

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
 Data File : BG049101.D
 Acq On : 25 Jun 2021 22:07
 Operator : CG/JU
 Sample : M2829-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 15B-DUP-01

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_G\METHODS\8270-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	14	21	30	rBV2	47704	127169	6.48%	0.921%
2	3.238	30	34	40	rVB	18384	31335	1.60%	0.227%
3	5.194	359	367	375	rBV2	16540	34213	1.74%	0.248%
4	5.664	440	447	457	rVB	610160	1030193	52.50%	7.461%
5	7.262	712	719	730	rVB	609128	1086495	55.37%	7.869%
6	8.108	854	863	869	rBV	153040	276944	14.11%	2.006%
7	9.272	1054	1061	1069	rBV	387802	700660	35.70%	5.075%
8	10.688	1295	1302	1311	rBV	320399	535907	27.31%	3.881%
9	10.929	1334	1343	1350	rBV	197514	366585	18.68%	2.655%
10	13.367	1751	1758	1769	rVB	933090	1522366	77.58%	11.026%
11	13.631	1797	1803	1810	rVB2	72770	119047	6.07%	0.862%
12	14.084	1873	1880	1885	rBV7	14832	24076	1.23%	0.174%
13	14.748	1986	1993	2000	rBV2	300979	488393	24.89%	3.537%
14	15.688	2149	2153	2165	rVB3	32002	50451	2.57%	0.365%
15	16.169	2230	2235	2239	rBV5	29906	54130	2.76%	0.392%
16	16.234	2239	2246	2253	rVB	798109	1215023	61.92%	8.800%
17	16.475	2283	2287	2291	rVB2	23939	34776	1.77%	0.252%
18	16.569	2298	2303	2307	rBV	27642	39315	2.00%	0.285%
19	16.622	2307	2312	2318	rVB4	35107	67089	3.42%	0.486%
20	16.687	2319	2323	2327	rBV2	27745	37671	1.92%	0.273%
21	16.734	2327	2331	2335	rVB2	20779	27626	1.41%	0.200%
22	16.892	2352	2358	2363	rVB5	29840	60136	3.06%	0.436%
23	16.951	2363	2368	2372	rBV	24738	37610	1.92%	0.272%
24	17.027	2378	2381	2387	rVB2	17710	23242	1.18%	0.168%
25	17.497	2453	2461	2465	rBV	342977	557225	28.40%	4.036%
26	17.538	2465	2468	2478	rVV	78411	124036	6.32%	0.898%
27	17.627	2478	2483	2489	rVB	18940	32602	1.66%	0.236%
