

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
 Data File : BG048957.D
 Acq On : 14 Jun 2021 20:14
 Operator : CG/JU
 Sample : M2678-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0241-AMND-COMP-F(CL-05)

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: BG048957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	17	21	38	rVB	222135	391778	3.09%	1.472%
2	3.287	38	42	54	rVB	112885	168874	1.33%	0.634%
3	4.591	258	264	271	rBV	96176	150036	1.19%	0.564%
4	5.244	361	375	379	rBV	4781384	12659190	100.00%	47.548%
5	7.282	713	722	732	rVB	132957	250729	1.98%	0.942%
6	8.117	858	864	871	rBV	152455	267016	2.11%	1.003%
7	9.286	1056	1063	1072	rVB	590612	1092974	8.63%	4.105%
8	10.708	1298	1305	1314	rBV	468550	771326	6.09%	2.897%
9	10.943	1334	1345	1351	rBV	200517	373393	2.95%	1.402%
10	13.387	1753	1761	1768	rBV	1214135	1883281	14.88%	7.074%
11	14.762	1984	1995	2002	rBV2	324315	540667	4.27%	2.031%
12	17.259	2414	2420	2425	rBV3	89883	134846	1.07%	0.506%
13	17.512	2457	2463	2467	rBV	394383	626414	4.95%	2.353%
14	17.553	2467	2470	2475	rVB	110689	156398	1.24%	0.587%
