

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
 Data File : BG049102.D
 Acq On : 25 Jun 2021 22:48
 Operator : CG/JU
 Sample : M2829-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 15B-STOCKPILE-2B

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: BG049102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.154	14	20	30	rBV4	47264	122976	7.02%	0.898%
2	3.237	30	34	40	rVB2	19365	34426	1.97%	0.251%
3	5.193	360	367	372	rBV3	14301	26344	1.50%	0.192%
4	5.663	440	447	457	rBV	529704	899822	51.39%	6.572%
5	7.261	709	719	729	rBV	540371	979351	55.93%	7.152%
6	8.107	855	863	870	rBV	155636	278936	15.93%	2.037%
7	9.277	1053	1062	1069	rBV	334391	628640	35.90%	4.591%
8	10.687	1296	1302	1313	rBV	231551	383362	21.89%	2.800%
9	10.928	1334	1343	1352	rBV	202612	375318	21.43%	2.741%
10	13.372	1750	1759	1769	rBV	890774	1386077	79.16%	10.123%
11	14.747	1983	1993	2000	rBV	316379	515994	29.47%	3.768%
12	16.233	2239	2246	2256	rVB	704112	1119081	63.91%	8.173%
13	16.874	2352	2355	2363	rVB9	10405	19844	1.13%	0.145%
14	17.373	2435	2440	2443	rBV5	22900	31893	1.82%	0.233%
15	17.496	2454	2461	2465	rBV	361854	558025	31.87%	4.075%
