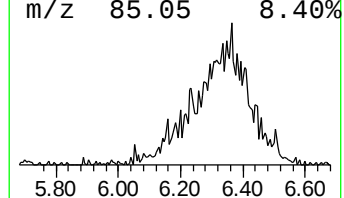
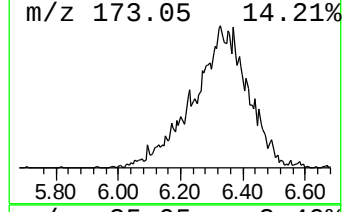
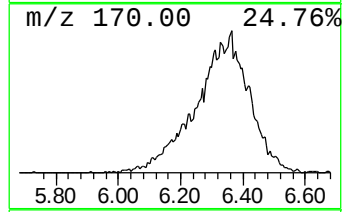
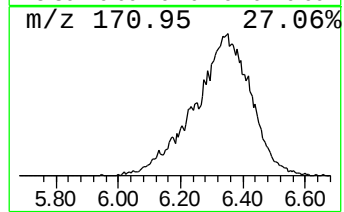
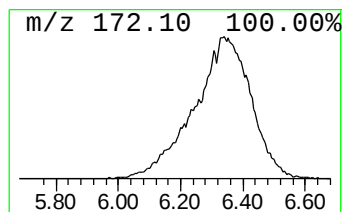
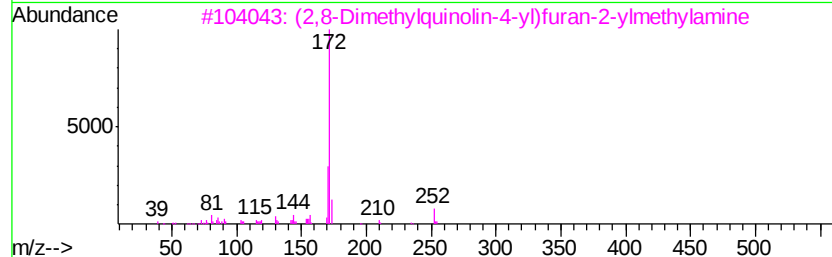
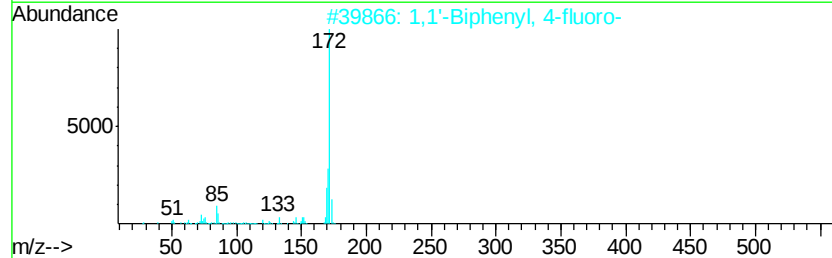
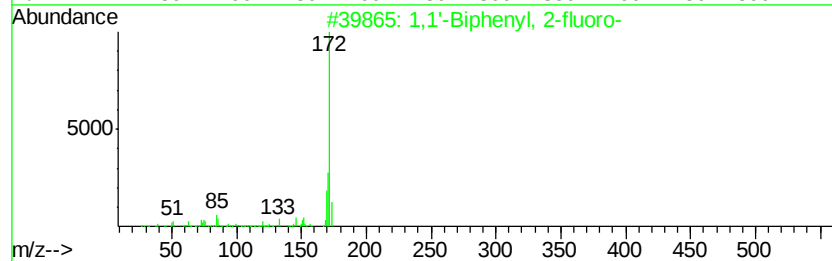
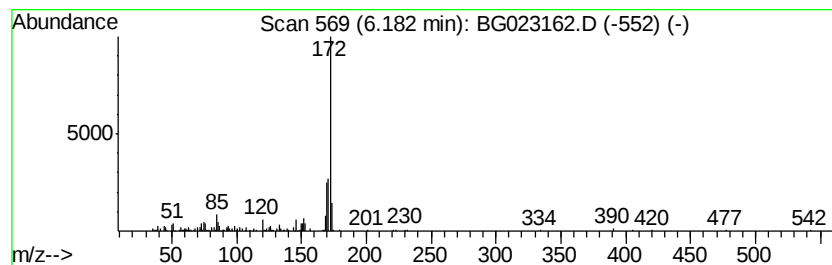
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1'-Biphenyl, 2-fluoro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.18	7.11 ng	353584	1,4-Dichlorobenzene-d4	8.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	000321-60-8	76
2	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	000324-74-3	76
3	(2,8-Dimethylquinolin-4-yl)furan...	252	C16H16N2O	1000322-13-0	59