15	19.339	2771	2774	2785	rVB5	106597	160049	1.26%	0.601%
16	19.556	2806	2811	2817	rBV	409005	592929	4.68%	2.227%
17	19.891	2863	2868	2869	rBV2	98417	136232	1.08%	0.512%
18	19.921	2869	2873	2881	rVB	335277	504291	3.98%	1.894%
19	20.120	2900	2907	2912	rVB	2158428	2838585	22.42%	10.662%
20	20.408	2953	2956	2963	rVB2	113641	174702	1.38%	0.656%
21	21.801	3185	3193	3198	rBV3	420850	1025275	8.10%	3.851%
22	21.848	3198	3201	3212	rVB	164982	315271	2.49%	1.184%
23	24.086	3574	3582	3589	rBV	93103	309006	2.44%	1.161%
24	24.827	3704	3708	3718	rVB2	64024	177407	1.40%	0.666%
25	24.979	3726	3734	3743	rVB2	95324	279319	2.21%	1.049%
26	25.144	3752	3762	3771	rBV	216248	643775	5.09%	2.418%

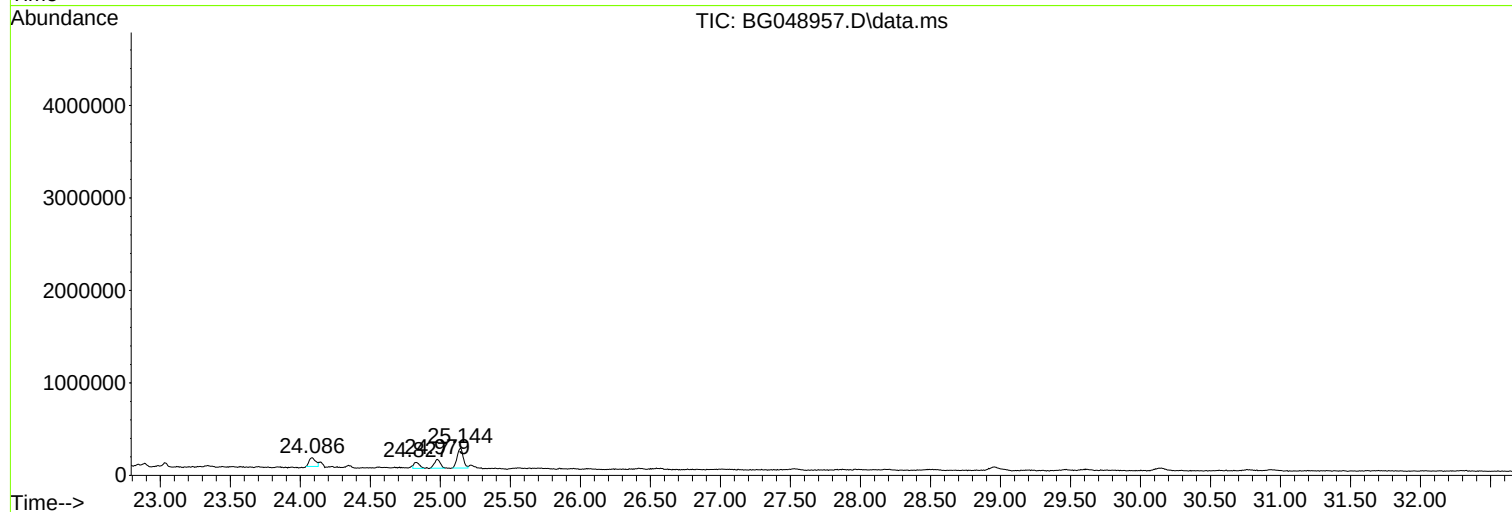
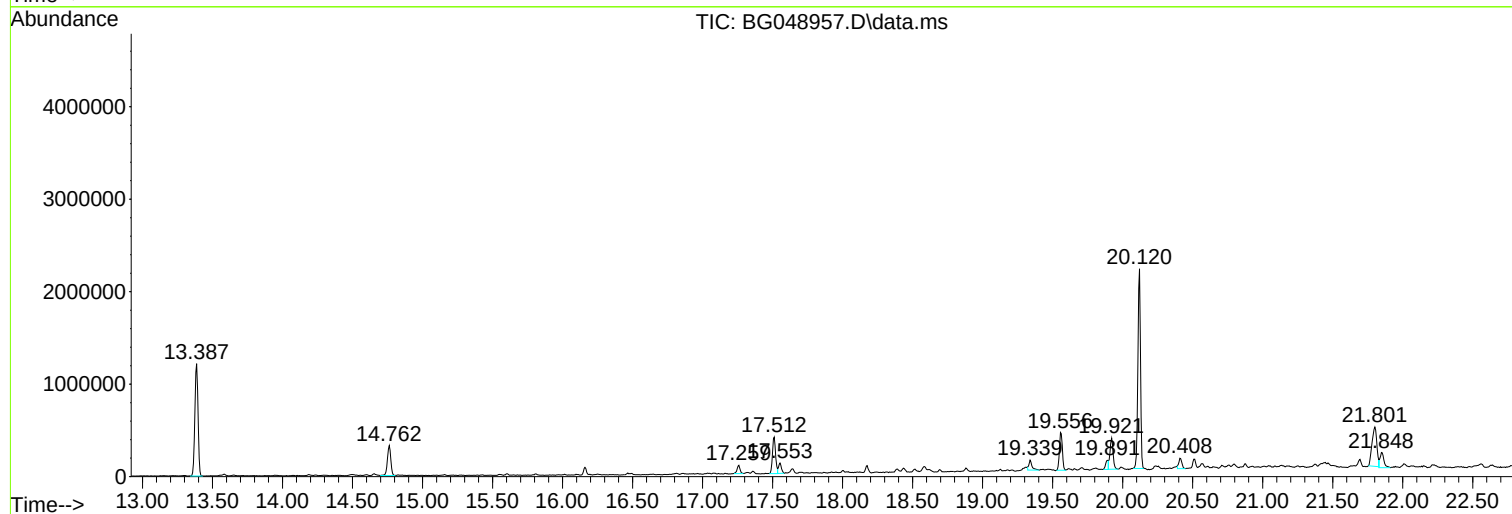
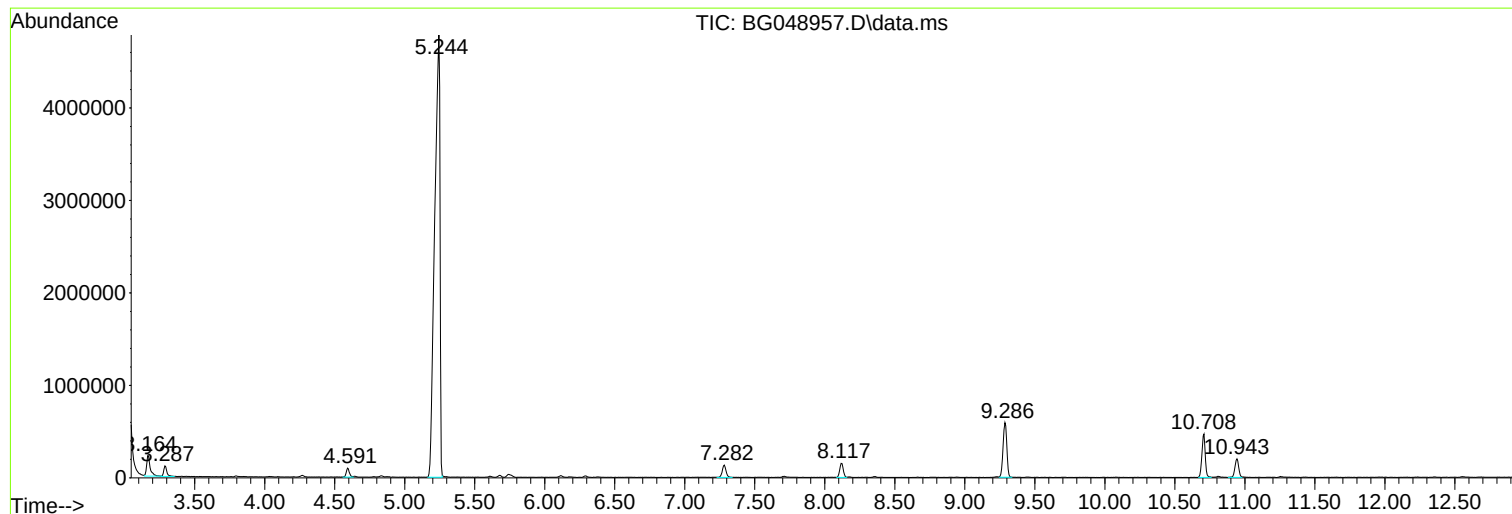
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ClientSampleId :
0241-AMND-COMP-F(CL-05)

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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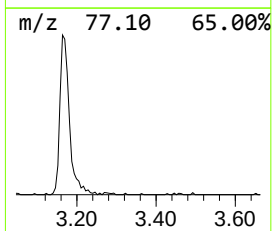
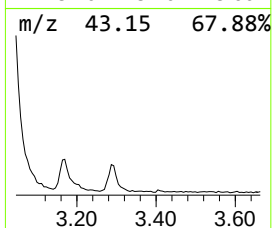
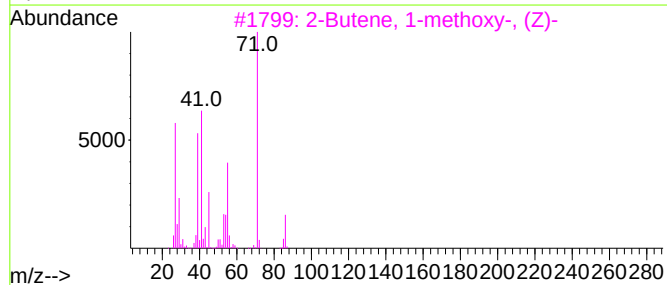