16	17.537	2465	2468	2476	rVV	99693	159786	9.13%	1.167%
17	17.626	2480	2483	2489	rVB	24419	37327	2.13%	0.273%
18	18.154	2568	2573	2577	rBV2	37556	55642	3.18%	0.406%
19	18.254	2585	2590	2594	rBV8	15744	29323	1.67%	0.214%
20	18.313	2597	2600	2605	rVV7	9724	17990	1.03%	0.131%
21	18.372	2605	2610	2615	rVV	139285	199186	11.38%	1.455%
22	18.419	2616	2618	2626	rVB2	26782	43048	2.46%	0.314%
23	18.572	2637	2644	2647	rBV3	29915	63620	3.63%	0.465%
24	18.901	2697	2700	2706	rVB6	16211	26269	1.50%	0.192%
25	19.100	2732	2734	2740	rVB5	25736	34288	1.96%	0.250%
26	19.282	2762	2765	2768	rBV5	12214	19097	1.09%	0.139%
27	19.547	2804	2810	2815	rBV	270850	385482	22.01%	2.815%
28	19.641	2823	2826	2830	rBV3	45615	55219	3.15%	0.403%
29	19.876	2862	2866	2867	rBV	41016	55789	3.19%	0.407%
30	19.905	2867	2871	2878	rVB	237673	351873	20.09%	2.570%
31	20.099	2899	2904	2910	rBV	1300832	1751052	100.00%	12.788%
32	20.393	2952	2954	2959	rVB2	41844	55855	3.19%	0.408%
33	21.409	3123	3127	3131	rBV3	92345	138102	7.89%	1.009%
34	21.785	3183	3191	3196	rBV3	368935	825931	47.17%	6.032%
35	21.832	3196	3199	3207	rVB	116385	183988	10.51%	1.344%