4	4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	45
5	1-Naphthalenecarboxylic acid	172	C11H8O2	000086-55-5	40



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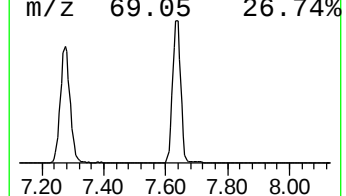
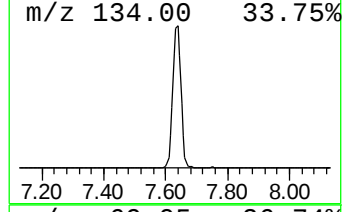
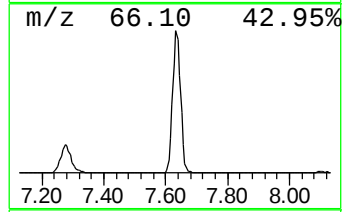
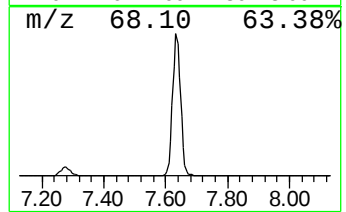
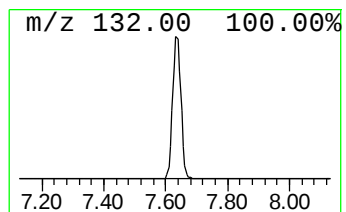
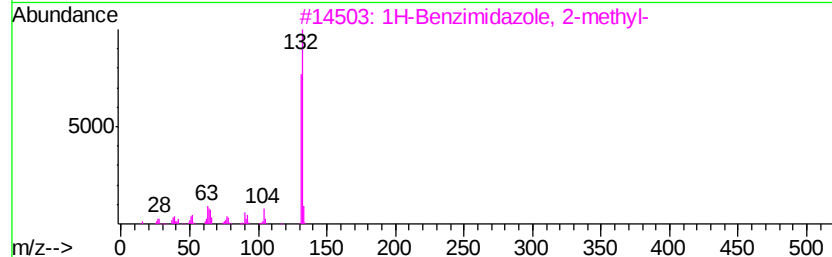
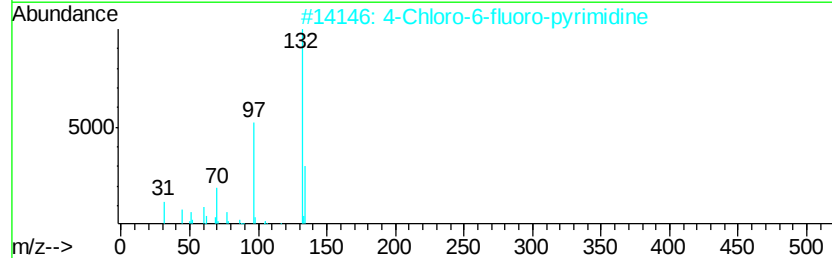
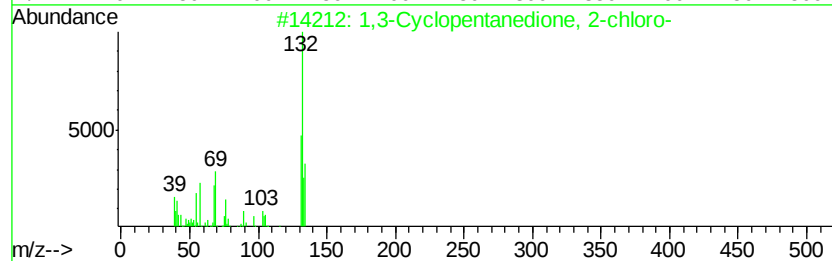
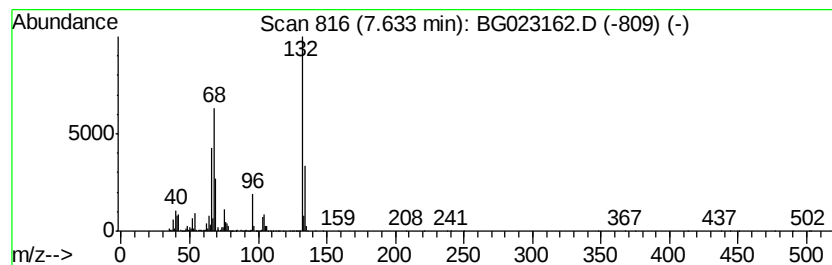
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown7.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	94.89 ng	4720480	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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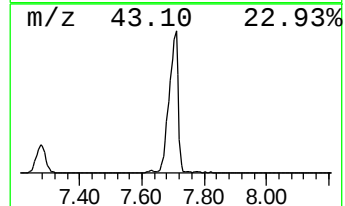