28	18.155	2568	2573	2577	rBV2	40676	55946	2.85%	0.405%
29	18.373	2604	2610	2615	rBV2	123902	188029	9.58%	1.362%
30	18.420	2615	2618	2626	rVB3	31747	53503	2.73%	0.388%
31	18.567	2638	2643	2647	rBV6	26389	52888	2.70%	0.383%
32	18.672	2656	2661	2665	rBV8	16742	32969	1.68%	0.239%
33	18.866	2690	2694	2697	rBV2	14643	21603	1.10%	0.156%
34	18.907	2698	2701	2706	rVB6	14414	19625	1.00%	0.142%
35	19.283	2762	2765	2767	rBV3	29433	36909	1.88%	0.267%
36	19.319	2767	2771	2778	rVB2	108089	141200	7.20%	1.023%

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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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37	19.430	2785	2790	2791	rBV3	18680	30059	1.53%	0.218%
38	19.448	2791	2793	2797	rVB2	41867	45346	2.31%	0.328%
39	19.548	2804	2810	2815	rVB	196127	297835	15.18%	2.157%
40	19.642	2823	2826	2829	rBV5	30709	37199	1.90%	0.269%
41	19.871	2862	2865	2867	rBV	36324	47817	2.44%	0.346%
42	19.906	2867	2871	2879	rVB	278546	418447	21.32%	3.031%
43	20.100	2898	2904	2910	rBV	1498608	1962379	100.00%	14.213%
44	20.729	3009	3011	3015	rVB4	34448	44437	2.26%	0.322%
45	21.410	3122	3127	3131	rBV3	77180	136104	6.94%	0.986%
46	21.781	3183	3190	3196	rBV3	343766	748325	38.13%	5.420%
47	24.049	3572	3576	3584	rBV2	50011	120464	6.14%	0.872%
48	24.225	3602	3606	3614	rVB6	83078	188639	9.61%	1.366%
49	25.112	3750	3757	3769	rVB3	148346	423023	21.56%	3.064%

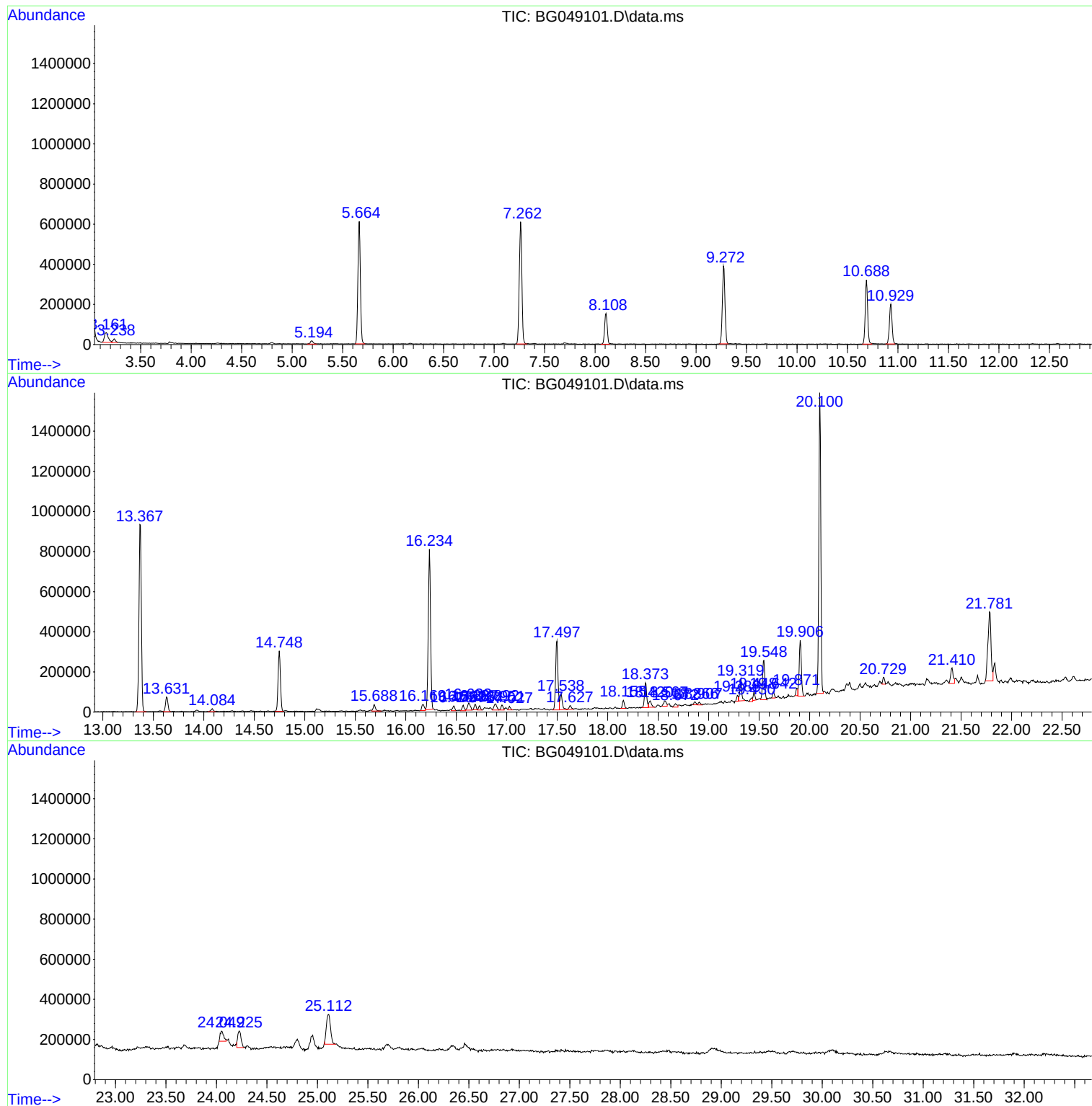
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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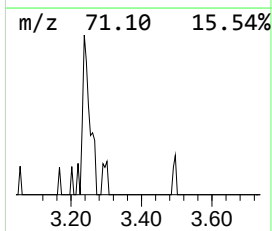
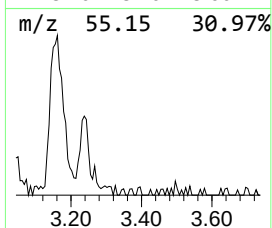
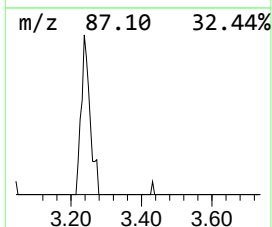
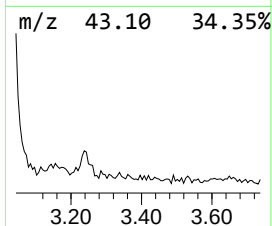
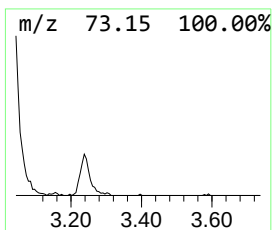
