

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
 Data File : BG023168.D
 Acq On : 18 Jul 2016 21:16
 Operator : UM/SJ
 Sample : H4044-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E9-B2(0-6)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	3.020	27	31	37	rVB	304561	423090	5.74%	0.732%
2	3.161	50	55	64	rBV2	202615	409472	5.56%	0.708%
3	4.272	238	244	247	rBV3	40922	77387	1.05%	0.134%
4	5.194	395	401	409	rBV	170295	292959	3.98%	0.507%
5	5.664	475	481	494	rBV	1839381	3163384	42.93%	5.473%
6	7.268	745	754	768	rBV	2112162	3871509	52.54%	6.698%
7	7.644	808	818	828	rBV	2080150	3773468	51.21%	6.529%
8	8.108	890	897	905	rBV	583490	1003322	13.62%	1.736%
9	8.437	942	953	961	rBV	1623536	2932189	39.80%	5.073%
10	9.278	1087	1096	1107	rBV	1483507	2756298	37.41%	4.769%
11	10.935	1370	1378	1386	rBV	814790	1499272	20.35%	2.594%
12	13.367	1783	1792	1801	rBV	3837555	6007371	81.53%	10.394%
13	14.190	1925	1932	1937	rBV	538558	825838	11.21%	1.429%
14	14.748	2018	2027	2033	rBV2	1255075	2092278	28.40%	3.620%
15	15.559	2161	2165	2171	rVB2	78358	115779	1.57%	0.200%
16	16.228	2272	2279	2290	rBV	2537930	4030345	54.70%	6.973%
17	16.416	2306	2311	2323	rBV2	100213	208885	2.83%	0.361%