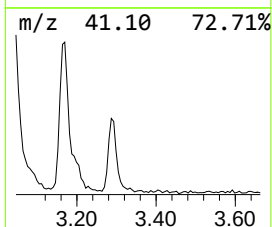
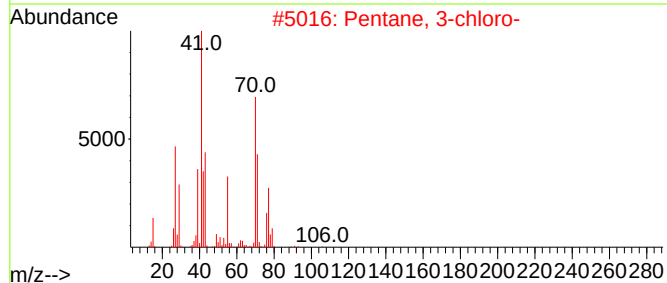
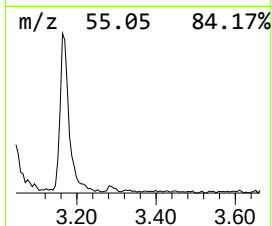
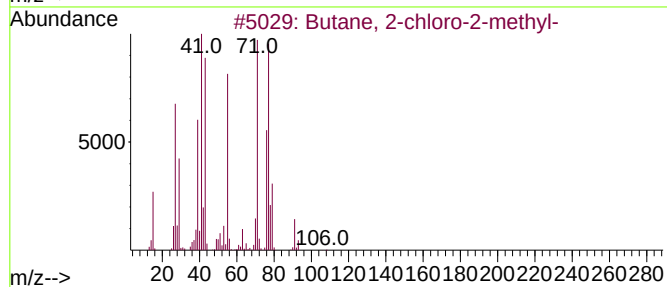
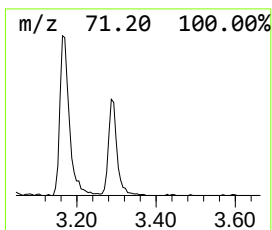
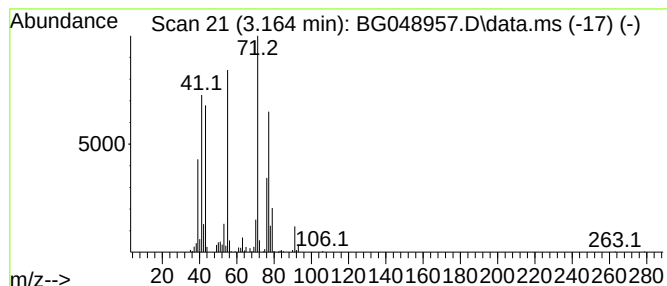
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-chloro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.164	29.34 ng	391778	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	72
2			Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	58
3			2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	38
4			Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	22
5			3-Penten-2-ol	86	C5H10O	001569-50-2	17



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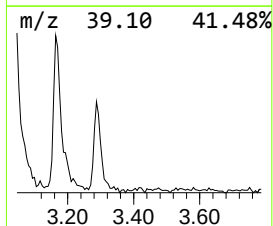
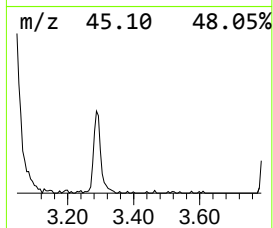
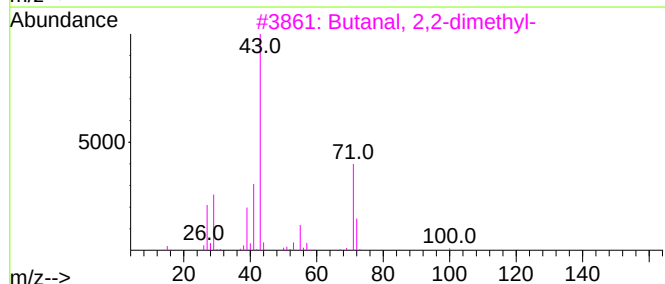
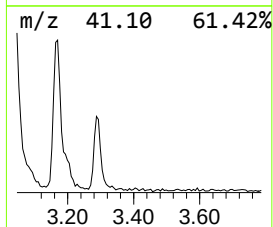
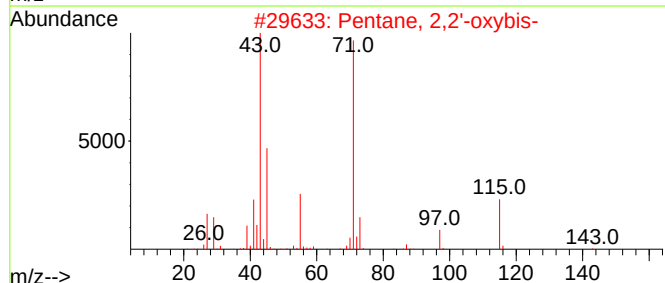
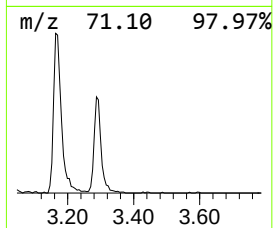
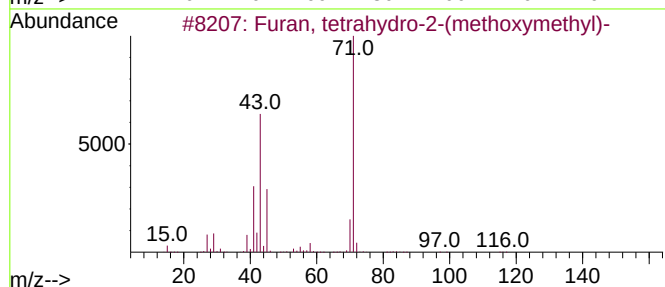
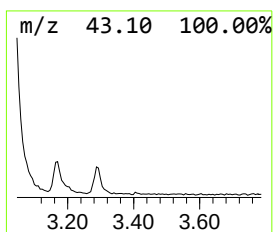
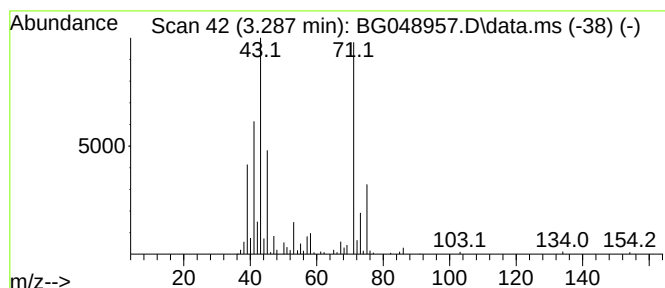