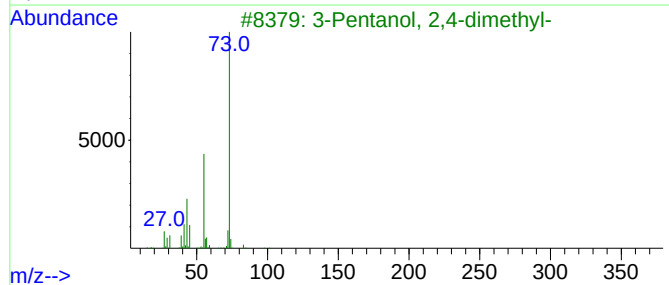
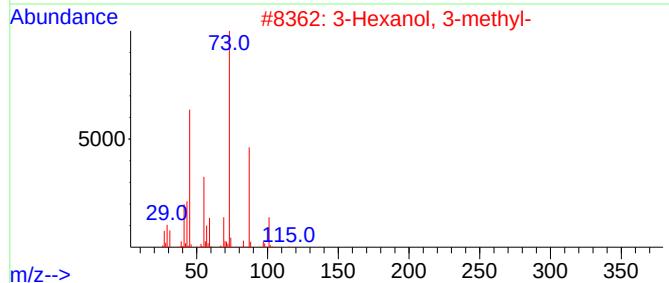
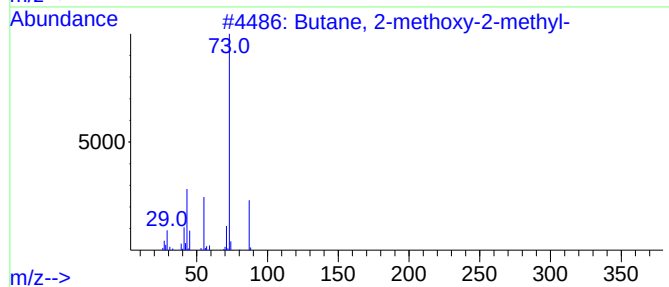
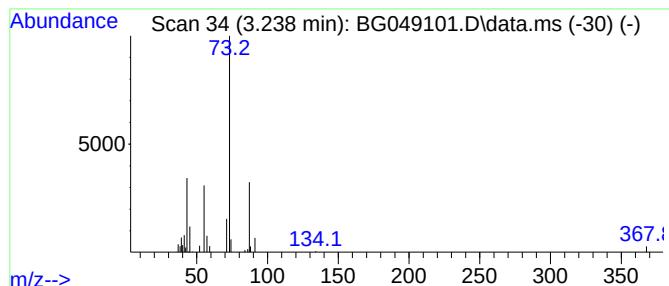
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.238	2.26 ng	31335	1,4-Dichlorobenzene-d4	8.108

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2			3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	12
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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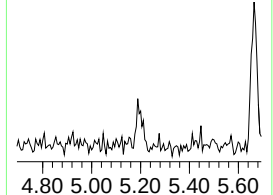
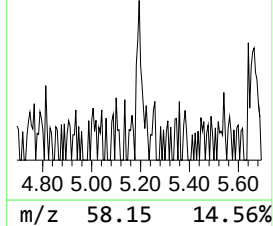
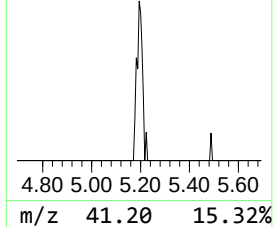
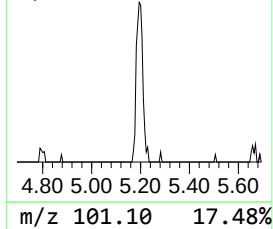
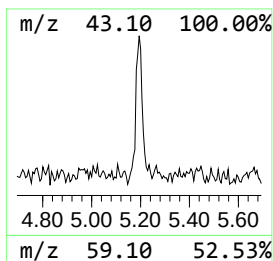
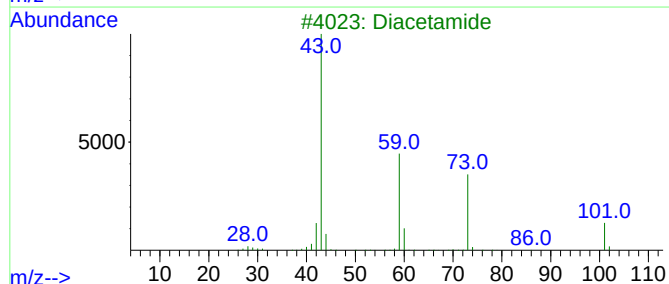
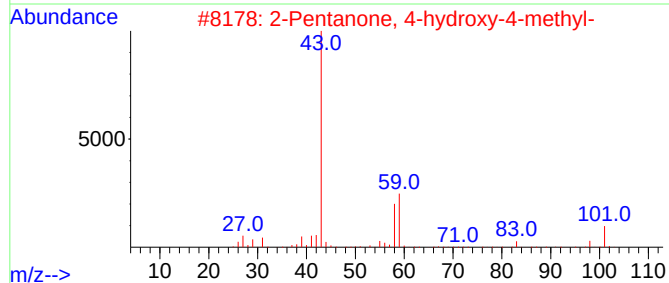
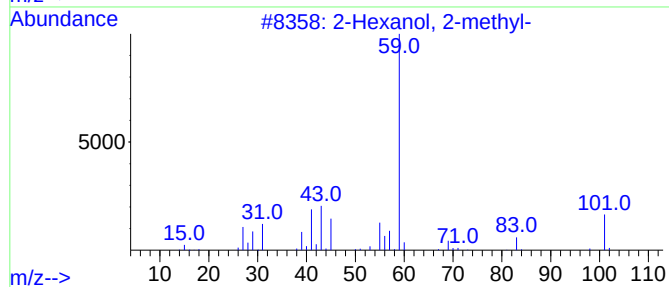
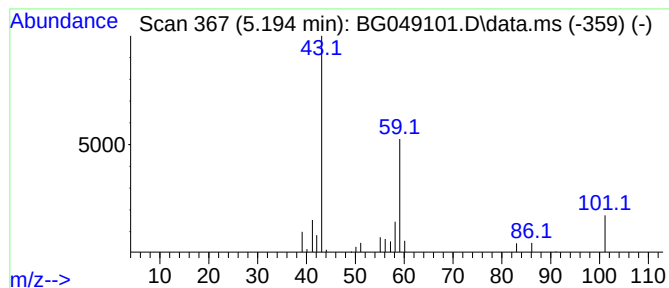
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.194 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	2.47 ng	34213	1,4-Dichlorobenzene-d4	8.108

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-			116	C7H16O	000625-23-0	33
2	2-Pentanone, 4-hydroxy-4-methyl-			116	C6H12O2	000123-42-2	28
3	Diacetamide			101	C4H7NO2	000625-77-4	9
4	Silane, dimethyl-			60	C2H8Si	001111-74-6	9
5	Ethanol, 1-(methylenecyclopropyl)-			98	C6H10O	1000152-74-6	9



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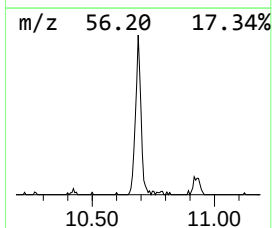
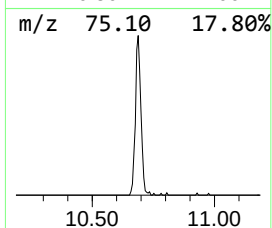
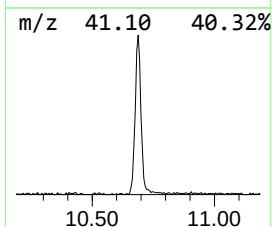
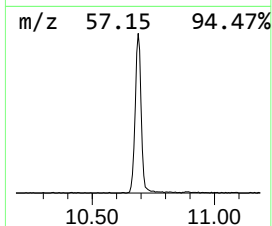
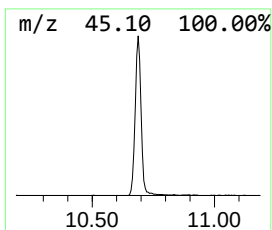
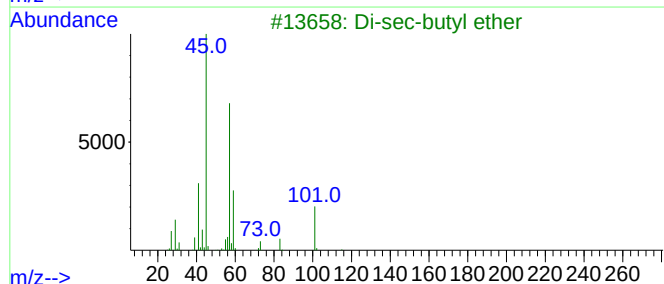
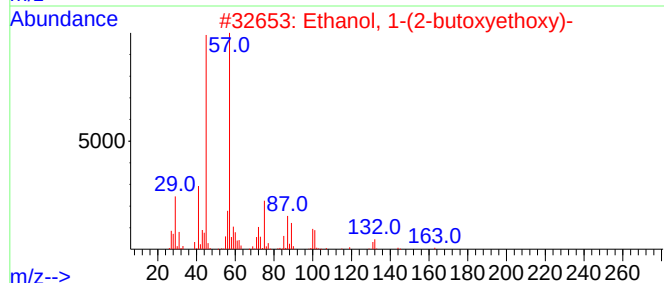
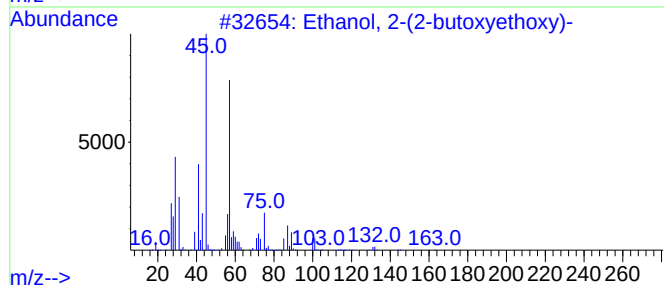
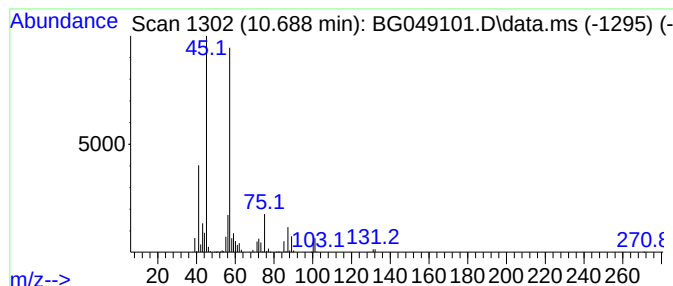
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.688	29.24 ng	535907	Naphthalene-d8	10.929