36	24.053	3571	3577	3585	rBV	90569	294869	16.84%	2.153%

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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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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37	24.165	3592	3596	3601	rVB2	96635	171135	9.77%	1.250%
38	24.958	3724	3731	3738	rVB2	69643	177921	10.16%	1.299%
39	25.111	3752	3757	3768	rVB2	136149	378707	21.63%	2.766%
40	26.339	3958	3966	3978	rVB2	246997	821201	46.90%	5.997%

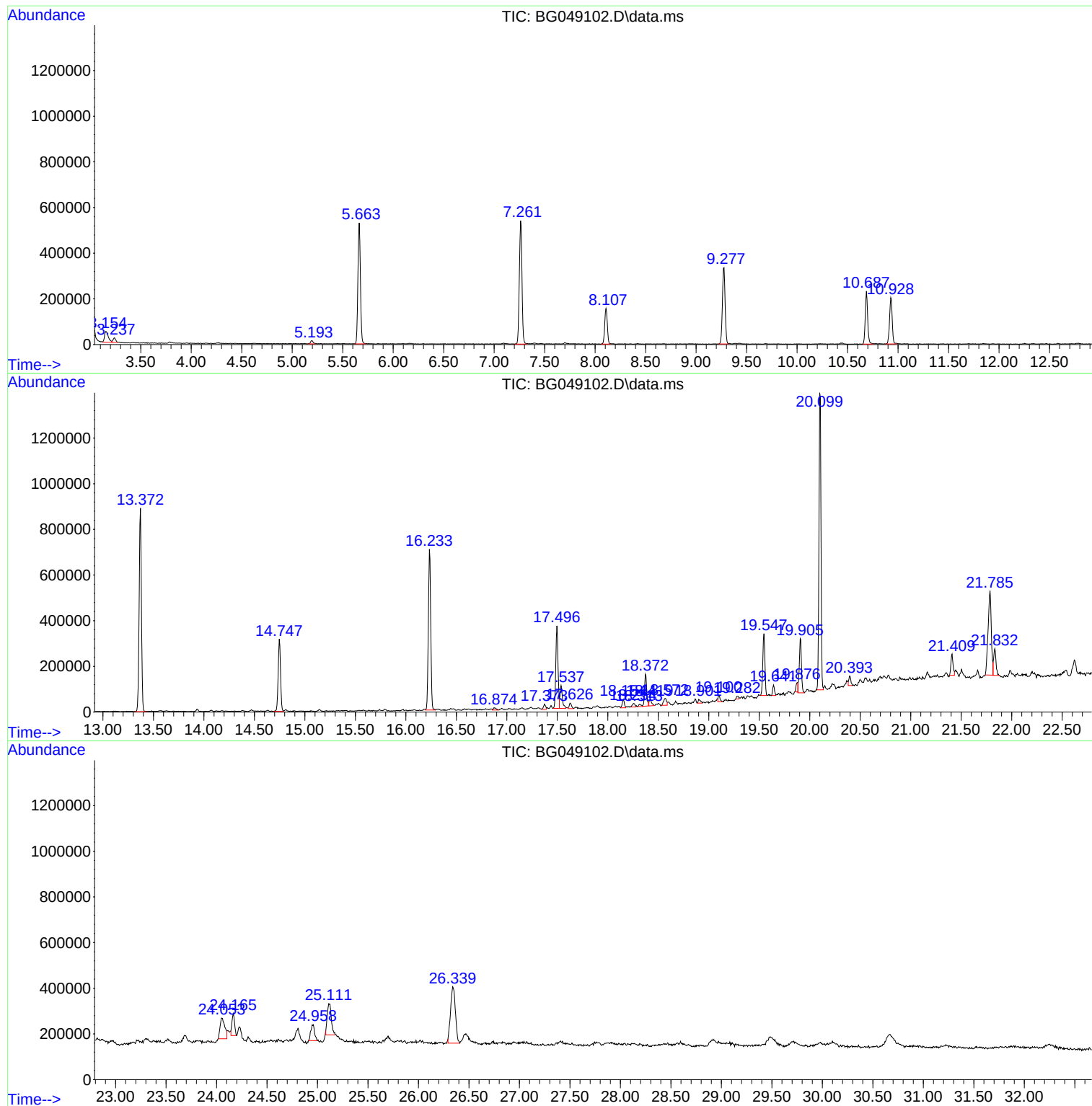
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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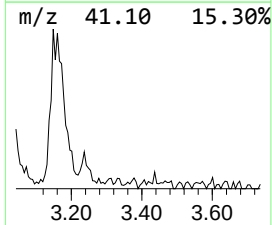
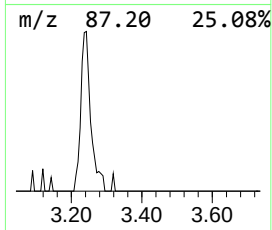
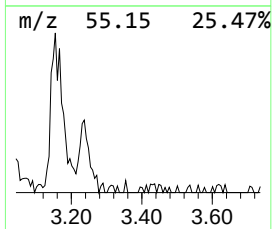
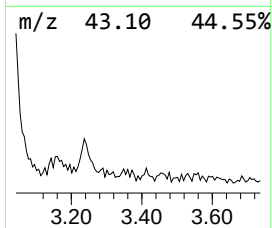
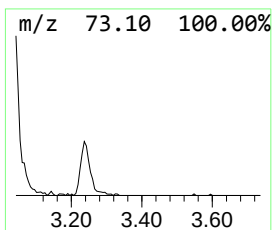
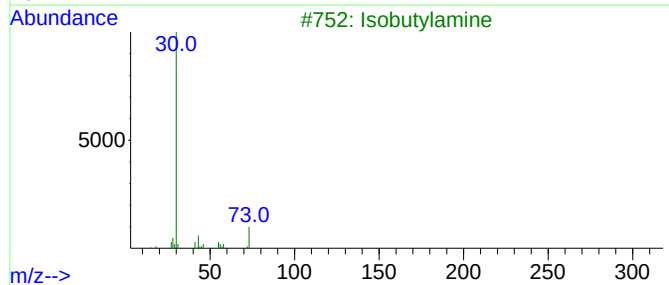
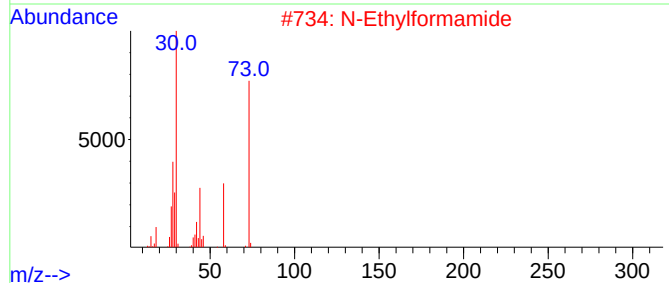
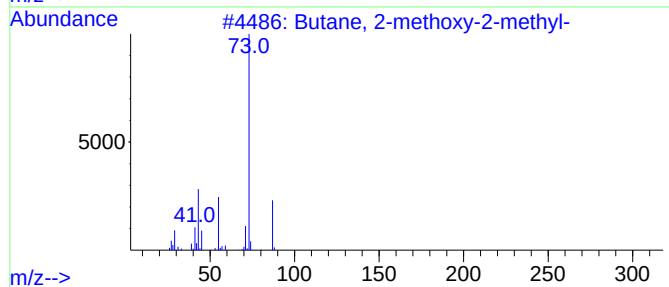
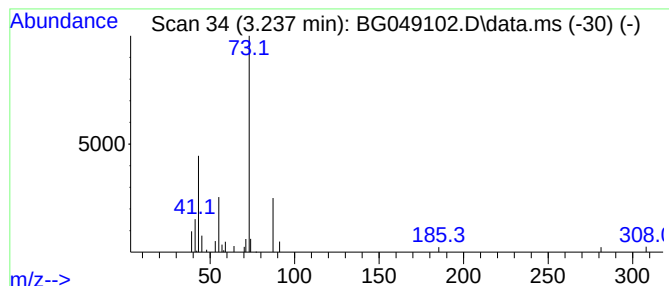
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.237 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.237	2.47 ng	34426	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