18	17.210	2441	2446	2449	rBV2	105223	139590	1.89%	0.242%
19	17.486	2486	2493	2497	rBV	1494785	2328067	31.60%	4.028%
20	17.527	2497	2500	2507	rVB	337335	493971	6.70%	0.855%
21	17.615	2512	2515	2520	rVB	54816	79779	1.08%	0.138%
22	18.344	2635	2639	2644	rBV3	122727	202472	2.75%	0.350%
23	18.402	2646	2649	2655	rVB3	79494	139470	1.89%	0.241%
24	18.549	2669	2674	2678	rBV2	78750	152392	2.07%	0.264%
25	19.254	2790	2794	2799	rBV4	71561	123412	1.67%	0.214%
26	19.524	2835	2840	2846	rVB	700753	967443	13.13%	1.674%
27	19.848	2892	2895	2897	rBV2	83732	110807	1.50%	0.192%
28	19.883	2897	2901	2909	rVB	636727	888590	12.06%	1.537%
29	20.077	2927	2934	2940	rBV	5169144	7368136	100.00%	12.748%
30	20.353	2978	2981	2983	rBV4	73879	101305	1.37%	0.175%
31	20.470	2997	3001	3005	rBV2	81828	122825	1.67%	0.213%
32	21.363	3149	3153	3160	rBV3	257208	466394	6.33%	0.807%
33	21.604	3191	3194	3200	rVB	240539	337912	4.59%	0.585%
34	21.745	3210	3218	3224	rBV2	1483739	3132267	42.51%	5.419%

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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
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35	21.792	3224	3226	3234	rVB	324936	493988	6.70%	0.855%