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.287 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.287	12.65 ng	168874	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	49
2			Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	47
3			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	43
4			Pantolactone	130	C6H10O3	000599-04-2	40
5			3-Penten-2-ol	86	C5H10O	001569-50-2	38



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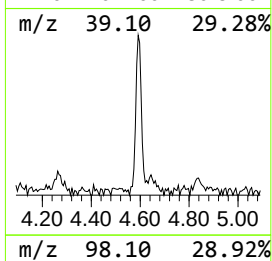
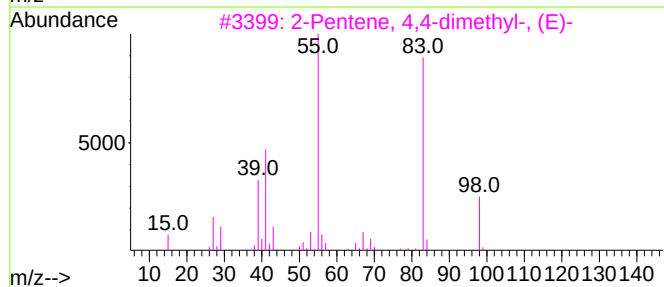
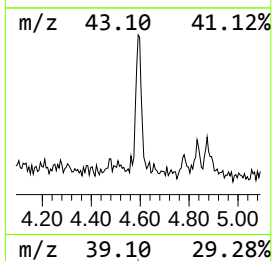
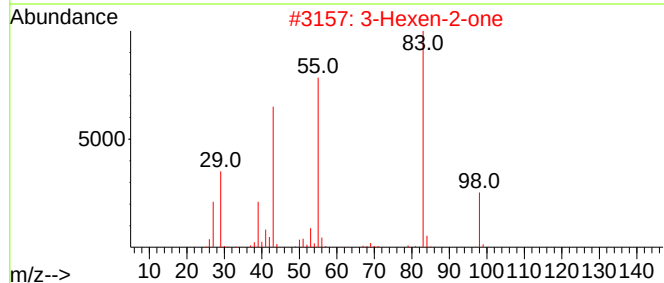
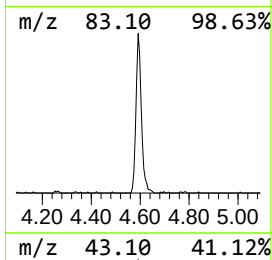
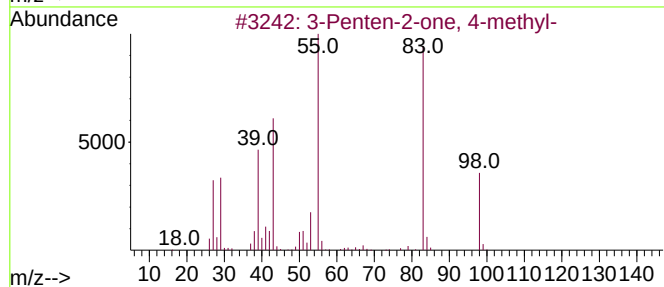
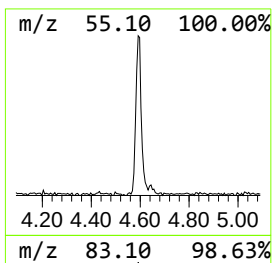
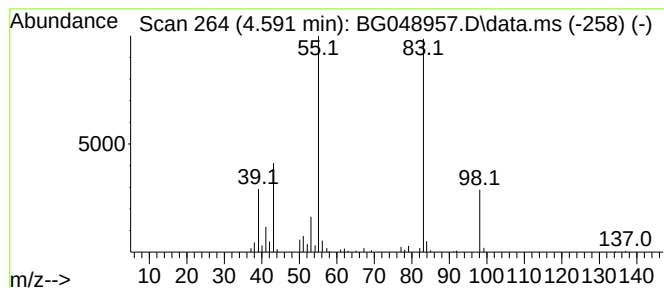
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.591	11.24 ng	150036	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	72



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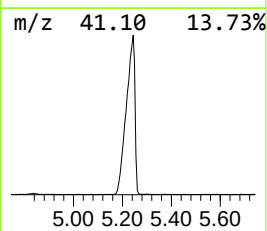
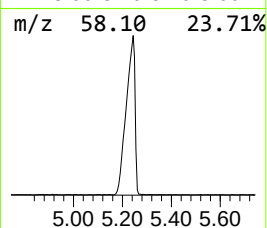
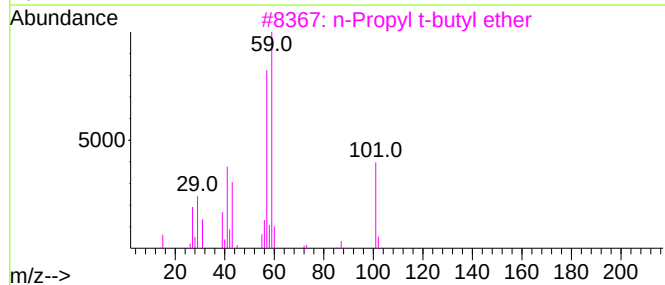
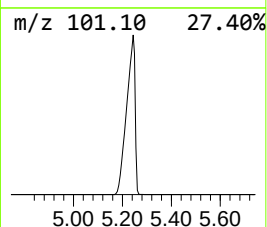