2			N-Ethylformamide	73	C3H7NO	000627-45-2	5
3			Isobutylamine	73	C4H11N	000078-81-9	5
4			1-Propene-1-thiol	74	C3H6S	000925-89-3	4
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	4



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Instrument :
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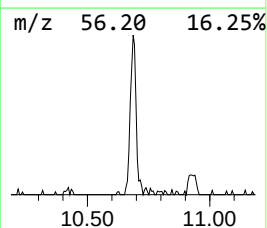
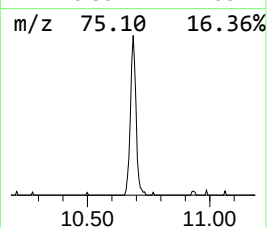
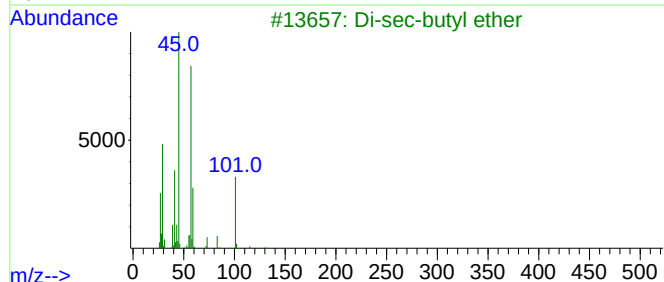
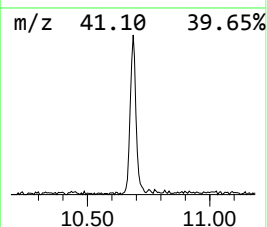
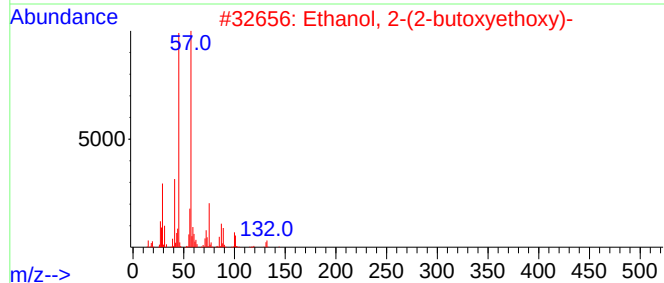
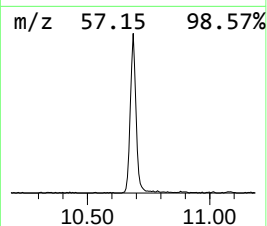
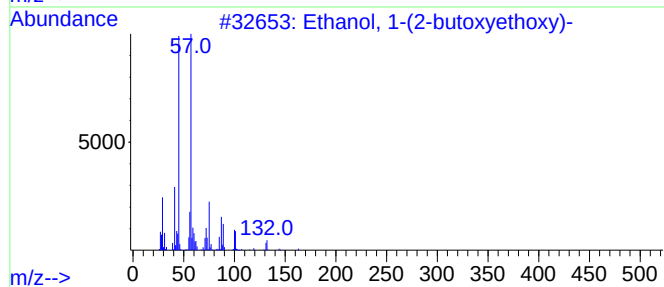
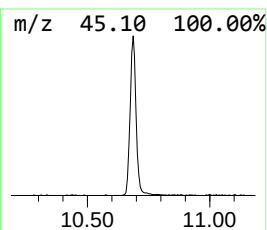
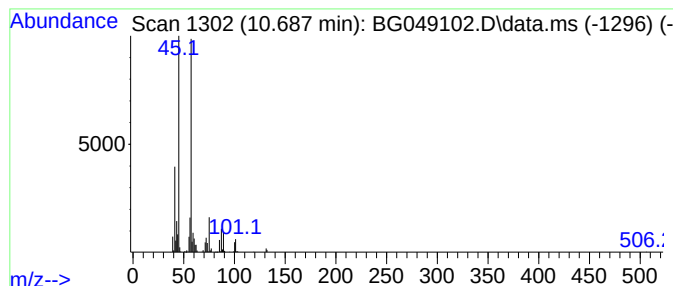
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Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.687	20.43 ng	383362	Naphthalene-d8	10.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Di-sec-butyl ether	130	C8H18O	006863-58-7	50
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	50



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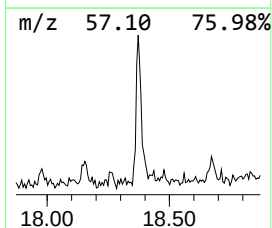