36	23.579	3524	3530	3540	rVB2	871478	1707312	23.17%	2.954%
37	24.119	3617	3622	3634	rVB5	184463	571497	7.76%	0.989%
38	25.036	3770	3778	3788	rVB2	616716	1774143	24.08%	3.070%
39	25.529	3856	3862	3872	rVB3	471200	1156381	15.69%	2.001%
40	26.134	3959	3965	3976	rVB3	532702	1456745	19.77%	2.520%

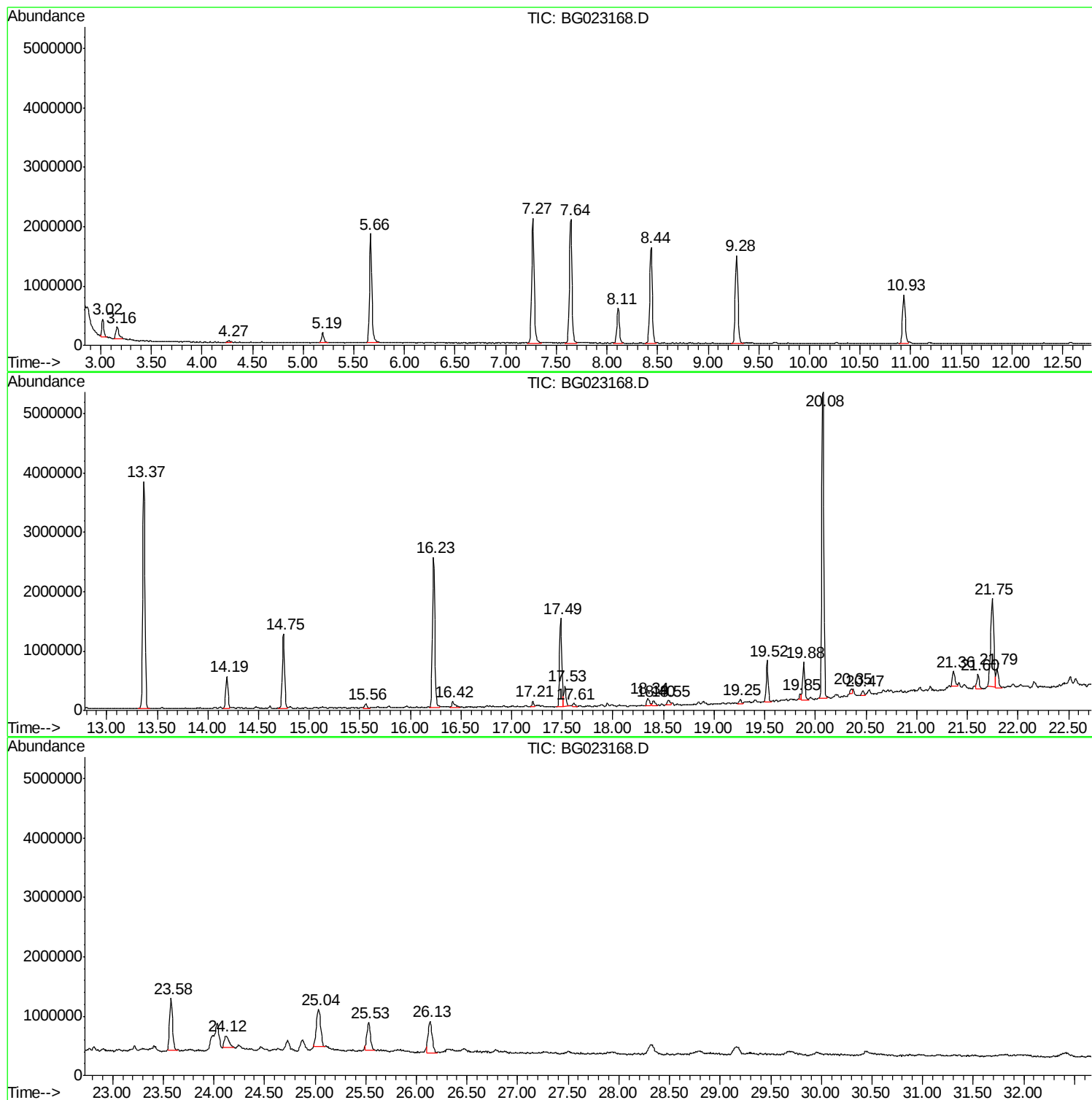
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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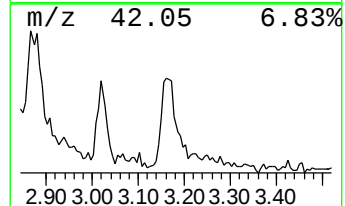
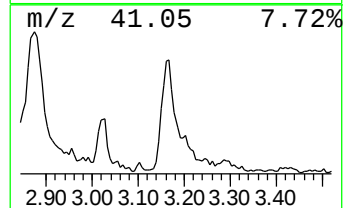
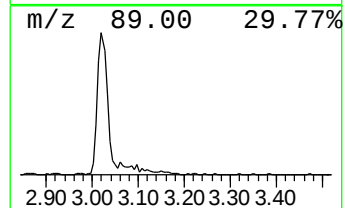
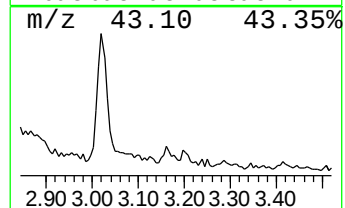
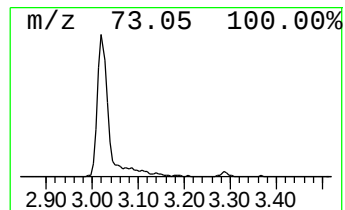
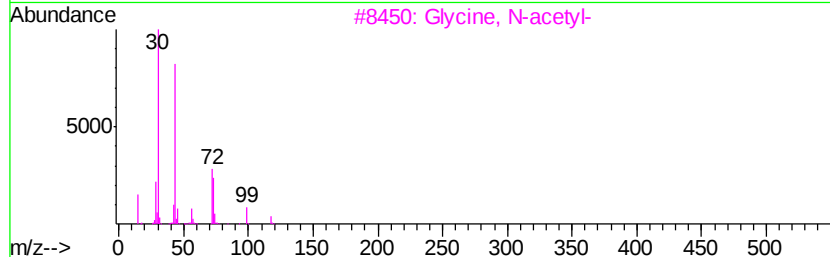
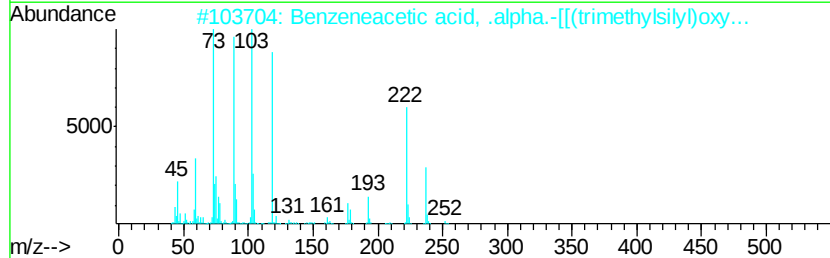
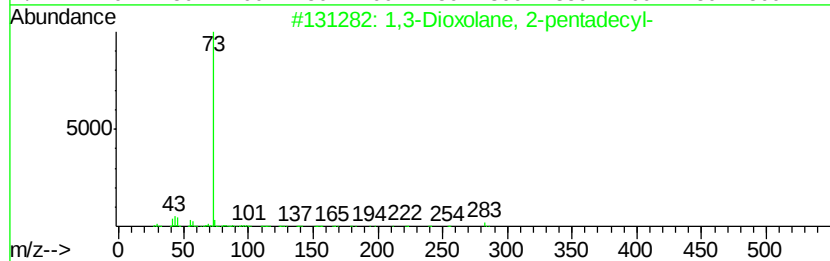
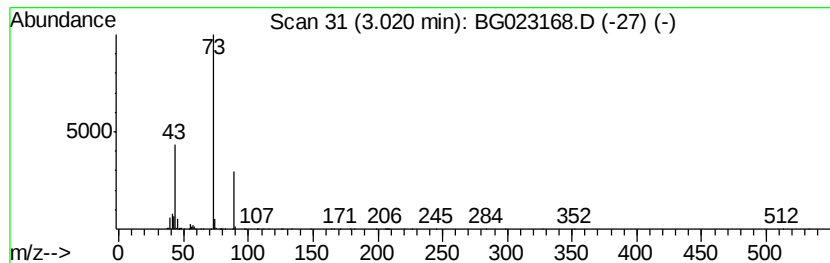
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	8.43 ng	423090	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	32
2		Benzeneacetic acid, .alpha.-[[(t...	252	C13H20O3Si	057397-46-3	9
3		Glycine, N-acetyl-	117	C4H7NO3	000543-24-8	9
4		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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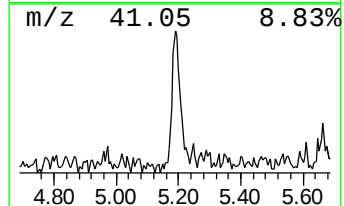
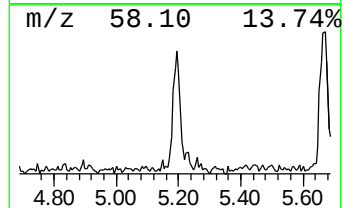