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Di-sec-butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Propanal, 3-methoxy-	88	C4H8O2	002806-84-0	47



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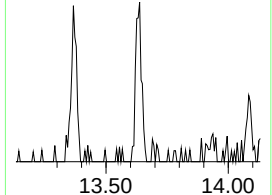
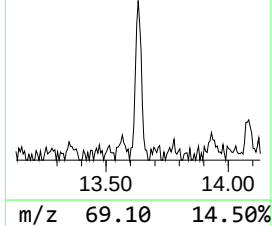
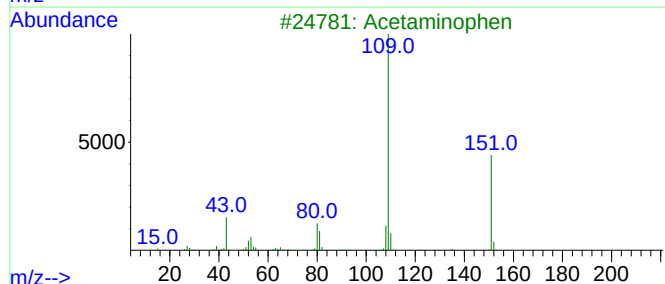
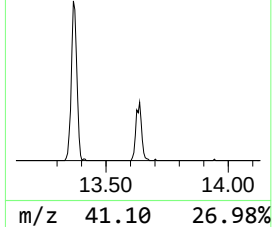
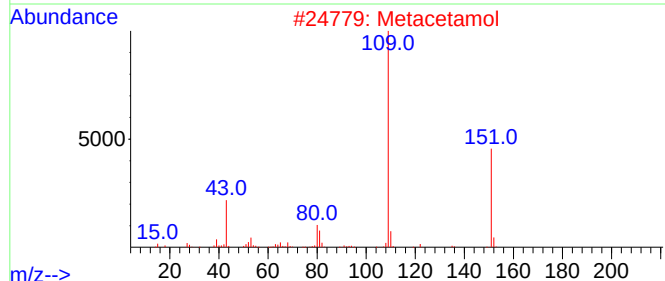
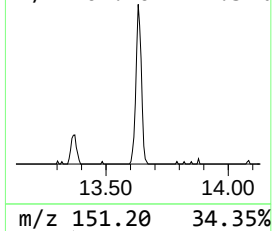
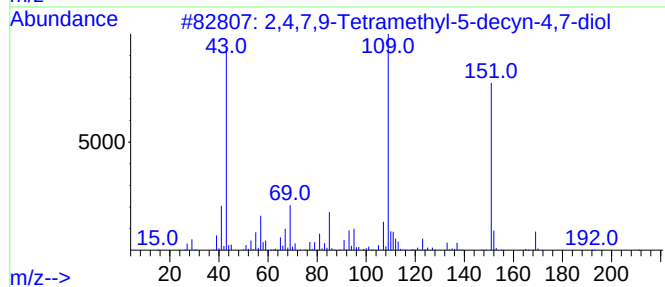
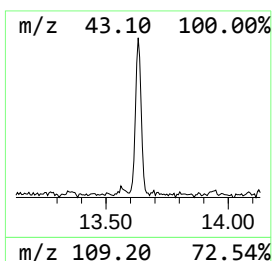
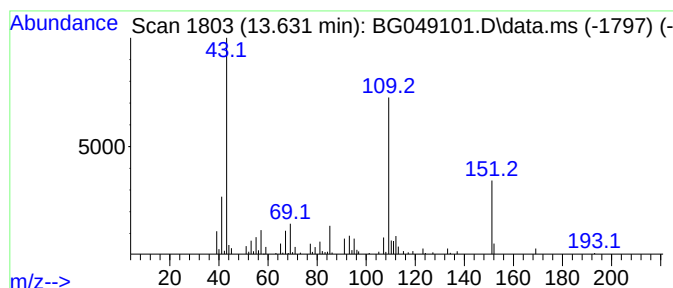
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.631	4.88 ng	119047	Acenaphthene-d10	14.748

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Metacetamol	151	C8H9NO2	000621-42-1	52	
3	Acetaminophen	151	C8H9NO2	000103-90-2	52	
4	Diacetamate	193	C10H11NO3	002623-33-8	50	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50	



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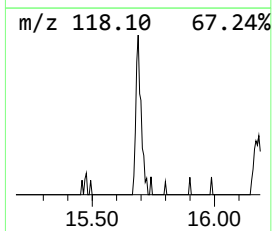
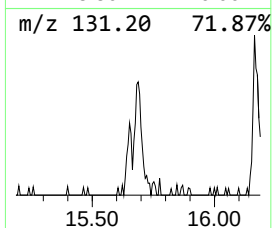
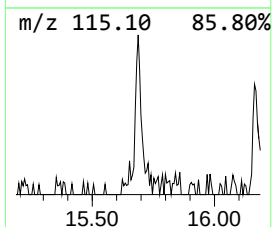
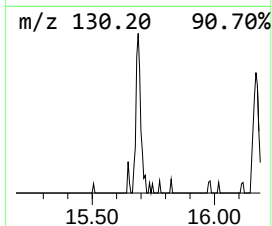
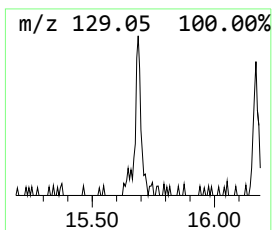
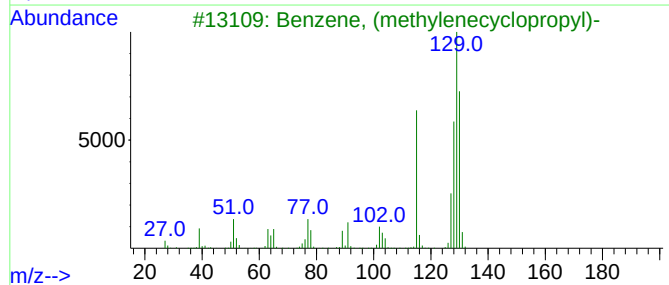
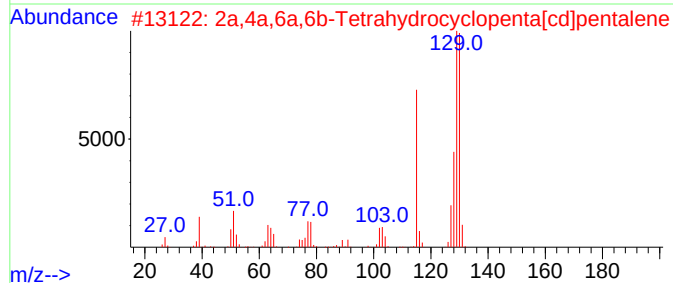
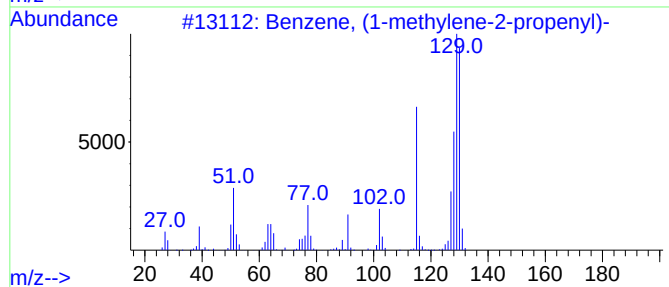
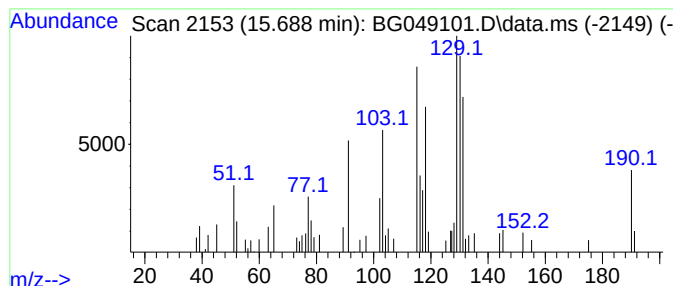
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, (1-methylene-2-pro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.688	2.07 ng	50451	Acenaphthene-d10	14.748

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylene-2-propenyl)-	130	C10H10	002288-18-8	55
2			2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	49
3			Benzene, (methylenecyclopropyl)-	130	C10H10	029817-09-2	46