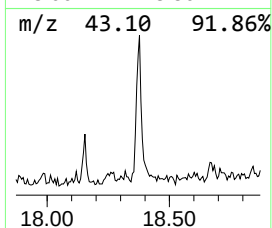
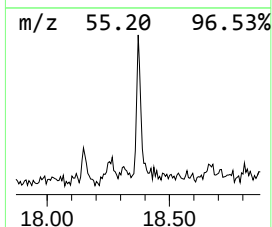
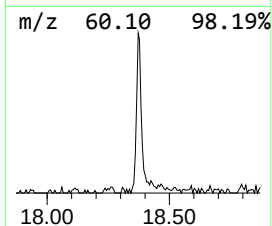
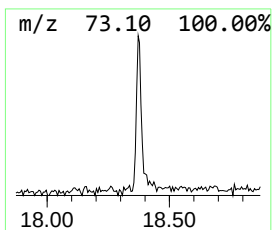
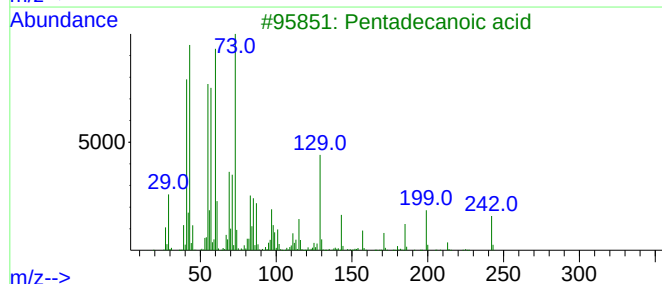
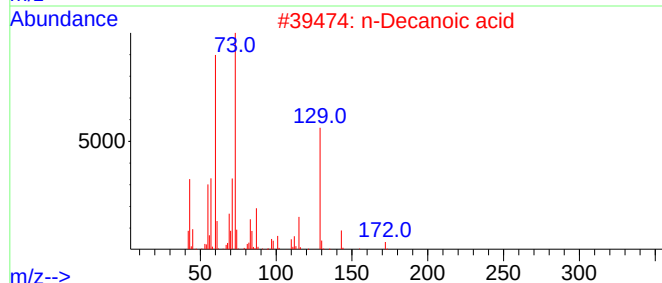
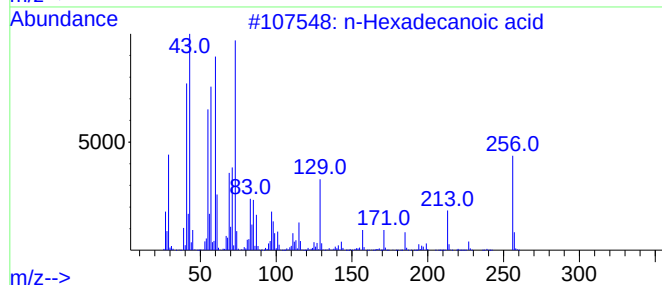
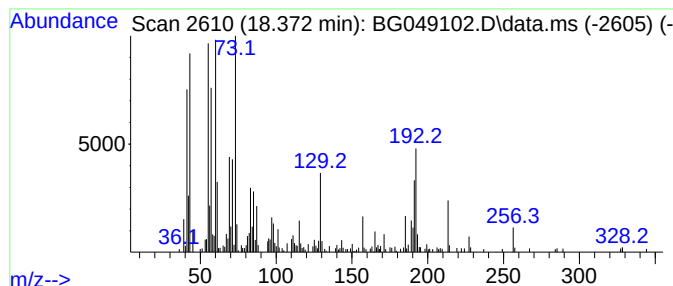
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.372	7.14 ng	199186	Phenanthrene-d10	17.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Decanoic acid	172	C10H20O2	000334-48-5	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5			Octadecanoic acid	284	C18H36O2	000057-11-4	62



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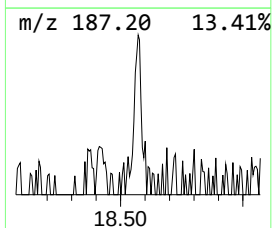
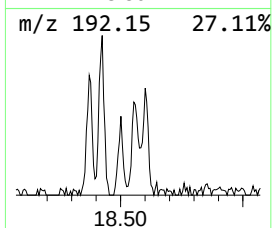
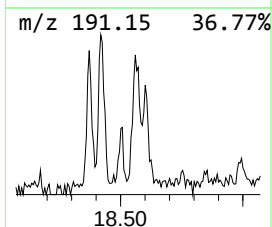
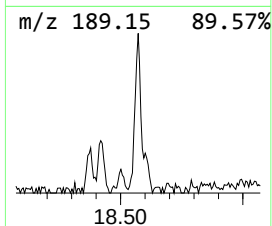
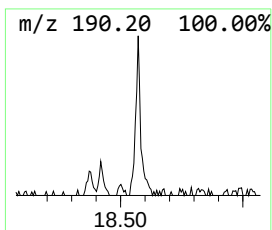
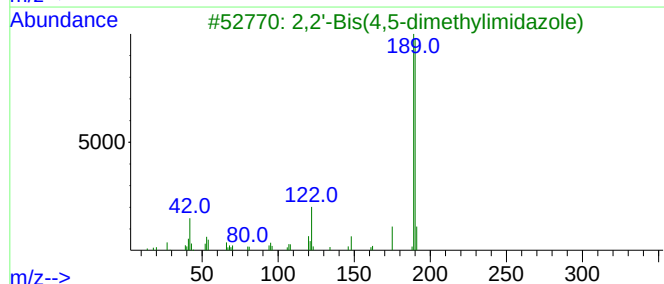
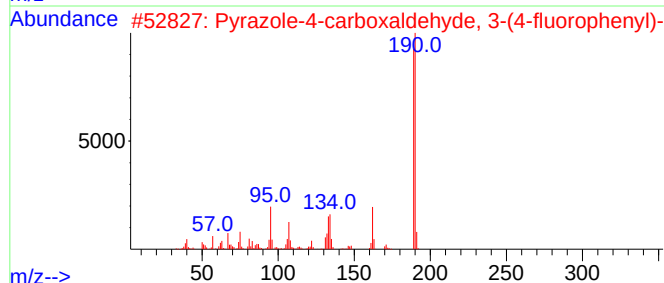
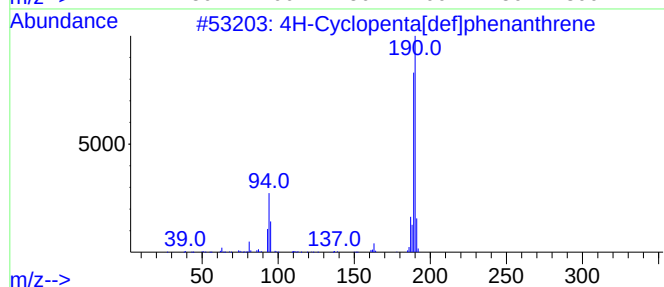
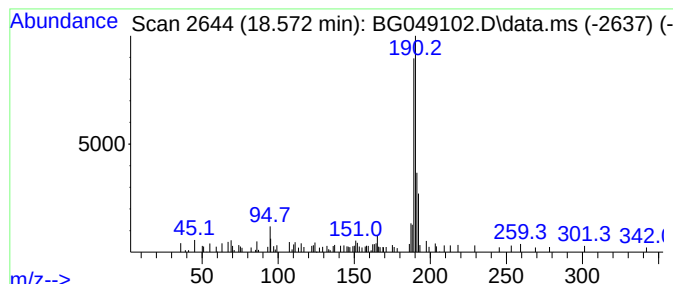