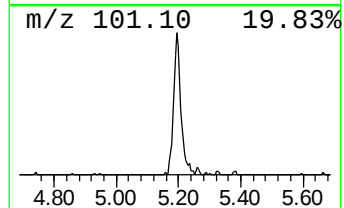
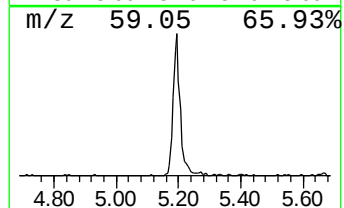
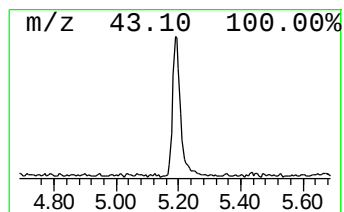
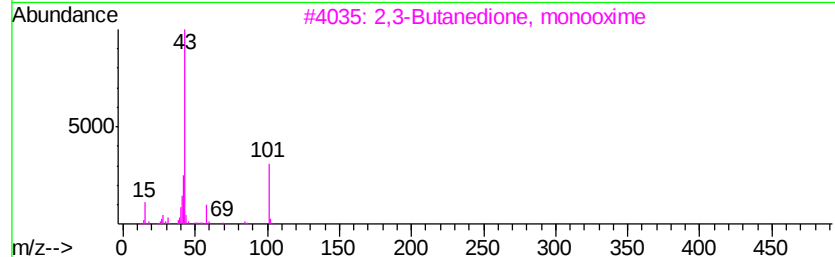
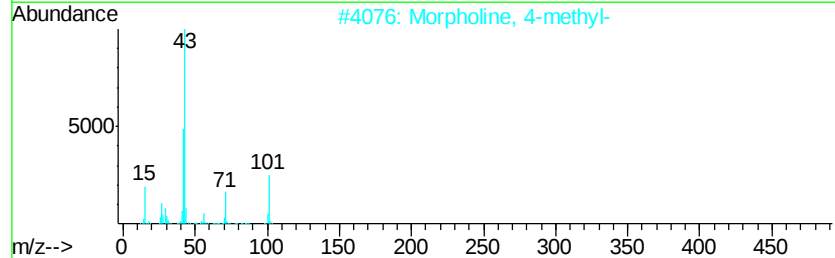
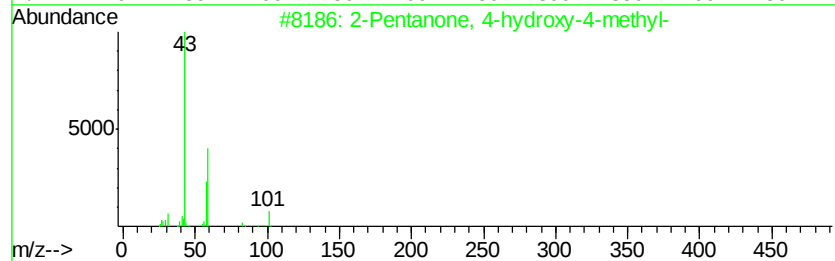
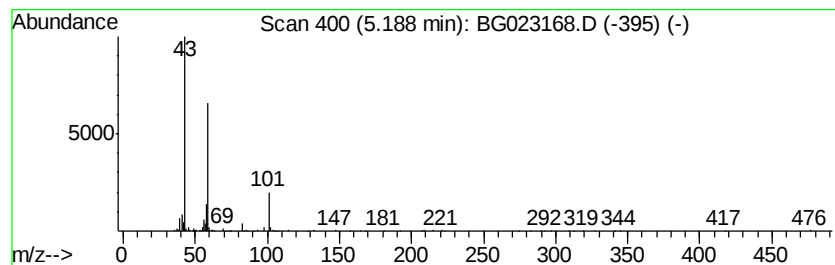
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.84 ng	292959	1,4-Dichlorobenzene-d4	8.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Guanidine	59	CH5N3	000113-00-8	9
5			3-Octanol	130	C8H18O	000589-98-0	9



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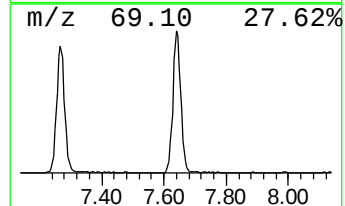
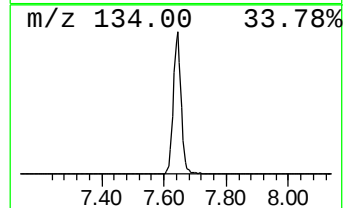
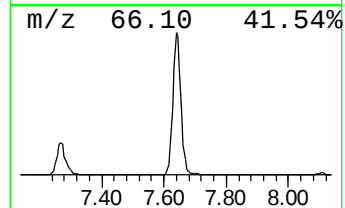
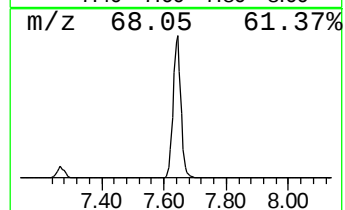
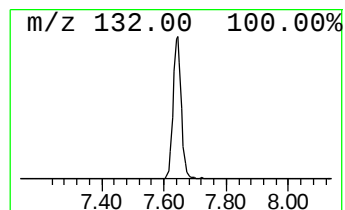
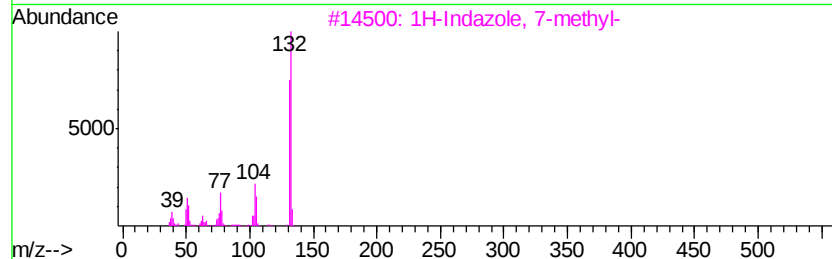
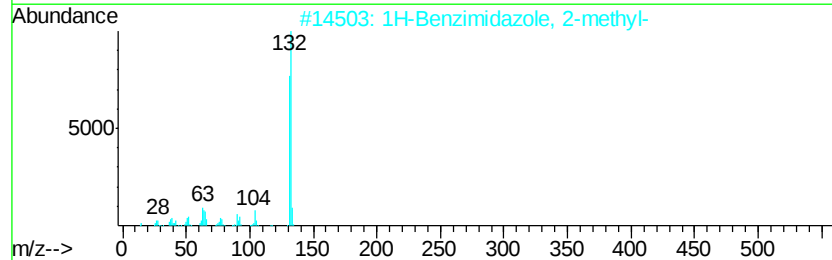
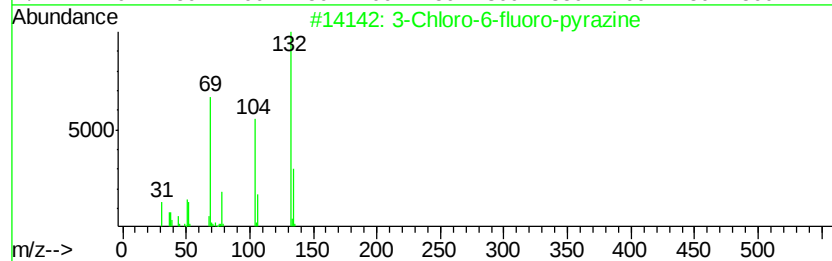
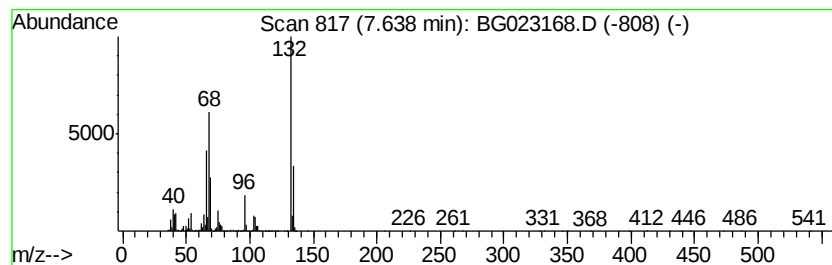
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	75.22 ng	3773470	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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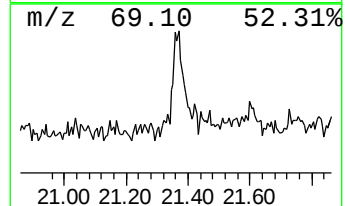
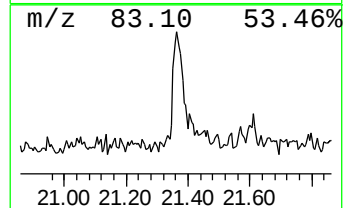