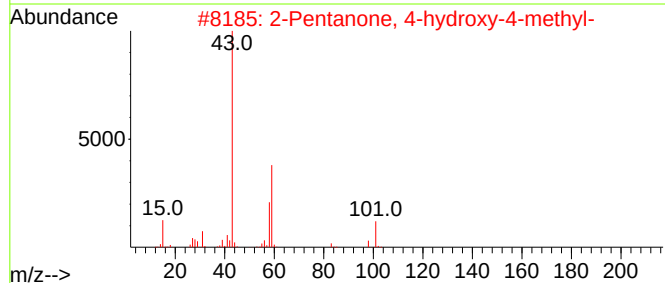
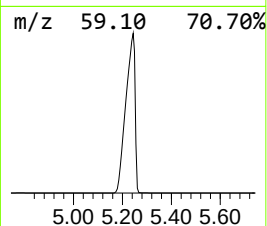
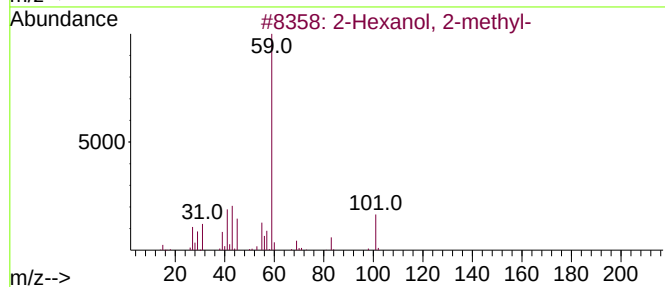
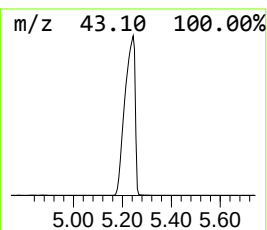
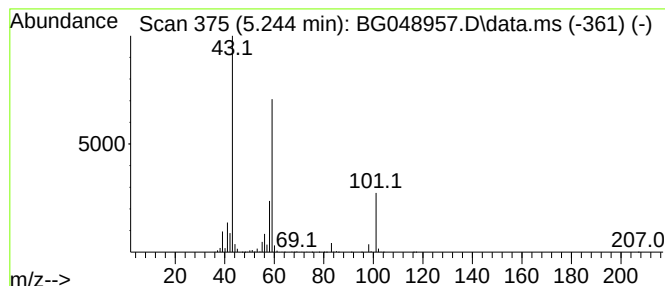
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown5.244 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.244	948.20 ng	12659200	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-		116	C7H16O		000625-23-0	47
2	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2		000123-42-2	43
3	n-Propyl t-butyl ether		116	C7H16O		1000334-81-9	25
4	2,3-Dimethyloxirane-2-carboxylic...		130	C6H10O3		1000306-64-4	25
5	2-Nonanone, 9-hydroxy-		158	C9H18O2		025368-56-3	25



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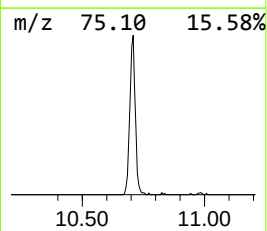
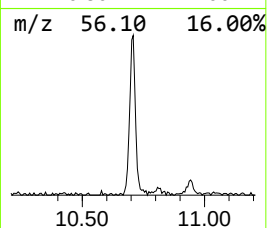
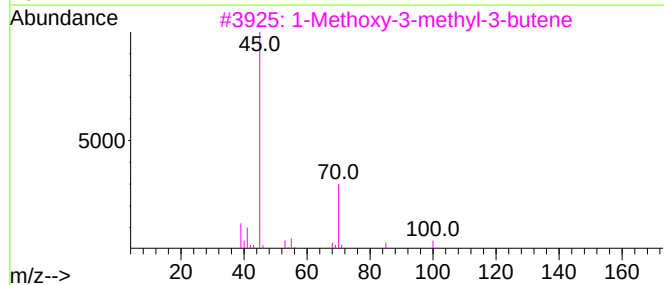
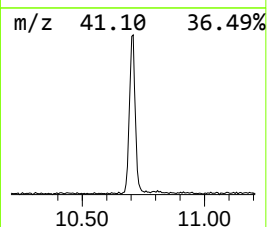
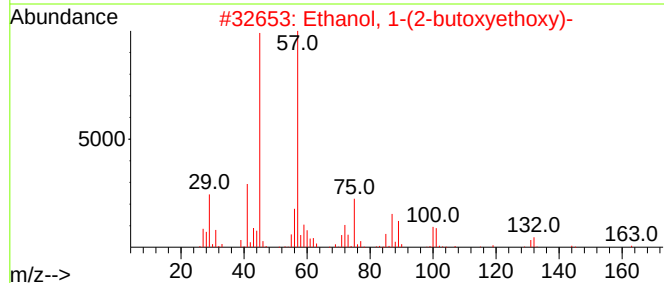
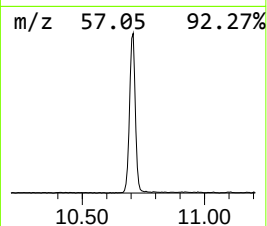
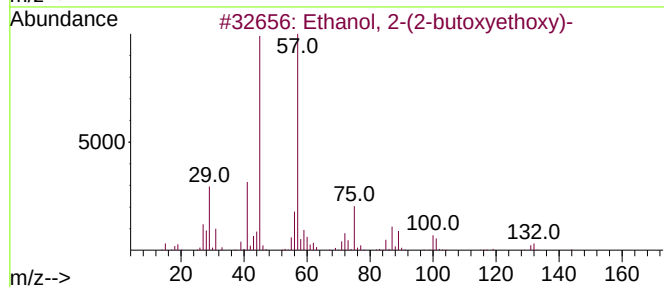
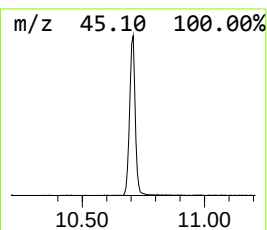
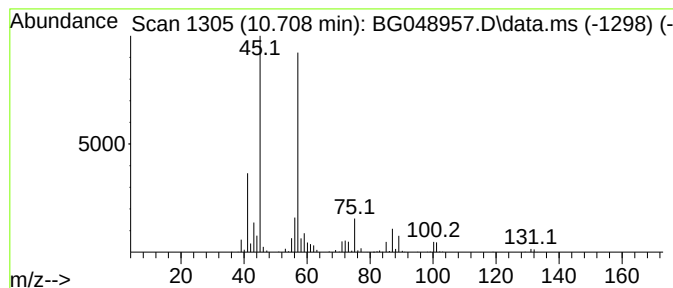