4			Benzene, (cyclopropylidenemethyl)-	130	C10H10	007555-67-1	46
5			Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
Operator : CG/JU
Sample : M2829-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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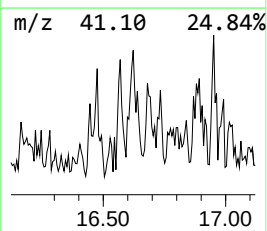
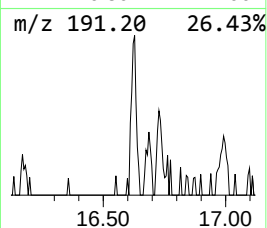
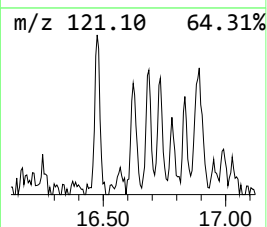
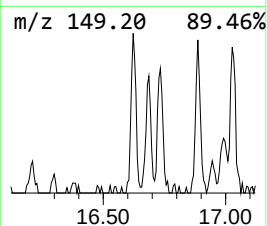
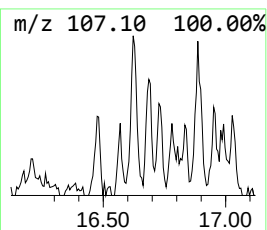
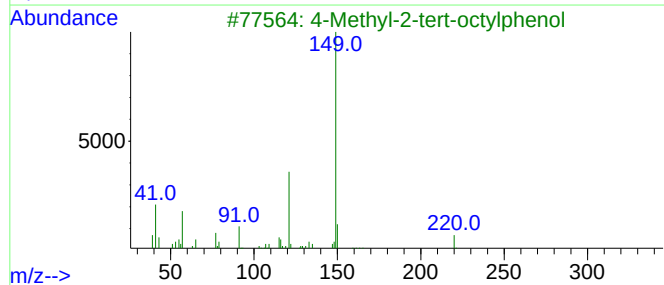
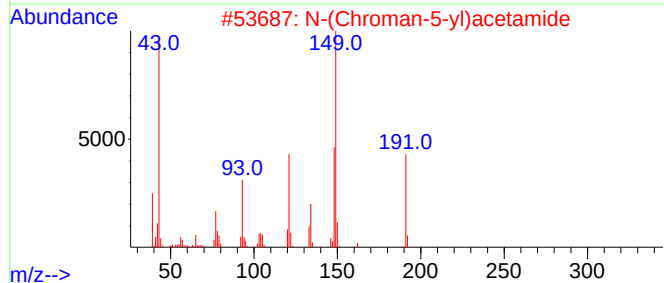
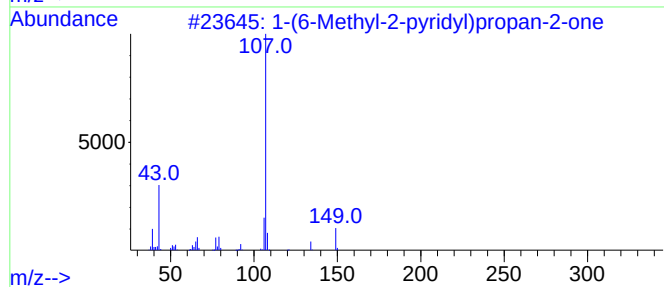
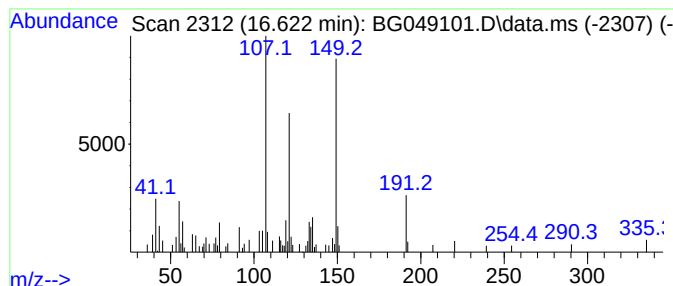
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.622 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.622	2.41 ng	67089	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	47		
2	N-(Chroman-5-yl)acetamide	191	C11H13NO2	1000306-69-8	43		
3	4-Methyl-2-tert-octylphenol	220	C15H24O	004979-46-8	38		
4	N-(Chroman-7-yl)acetamide	191	C11H13NO2	1000306-69-7	38		
5	Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
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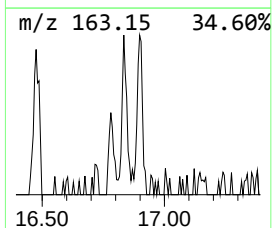
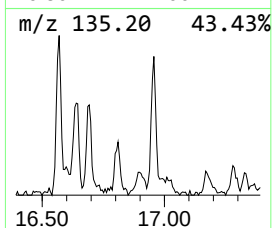
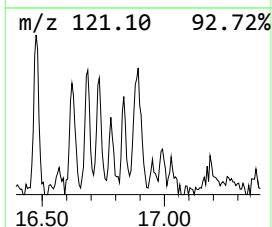
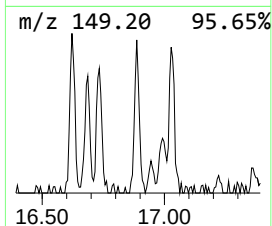
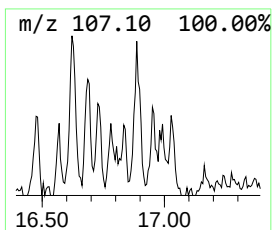
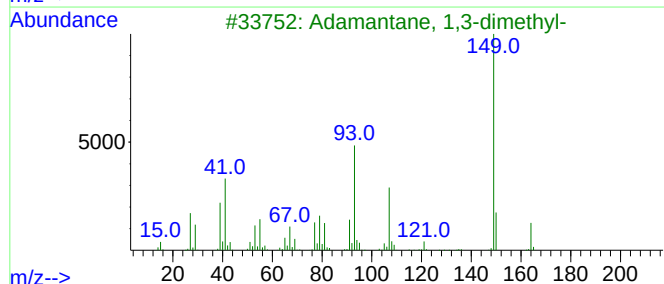
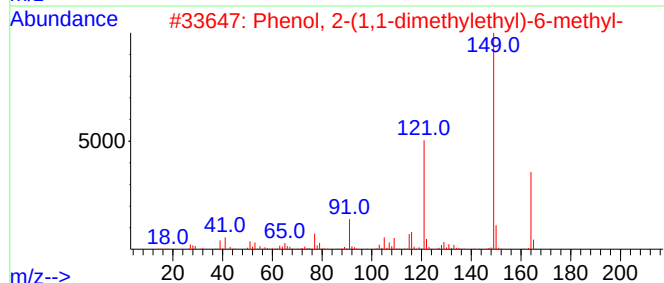
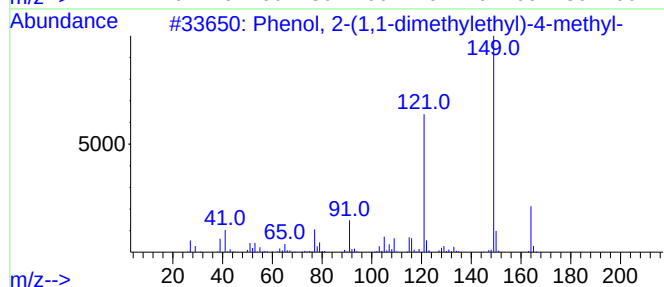
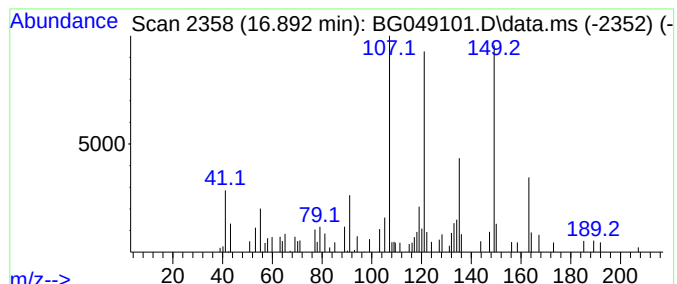
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.892 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	2.16 ng	60136	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	43
2			Phenol, 2-(1,1-dimethylethyl)-6-...	164	C11H16O	002219-82-1	38
3			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	25