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Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.572	2.28 ng	63620	Phenanthrene-d10	17.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	53
4			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
5			4-(4-Methyl-piperidin-1-yl)-phen...	190	C12H18N2	342013-25-6	53



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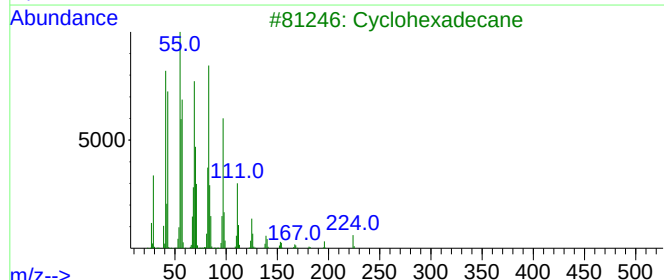
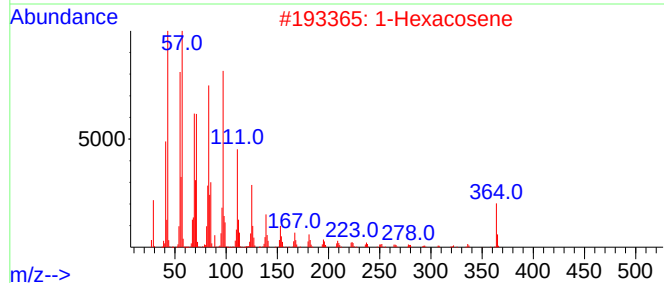
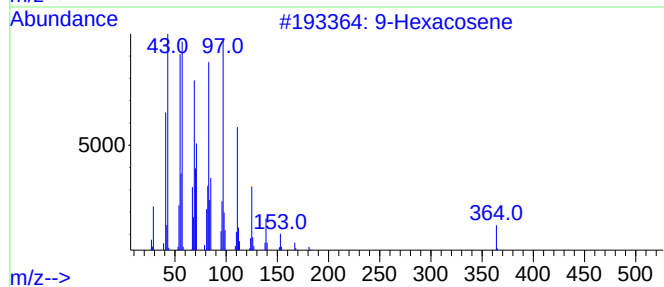
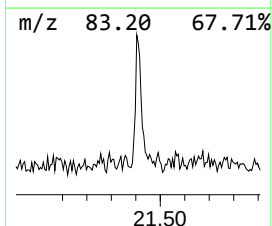
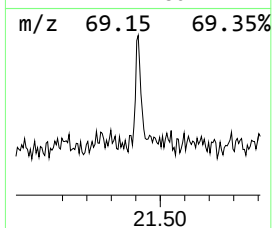
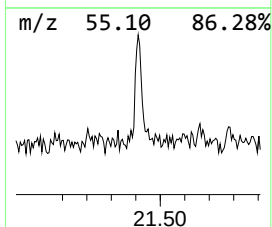
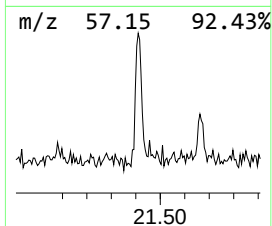
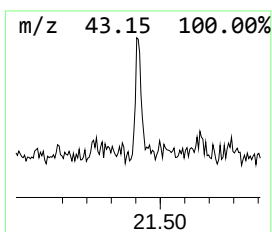
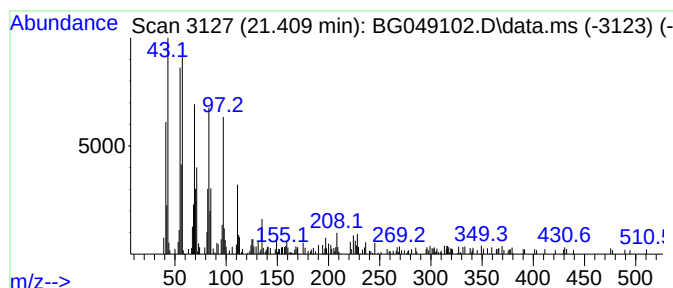
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 9-Hexacosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.409	3.34 ng	138102	Chrysene-d12	21.785

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexacosene			364	C26H52	071502-22-2	93
2	1-Hexacosene			364	C26H52	018835-33-1	93
3	Cyclohexadecane			224	C16H32	000295-65-8	93
4	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	91
5	1-Heneicosanol			312	C21H44O	015594-90-8	90