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.708	41.31 ng	771326	Naphthalene-d8	10.943

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	50
3			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
4			Propanoic acid, 2-hydroxy-, buty...	146	C7H14O3	000138-22-7	47
5			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47



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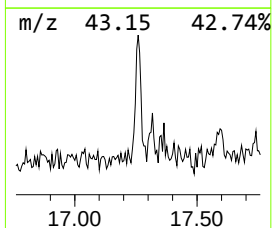
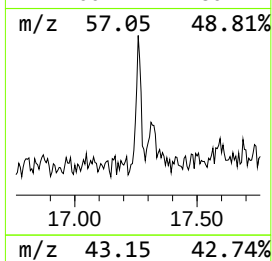
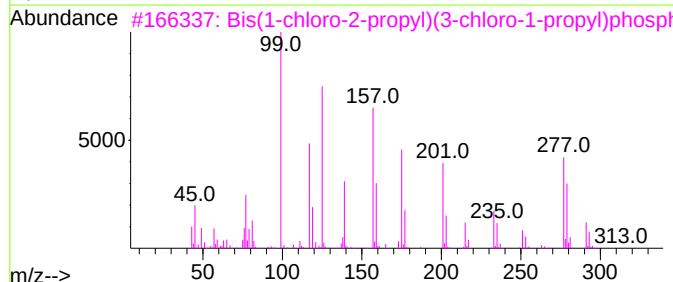
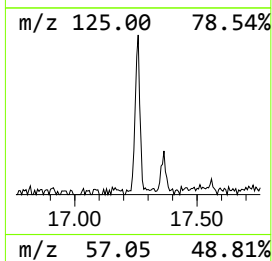
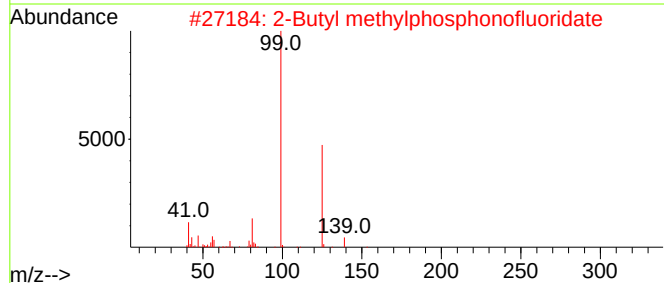
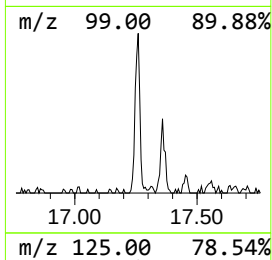
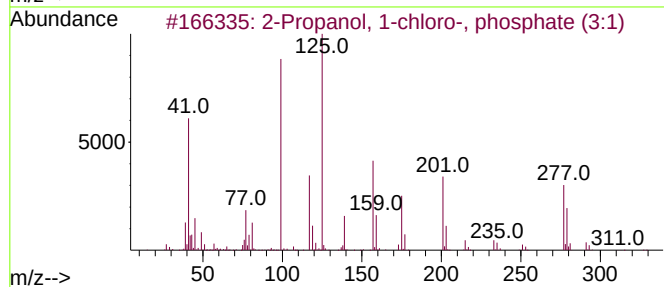
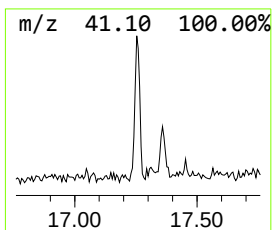
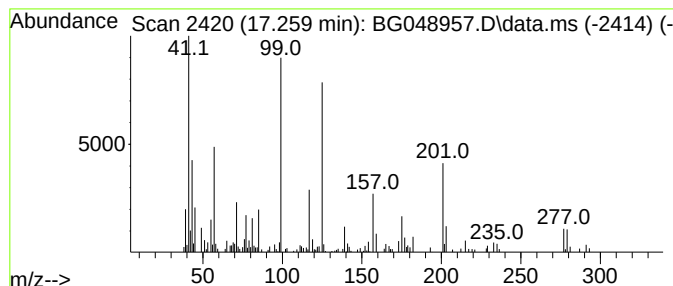
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Propanol, 1-chloro-, phos... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.259	4.31 ng	134846	Phenanthrene-d10	17.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	50		
2	2-Butyl methylphosphonofluoridate	154	C5H12FO2P	000352-52-3	43		
3	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	18		