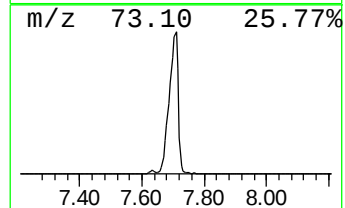
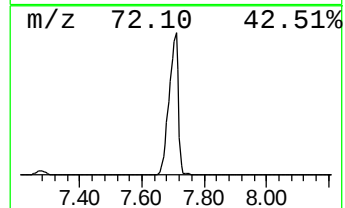
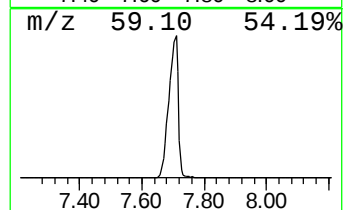
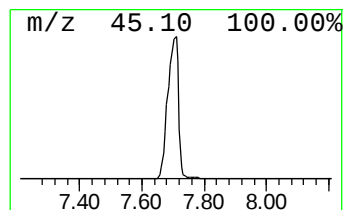
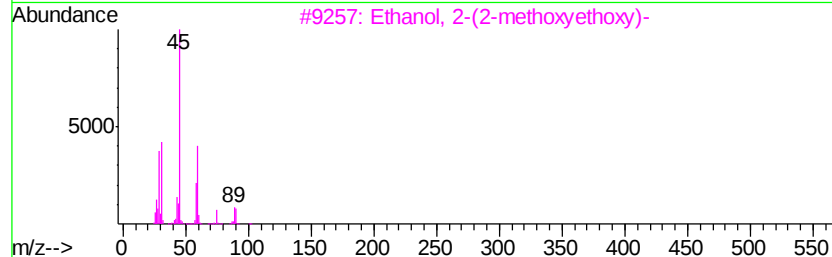
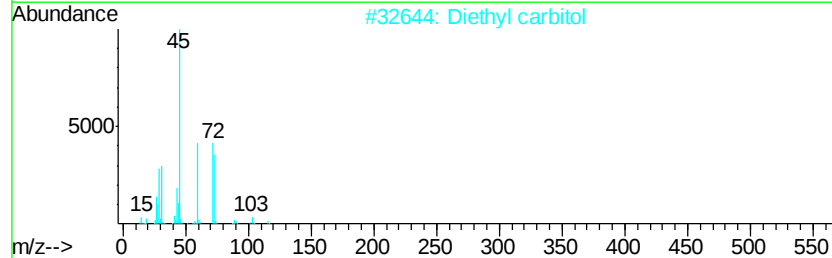
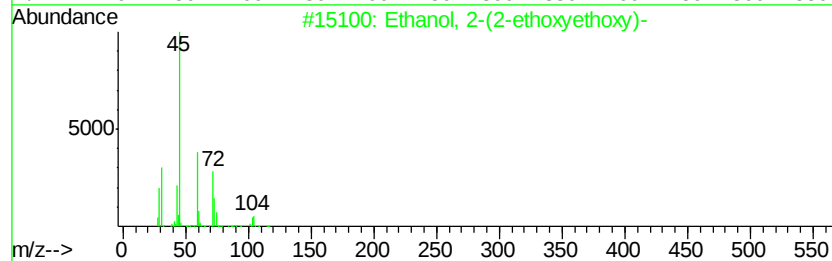
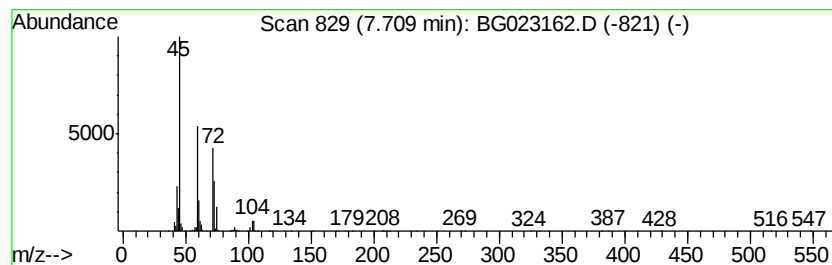
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	240.81 ng	11980200	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2		Diethyl carbitol	162	C8H18O3	000112-36-7	56
3		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	47
4		Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	47
5		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023162.D
Acq On : 18 Jul 2016 17:14
Operator : UM/SJ