4			Benzaldehyde, 3-(4-nitrophenoxy...	287	C15H13NO5	1000273-81-9	14
5			Benzaldehyde, 3-(4-bromophenoxy...	320	C15H13BrO3	351365-97-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
Operator : CG/JU
Sample : M2829-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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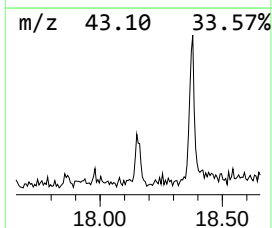
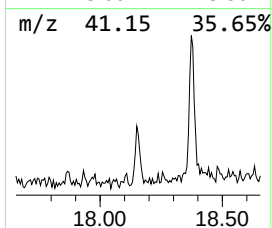
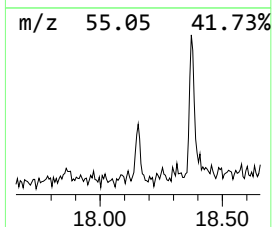
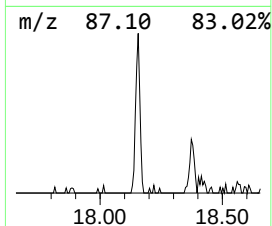
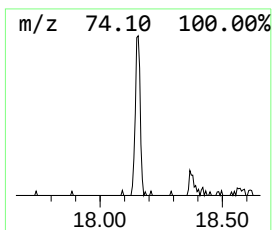
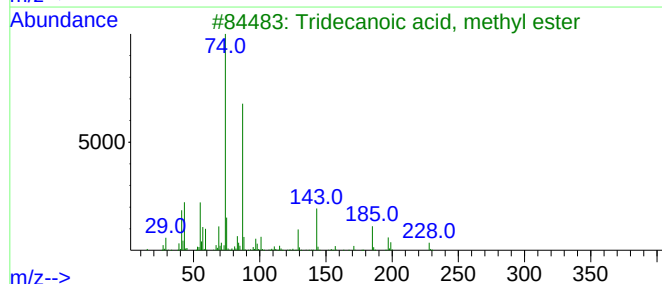
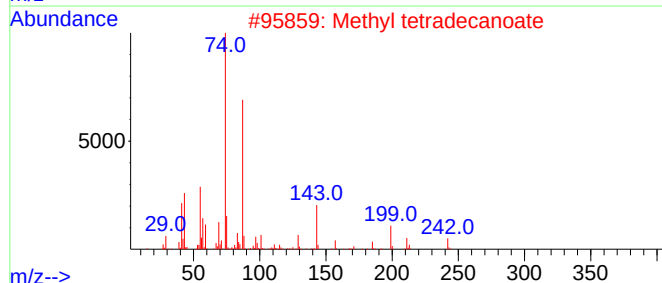
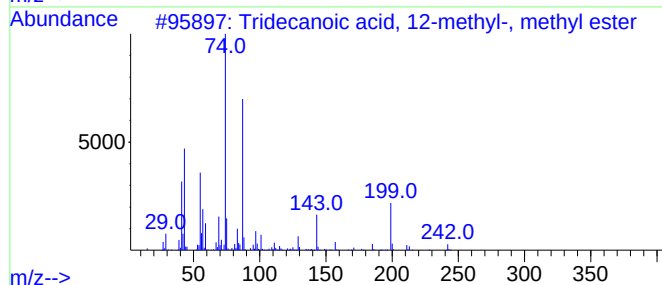
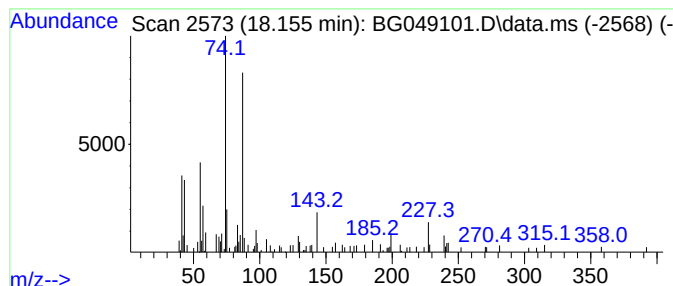
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecanoic acid, 12-methyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.155	2.01 ng	55946	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	90
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5			Methyl stearate	298	C19H38O2	000112-61-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
Operator : CG/JU
Sample : M2829-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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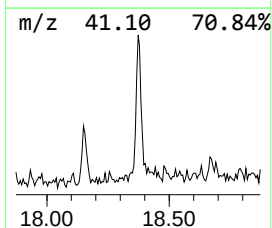
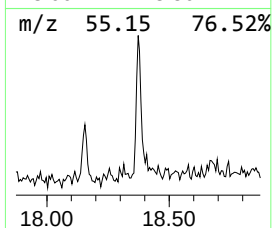
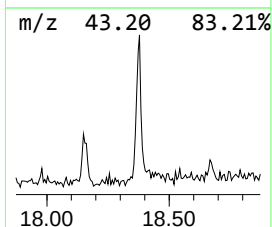
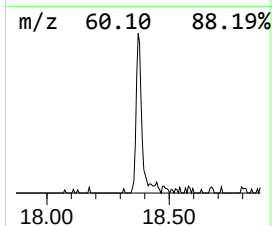
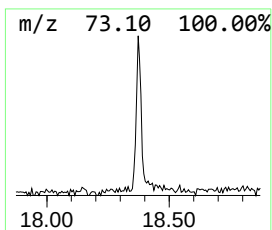
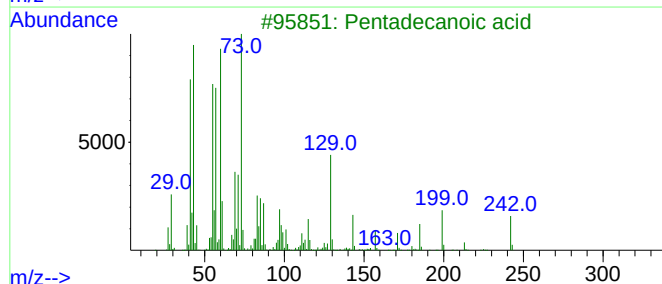
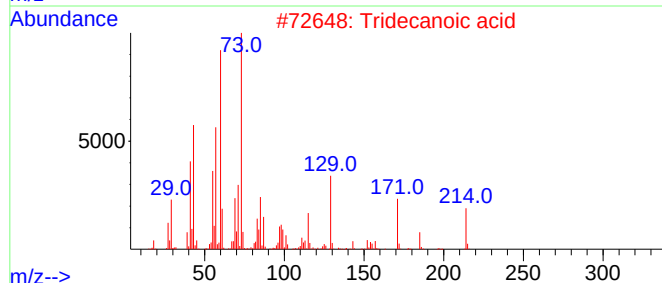
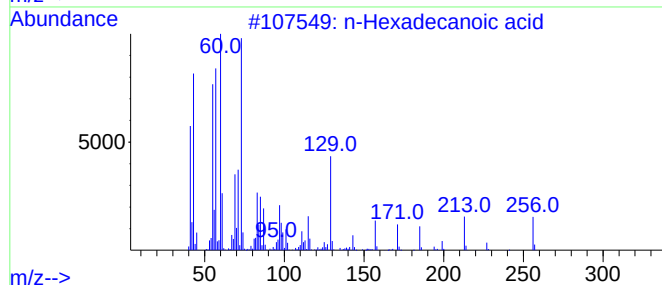
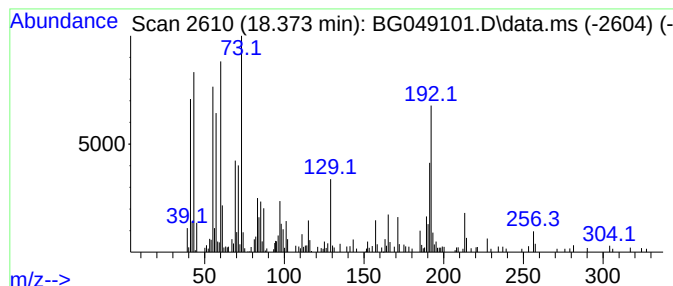
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	6.75 ng	188029	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
Operator : CG/JU