4	Sarin	140	C4H10FO2P	000107-44-8	14		
5	2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048957.D
Acq On : 14 Jun 2021 20:14
Operator : CG/JU
Sample : M2678-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

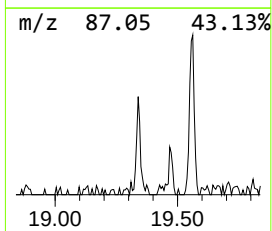
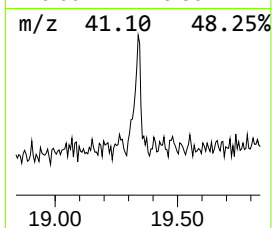
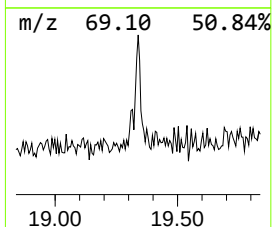
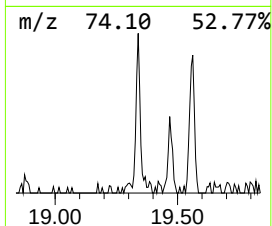
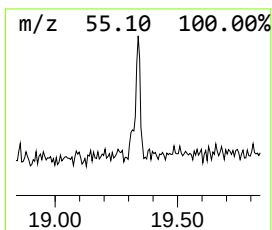
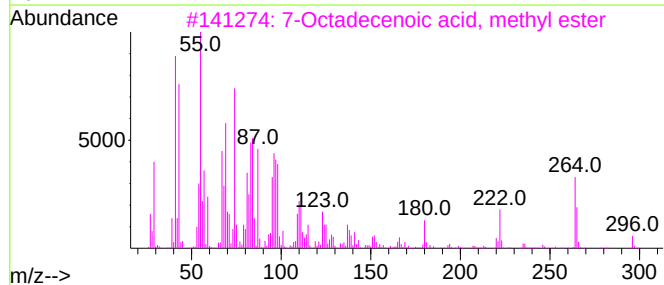
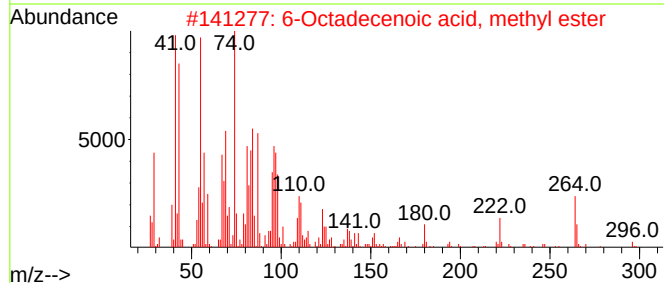
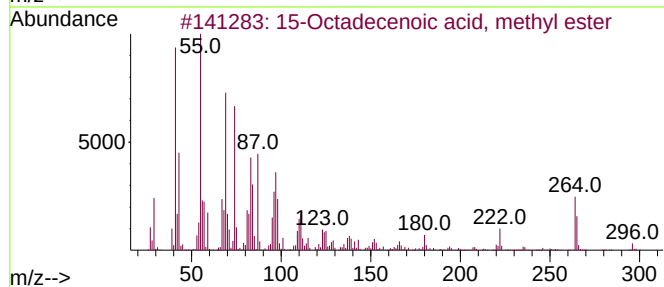
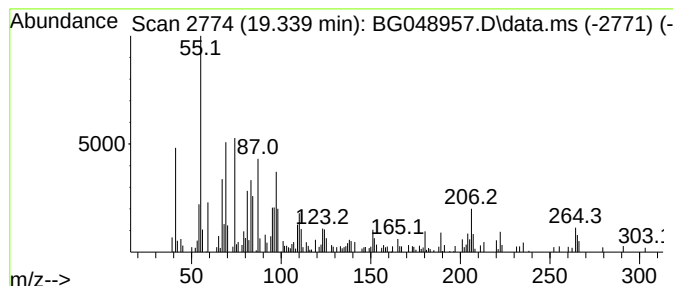
Instrument :
BNA_G
ClientSampleId :
0241-AMND-COMP-F(CL-05)

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 7 15-Octadecenoic acid, methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.339	5.11 ng	160049	Phenanthrene-d10	17.512	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	80
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	74
3	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	68
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	68
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048957.D