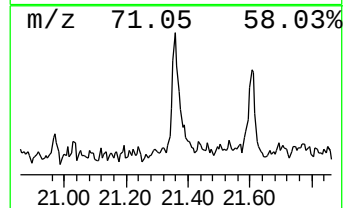
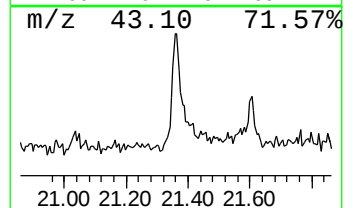
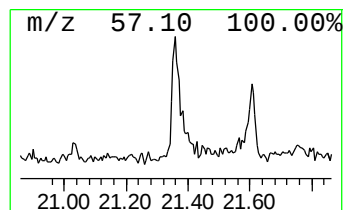
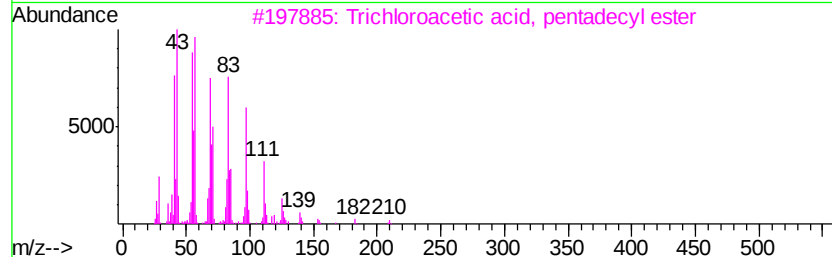
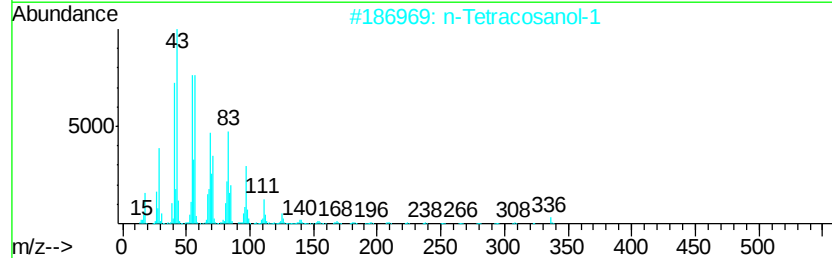
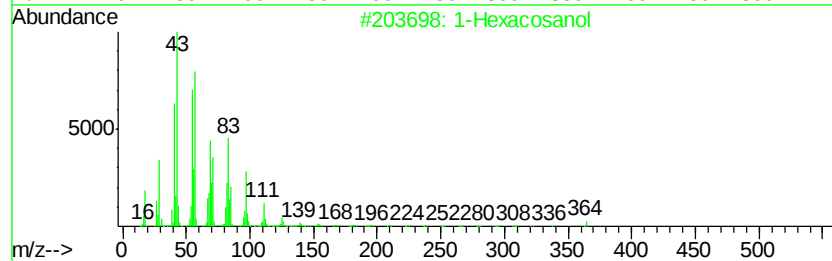
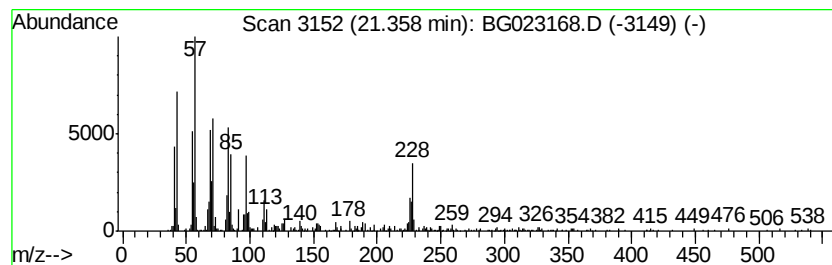
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Peak Number 6 1-Hexacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.36	2.98 ng	466394	Chrysene-d12	21.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	70
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62
4	Octacosanol	410	C28H58O	000557-61-9	58
5	1-Hexadecanol	242	C16H34O	036653-82-4	53



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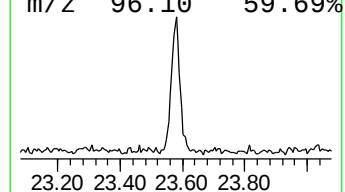
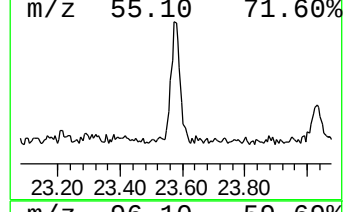
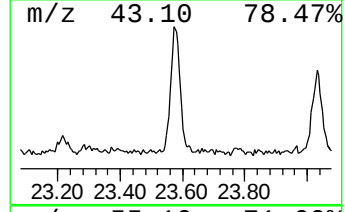
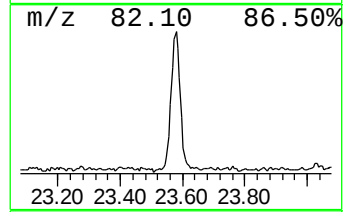
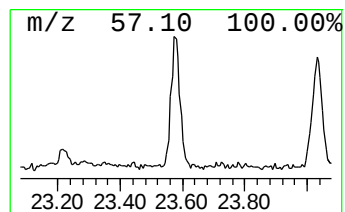
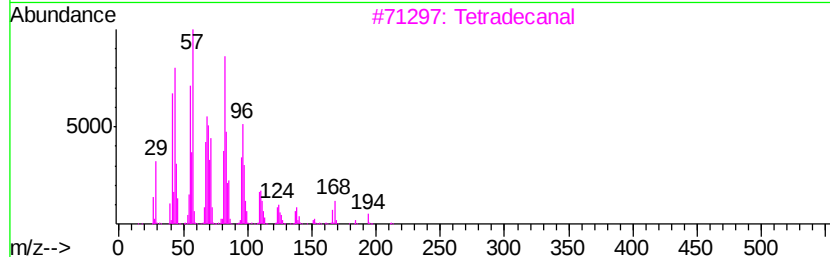
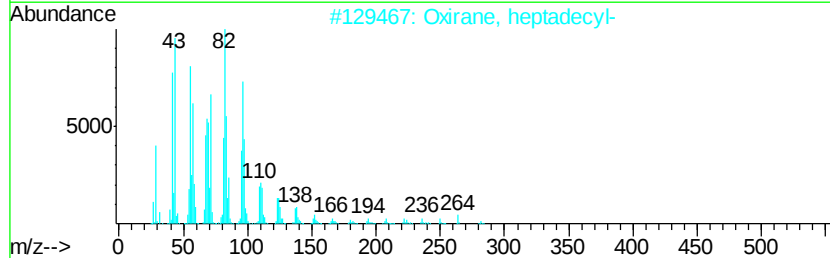
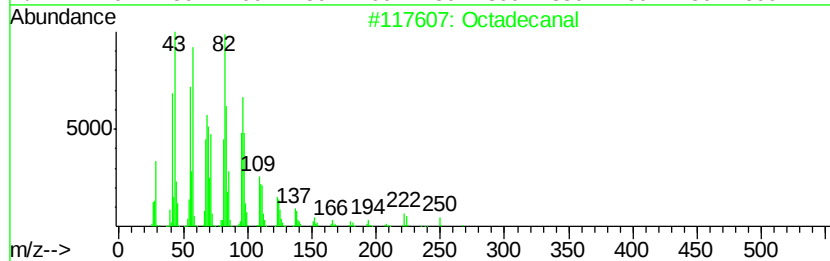
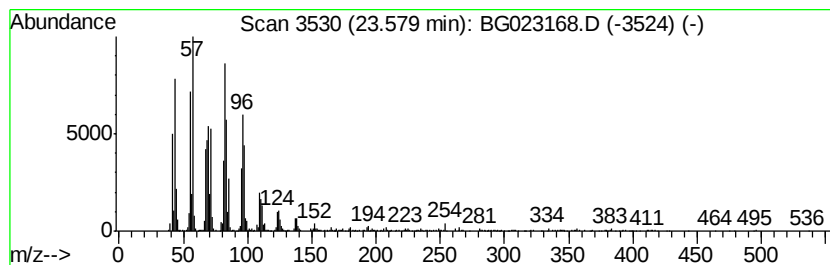
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	19.25 ng	1707310	Perylene-d12	25.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octadecanal	268 C18H36O	000638-66-4 96