Sample : H4044-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B1(6-12)C

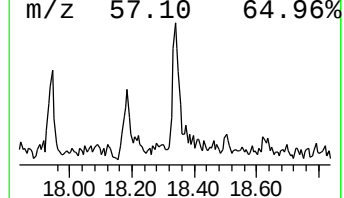
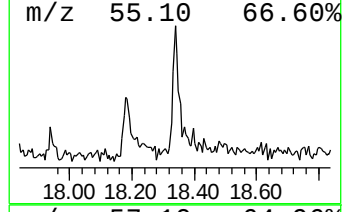
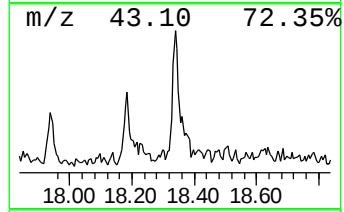
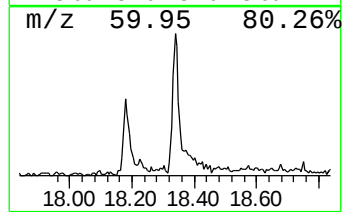
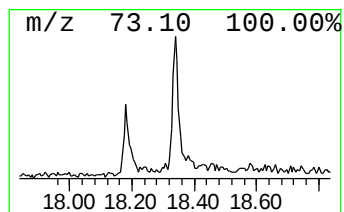
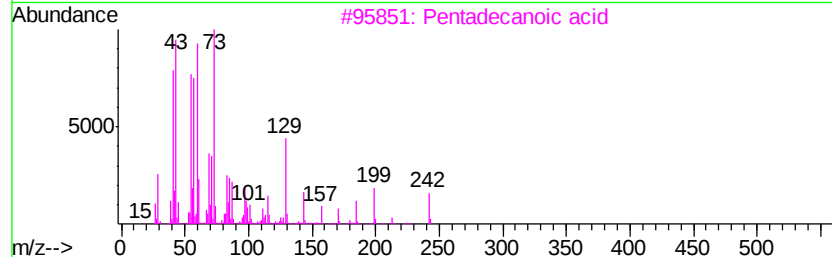
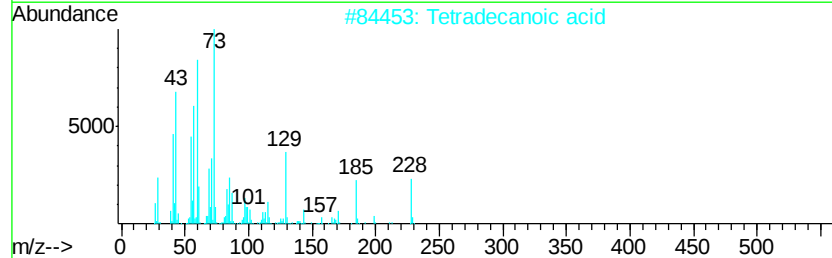
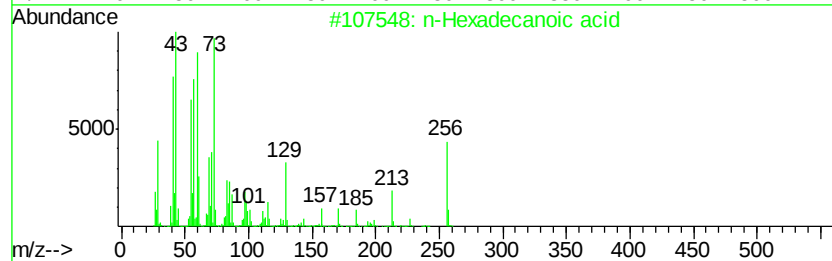
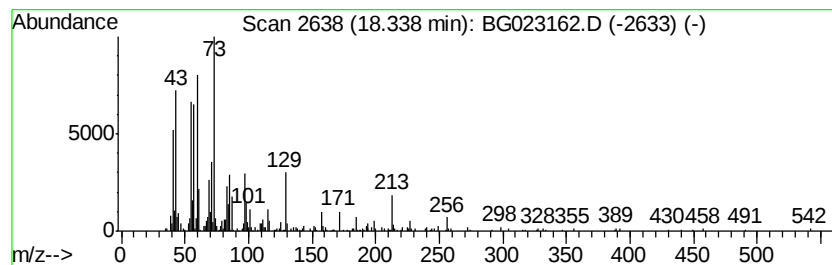
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	2.86 ng	381678	Phenanthrene-d10	17.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Octadecanoic acid	284	C18H36O2	000057-11-4	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023162.D
Acq On : 18 Jul 2016 17:14
Operator : UM/SJ
Sample : H4044-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