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Data File : BG049102.D
Acq On : 25 Jun 2021 22:48
Operator : CG/JU
Sample : M2829-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-2B

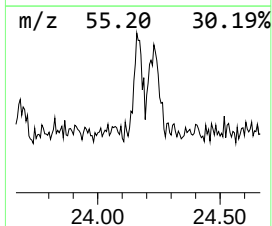
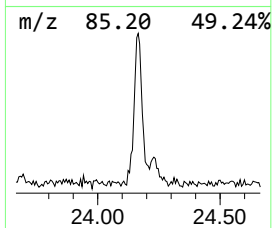
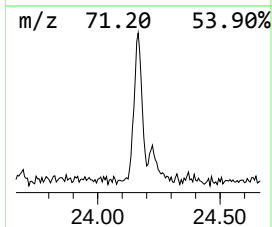
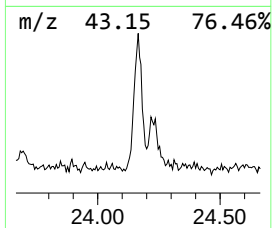
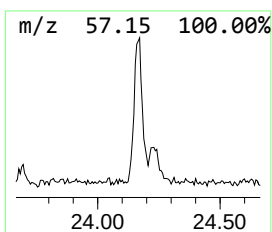
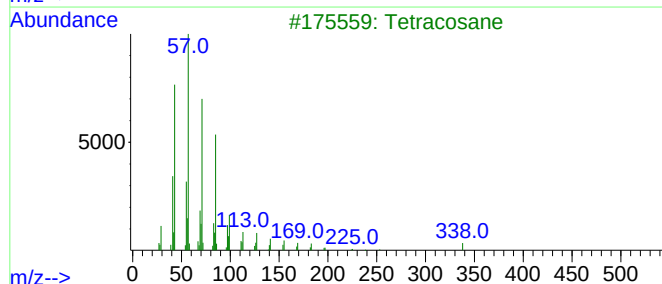
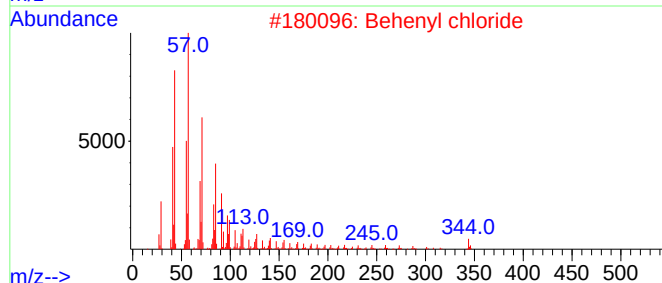
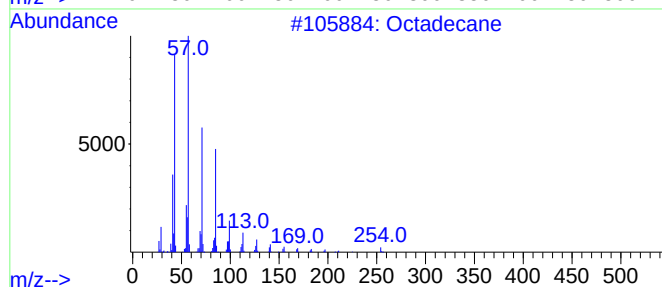
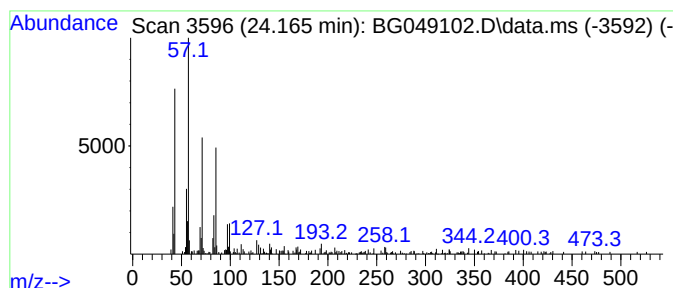
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.165	9.04 ng	171135	Perylene-d12	25.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	90
2			Behenyl chloride	344	C22H45Cl	042217-03-8	81
3			Tetracosane	338	C24H50	000646-31-1	81
4			Tricosane	324	C23H48	000638-67-5	81
5			Nonacosane	408	C29H60	000630-03-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049102.D
Acq On : 25 Jun 2021 22:48
Operator : CG/JU
Sample : M2829-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-2B

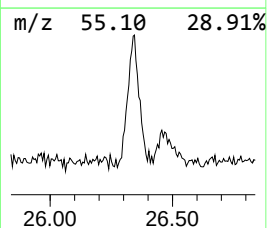