2		Oxirane, heptadecyl-	282 C19H38O	067860-04-2 94
3		Tetradecanal	212 C14H28O	000124-25-4 94
4		Oxirane, hexadecyl-	268 C18H36O	007390-81-0 94
5		Oleyl alcohol, methyl ether	282 C19H38O	1000352-68-0 91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023168.D
Acq On : 18 Jul 2016 21:16
Operator : UM/SJ
Sample : H4044-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

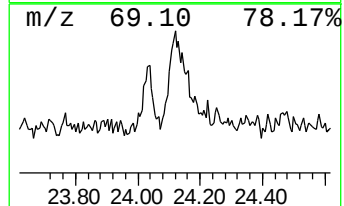
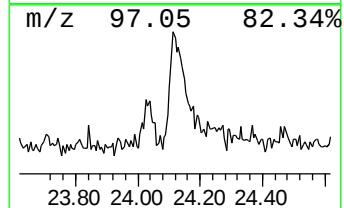
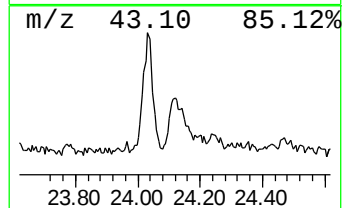
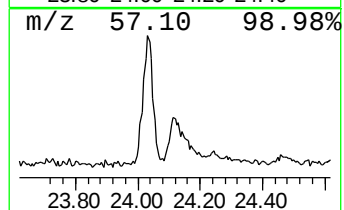
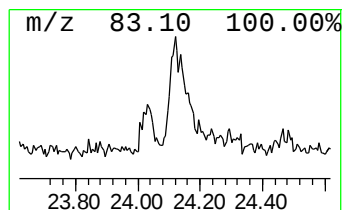
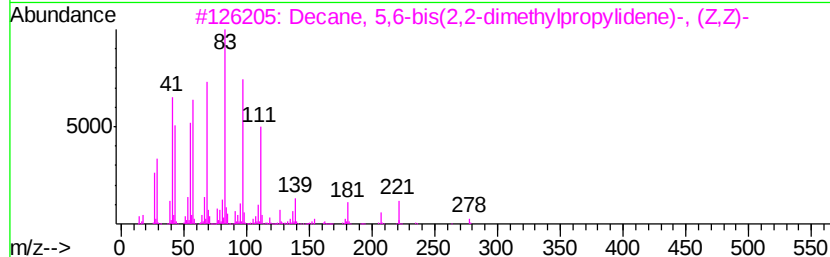
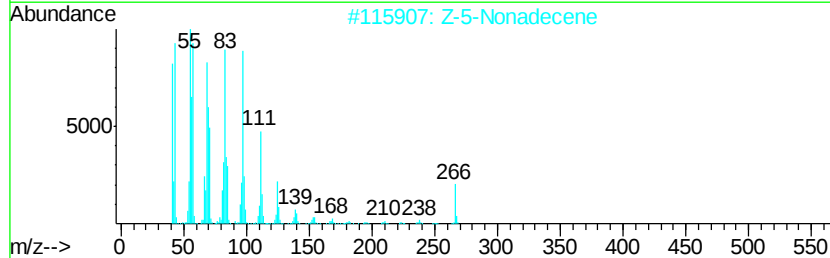
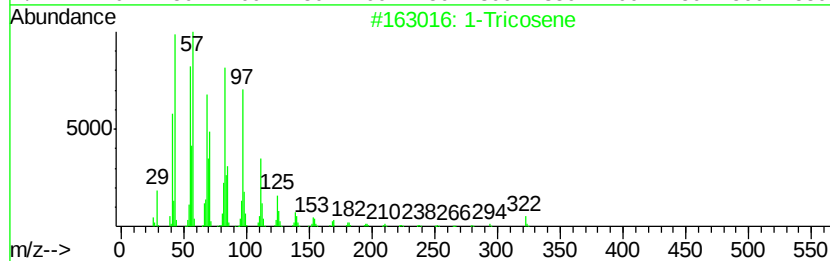
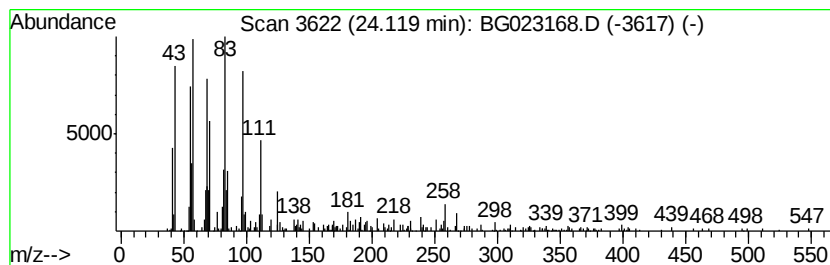
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ClientSampleId :
E9-B2(0-6)C

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 9 1-Tricosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	6.44 ng	571497	Perylene-d12	25.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Tricosene	322 C23H46	018835-32-0	91
2	Z-5-Nonadecene	266 C19H38	1000131-11-8	90
3	Decane, 5,6-bis(2,2-dimethylprop...	278 C20H38	073002-85-4	90