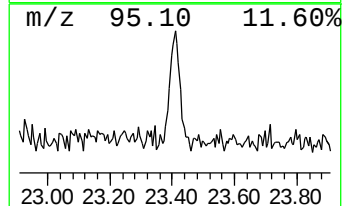
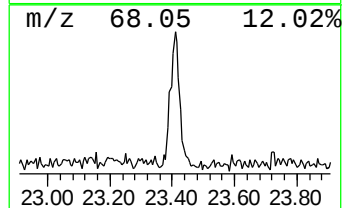
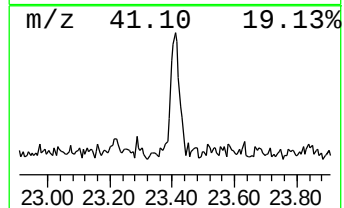
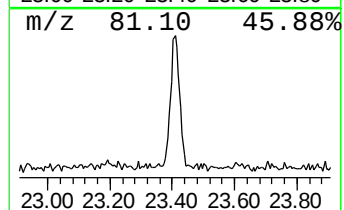
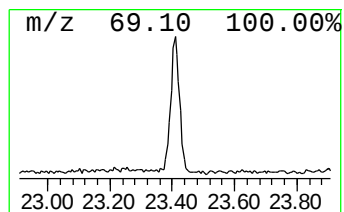
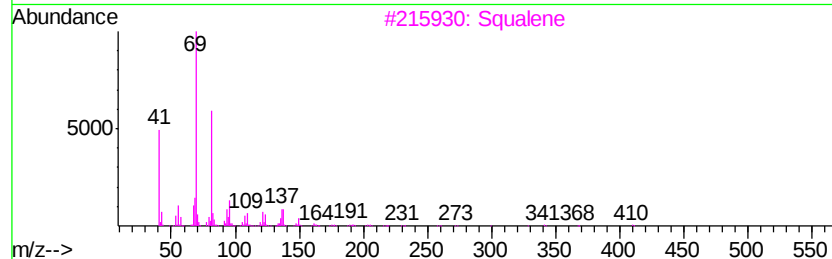
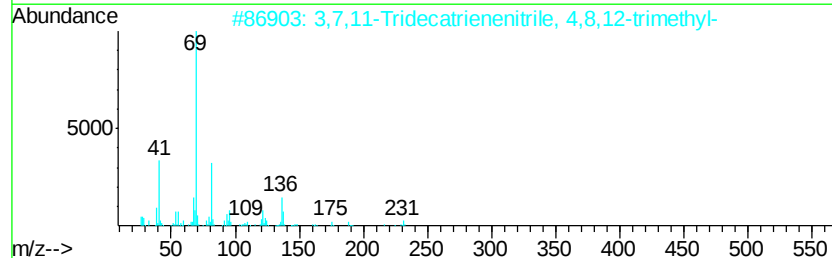
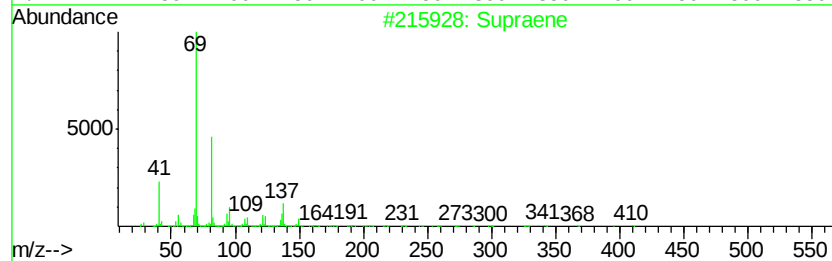
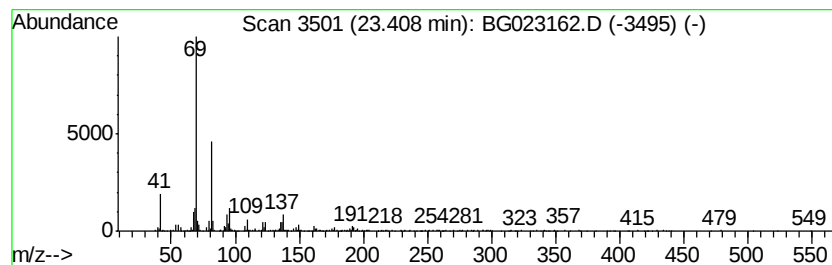
Instrument :
BNA_G
ClientSampleId :
H10-B1(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Supraene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.41	2.48 ng	619696	Perylene-d12	25.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene		410 C30H50	007683-64-9 72
2	3,7,11-Tridecatrienitrile, 4,8...		231 C16H25N	006006-01-5 64
3	Squalene		410 C30H50	000111-02-4 64
4	(E)-2-Butenoic acid, 2-(methylen...		180 C11H16O2	1000158-24-3 64
5	2,6-Octadiene, 4-methyl-		124 C9H16	074498-94-5 59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
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Operator : UM/SJ
Sample : H4044-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H10-B1(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
unknown3.01	3.01	169.6	ng	8435200	1	8.10	994973	20.0
unknown5.18	5.18	5.3	ng	262744	1	8.10	994973	20.0
1,1'-Biphenyl, 2-...	6.18	7.1	ng	353584	1	8.10	994973	20.0
unknown7.63	7.63	94.9	ng	4720480	1	8.10	994973	20.0
Ethanol, 2-(2-eth...	7.71	240.8	ng	11980200	1	8.10	994973	20.0
n-Hexadecanoic acid	18.34	2.9	ng	381678	4	17.48	2664890	20.0
Supraene	23.41	2.5	ng	619696	6	25.02	4993400	20.0