Sample : M2829-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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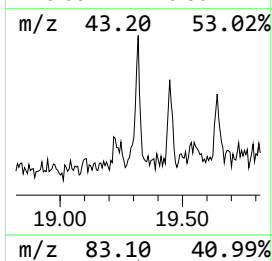
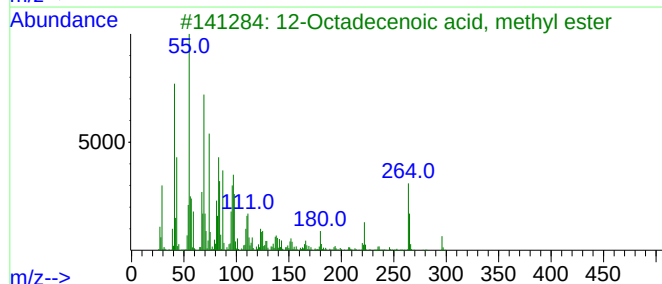
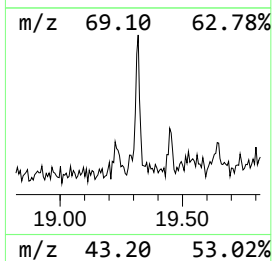
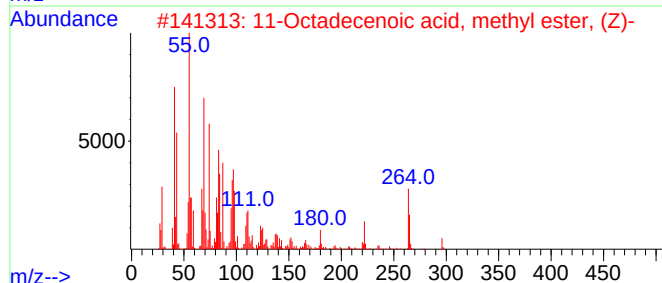
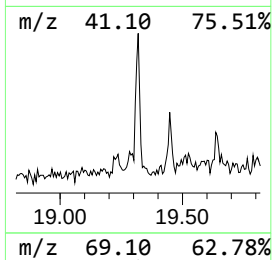
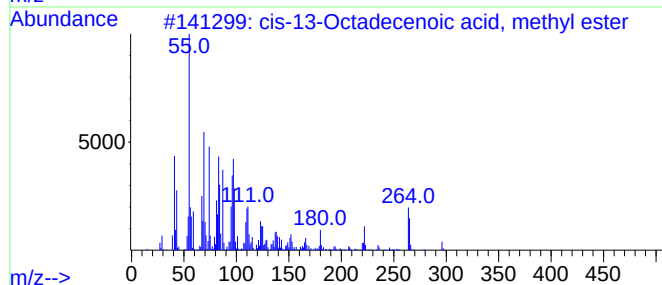
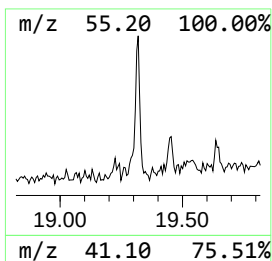
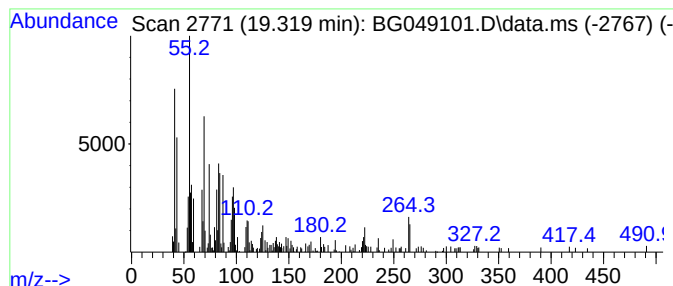
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 cis-13-Octadecenoic acid, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.319	5.07 ng	141200	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	91
2			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	91
3			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
4			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
5			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
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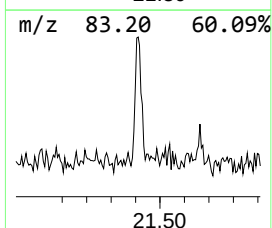
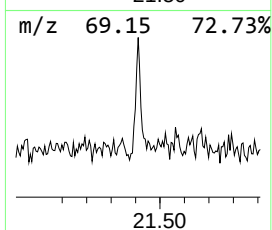
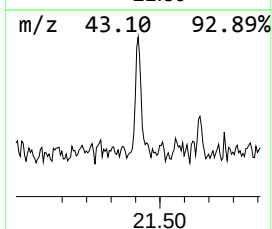
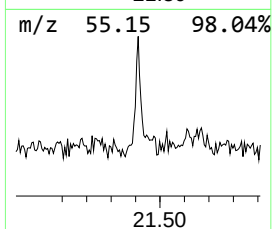
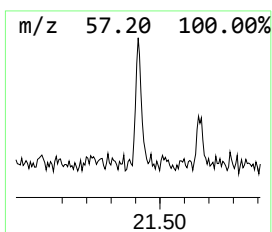
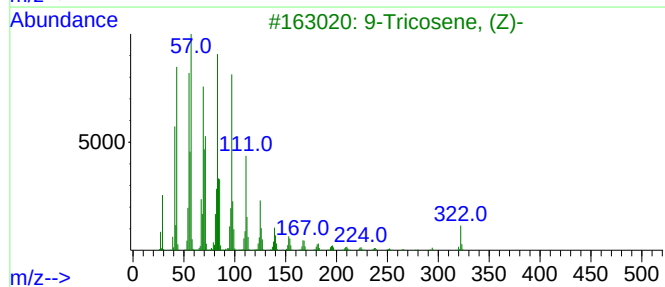
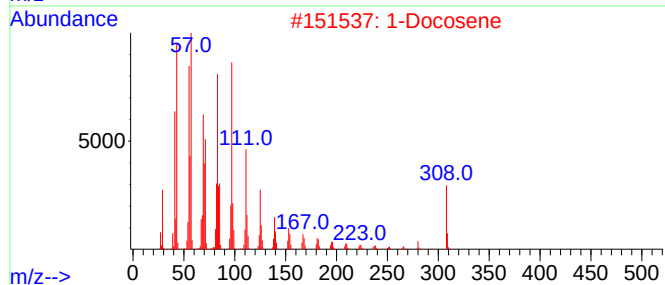
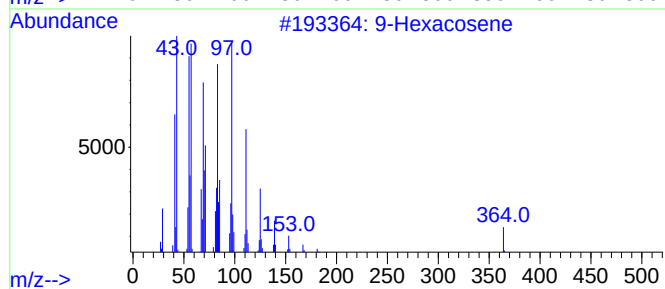
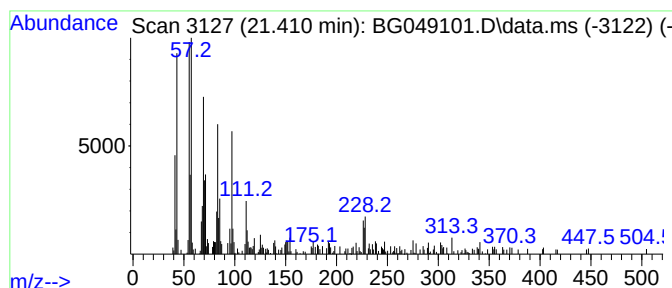
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Hexacosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	3.64 ng	136104	Chrysene-d12	21.786

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexacosene		364	C26H52	071502-22-2	91
2	1-Docosene		308	C22H44	001599-67-3	91
3	9-Tricosene, (Z)-		322	C23H46	027519-02-4	91
4	E-14-Hexadecenal		238	C16H30O	330207-53-9	90
5	1-Hexacosene		364	C26H52	018835-33-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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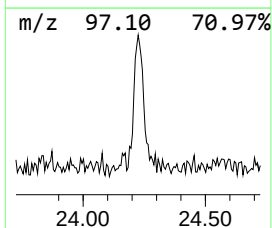