4	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	87
5	1-Docosene	308 C22H44	001599-67-3	83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023168.D
Acq On : 18 Jul 2016 21:16
Operator : UM/SJ
Sample : H4044-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E9-B2(0-6)C

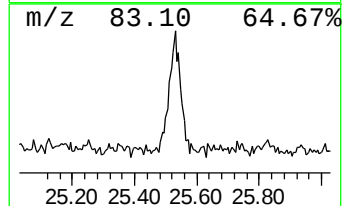
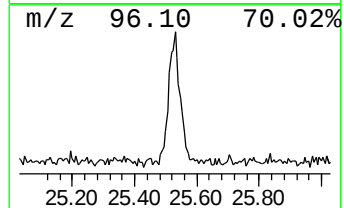
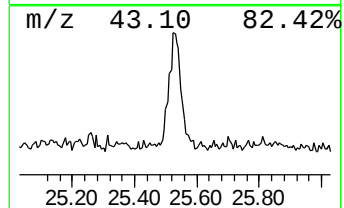
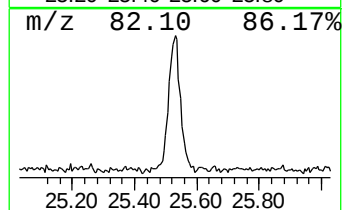
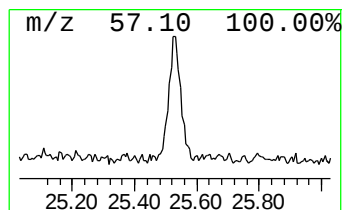
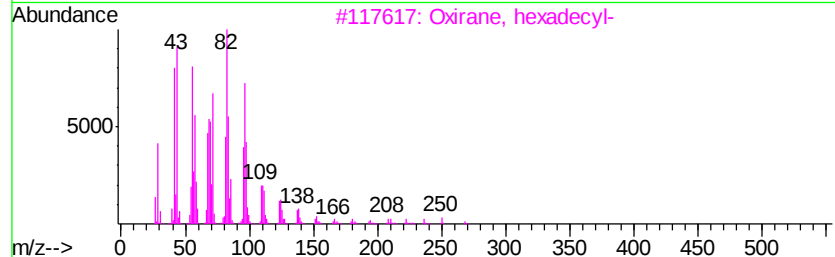
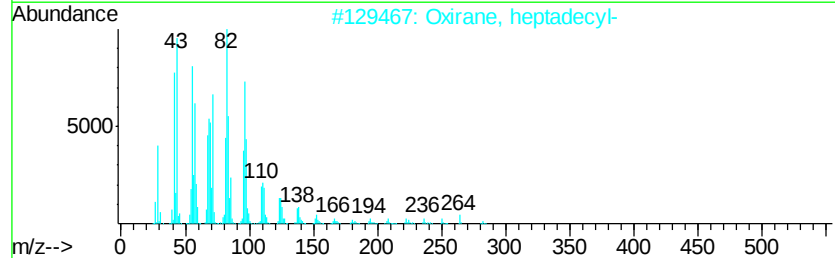
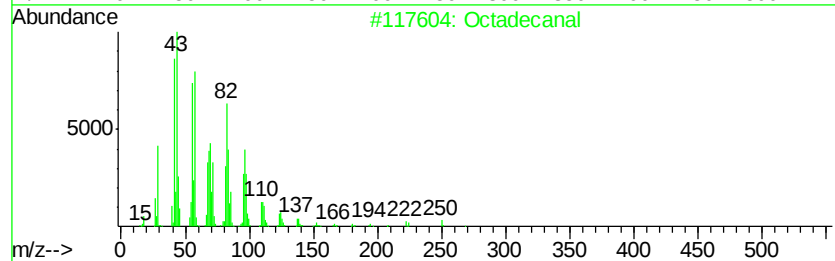
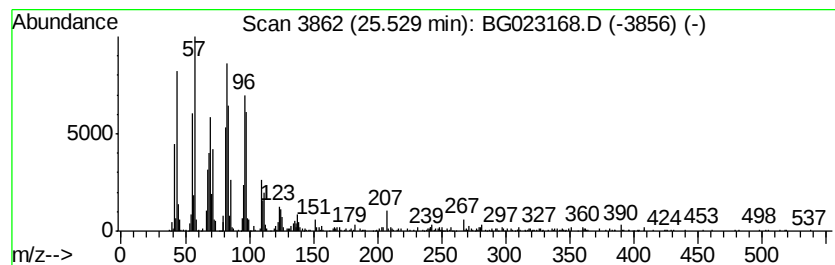
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.53	13.04 ng	1156380	Perylene-d12	25.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	76
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
4		Tetradecanal	212	C14H28O	000124-25-4	70
5		2-Heptadecenal	252	C17H32O	1000143-48-6	62



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023168.D
Acq On : 18 Jul 2016 21:16
Operator : UM/SJ
Sample : H4044-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E9-B2(0-6)C

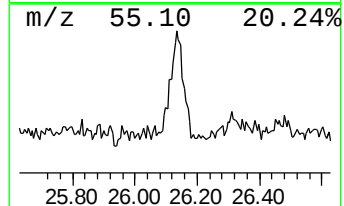