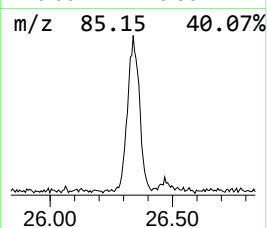
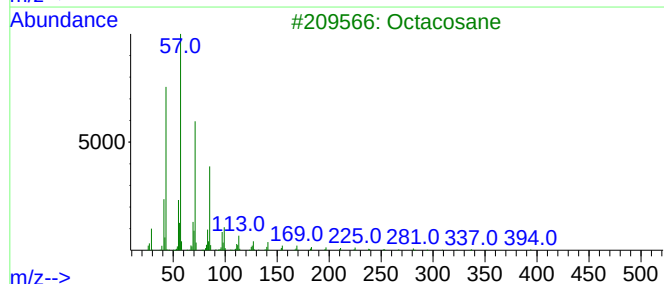
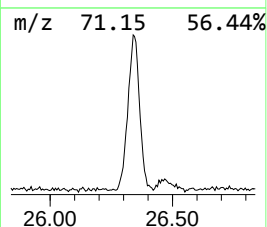
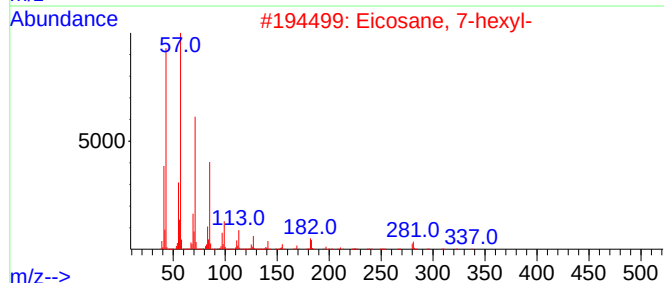
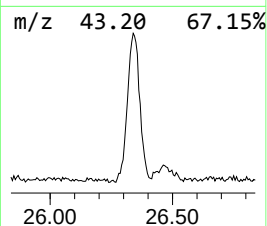
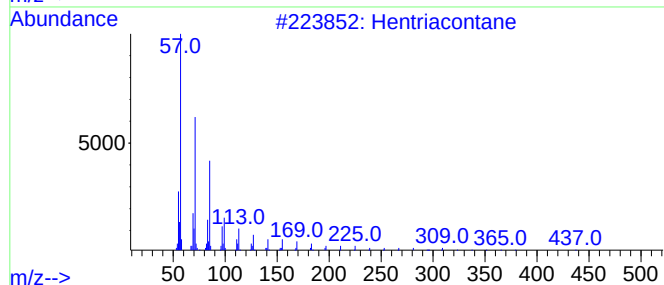
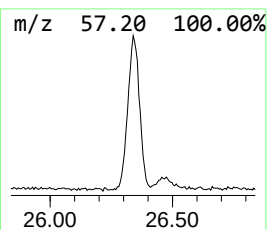
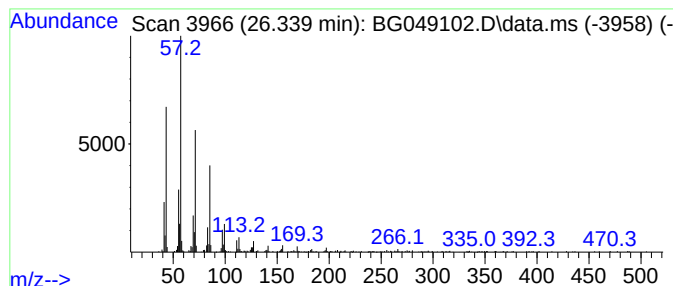
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.339	43.37 ng	821201	Perylene-d12	25.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptacosane	380	C27H56	000593-49-7	83
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049102.D
Acq On : 25 Jun 2021 22:48
Operator : CG/JU
Sample : M2829-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-2B

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
unknown3.237	3.237	2.5	ng	34426	1	8.107	278936	20.0
Ethanol, 1-(2-b...	10.687	20.4	ng	383362	2	10.928	375318	20.0
n-Hexadecanoic ...	18.372	7.1	ng	199186	4	17.496	558025	20.0
4H-Cyclopenta[d...	18.572	2.3	ng	63620	4	17.496	558025	20.0
9-Hexacosene	21.409	3.3	ng	138102	5	21.785	825931	20.0
Octadecane	24.165	9.0	ng	171135	6	25.117	378707	20.0
Hentriacontane	26.339	43.4	ng	821201	6	25.117	378707	20.0