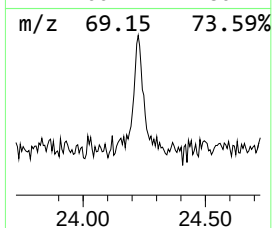
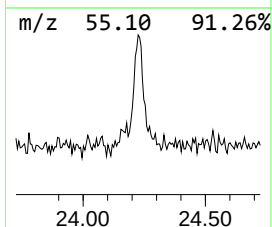
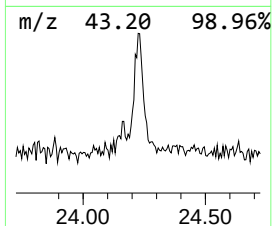
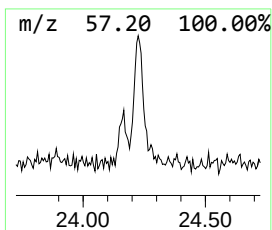
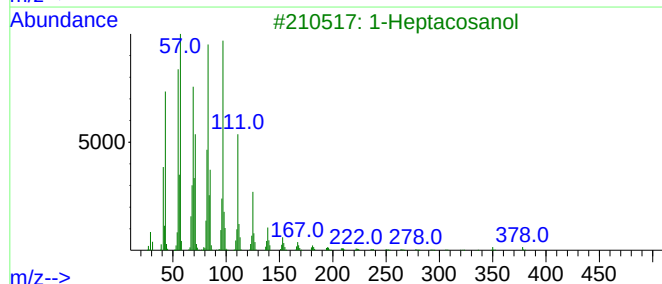
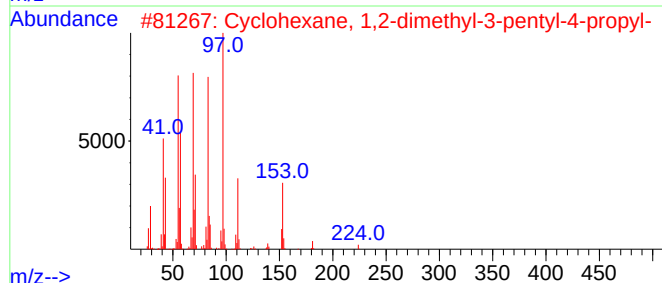
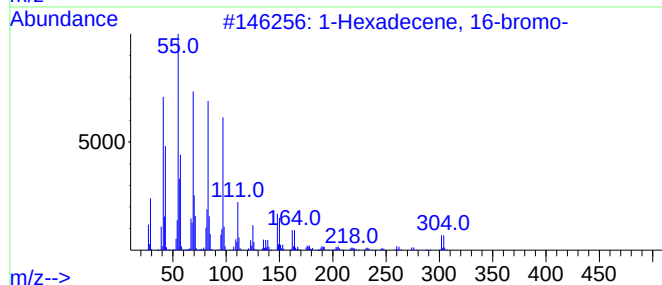
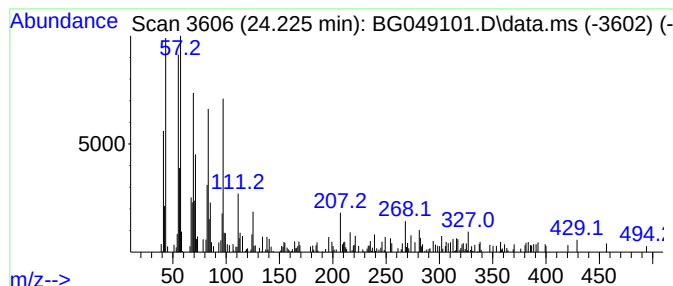
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Hexadecene, 16-bromo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.225	8.92 ng	188639	Perylene-d12	25.106

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	86
2		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	70
3		1-Heptacosanol	396	C27H56O	002004-39-9	70
4		11-Tricosene	322	C23H46	052078-56-5	62
5		9-Tricosene, (Z)-	322	C23H46	027519-02-4	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049101.D
Acq On : 25 Jun 2021 22:07
Operator : CG/JU
Sample : M2829-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-DUP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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
Butane, 2-metho...	3.238	2.3	ng	31335	1	8.108	276944	20.0
unknown5.194	5.194	2.5	ng	34213	1	8.108	276944	20.0
Ethanol, 2-(2-b...	10.688	29.2	ng	535907	2	10.929	366585	20.0
2,4,7,9-Tetrame...	13.631	4.9	ng	119047	3	14.748	488393	20.0
Benzene, (1-met...	15.688	2.1	ng	50451	3	14.748	488393	20.0
unknown16.622	16.622	2.4	ng	67089	4	17.497	557225	20.0
unknown16.892	16.892	2.2	ng	60136	4	17.497	557225	20.0
Tridecanoic aci...	18.155	2.0	ng	55946	4	17.497	557225	20.0
n-Hexadecanoic ...	18.373	6.8	ng	188029	4	17.497	557225	20.0
cis-13-Octadece...	19.319	5.1	ng	141200	4	17.497	557225	20.0
9-Hexacosene	21.410	3.6	ng	136104	5	21.786	748325	20.0
1-Hexadecene, 1...	24.225	8.9	ng	188639	6	25.106	423023	20.0