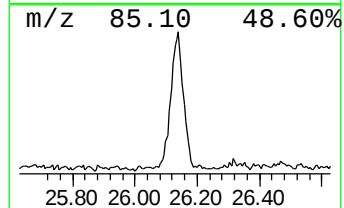
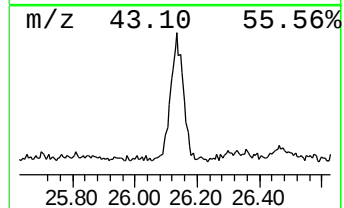
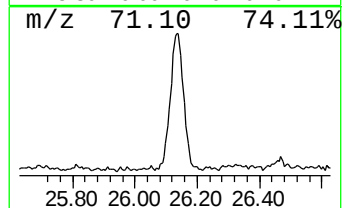
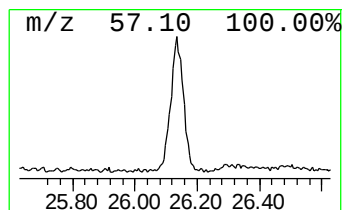
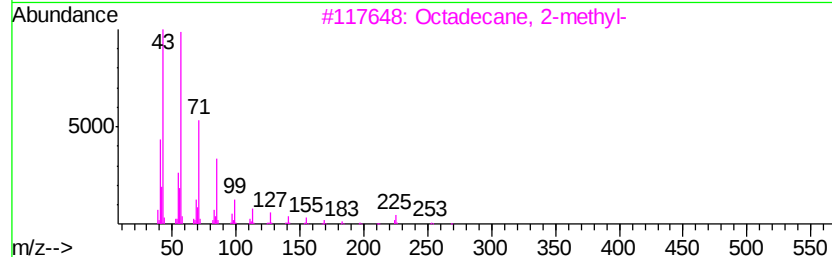
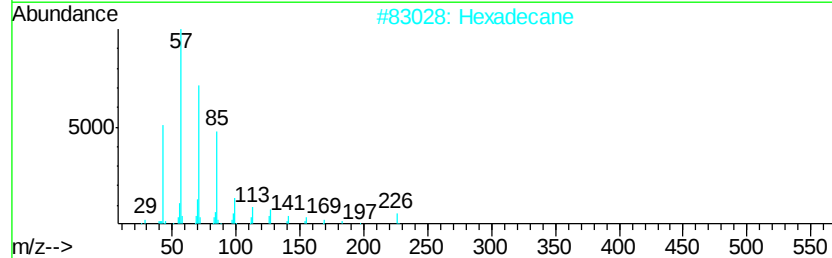
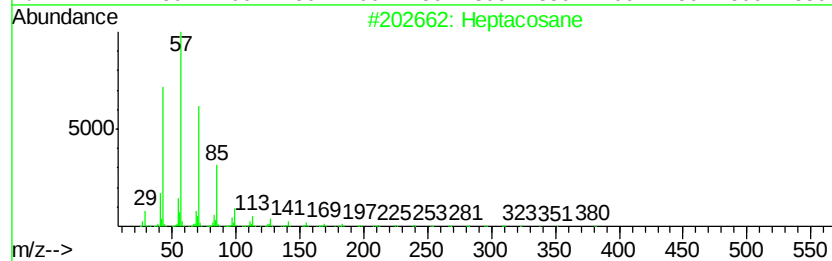
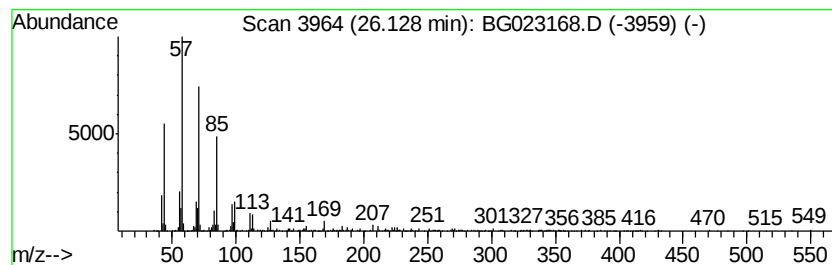
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.13	16.42 ng	1456750	Perylene-d12	25.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	93
2		Hexadecane	226	C16H34	000544-76-3	91
3		Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023168.D
Acq On : 18 Jul 2016 21:16
Operator : UM/SJ
Sample : H4044-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E9-B2(0-6)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
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2-Pentanone, 4-hy...	5.19	5.8	ng	292959	1	8.11	1003320	20.0
unknown7.64	7.64	75.2	ng	3773470	1	8.11	1003320	20.0
1-Hexacosanol	21.36	3.0	ng	466394	5	21.75	3132270	20.0
Oxirane, heptadecyl-	23.58	19.3	ng	1707310	6	25.04	1774140	20.0
1-Tricosene	24.12	6.4	ng	571497	6	25.04	1774140	20.0
Octadecanal	25.53	13.0	ng	1156380	6	25.04	1774140	20.0
Heptacosane	26.13	16.4	ng	1456750	6	25.04	1774140	20.0