Acq On : 14 Jun 2021 20:14
Operator : CG/JU
Sample : M2678-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0241-AMND-COMP-F(CL-05)

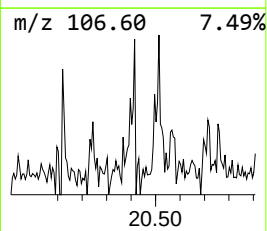
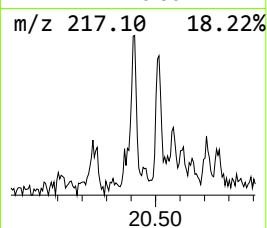
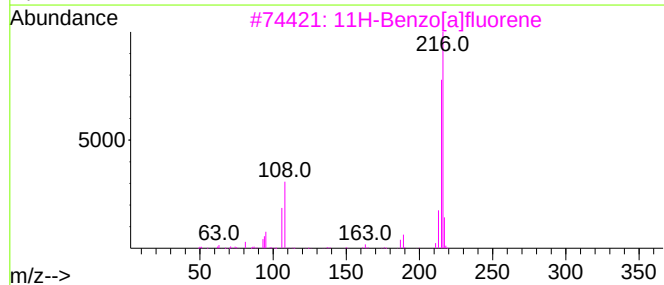
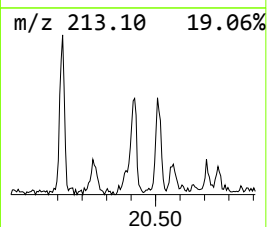
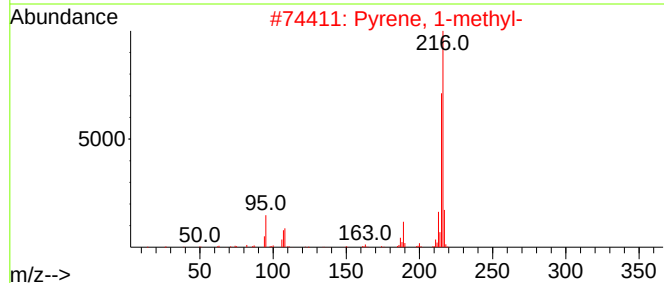
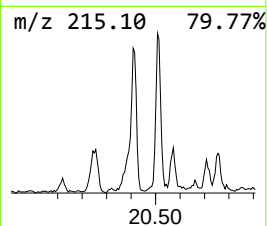
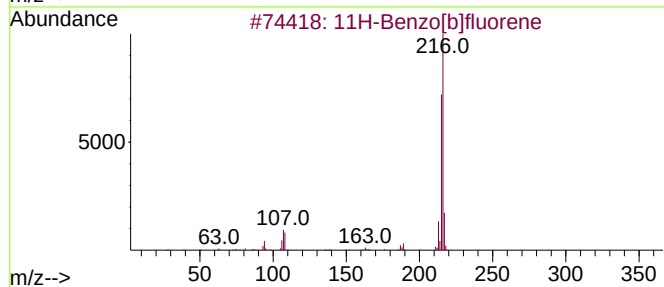
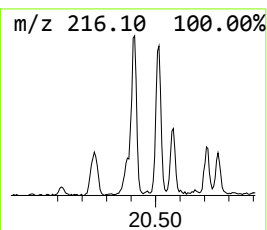
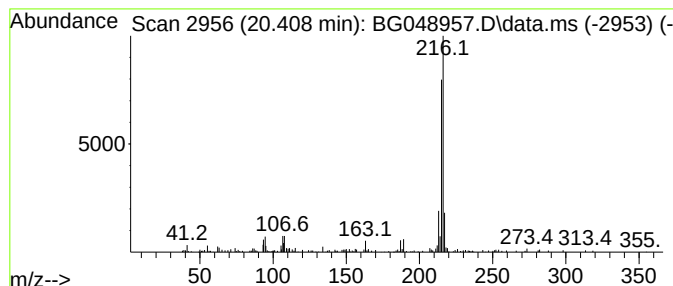
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.408	3.41 ng	174702	Chrysene-d12	21.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048957.D
Acq On : 14 Jun 2021 20:14
Operator : CG/JU
Sample : M2678-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

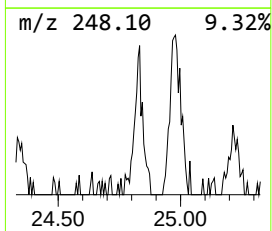
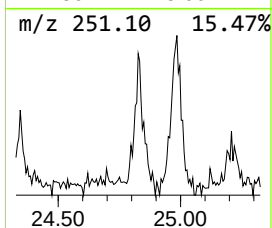
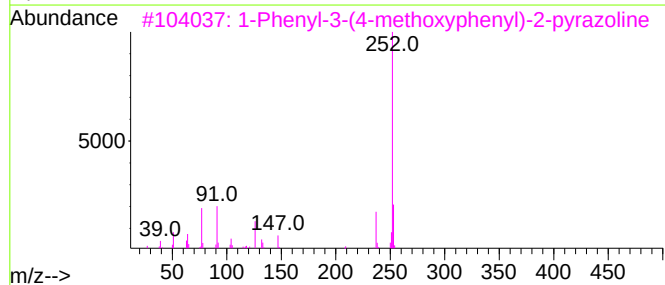
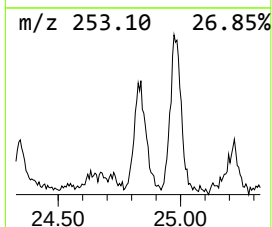
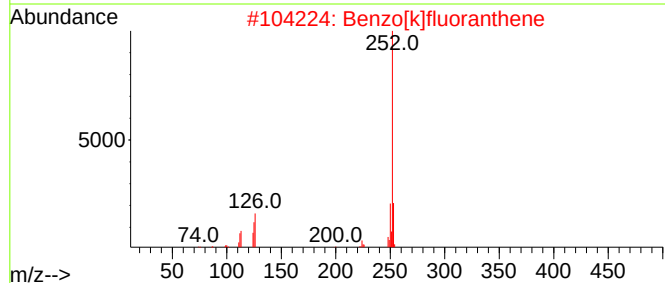
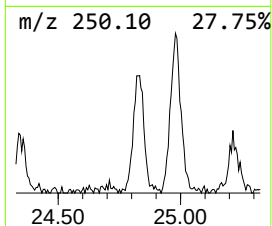
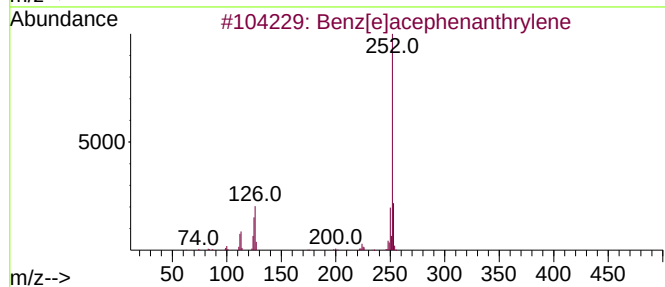
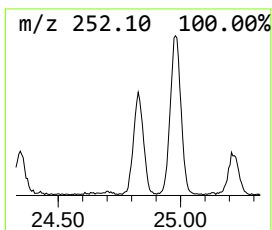
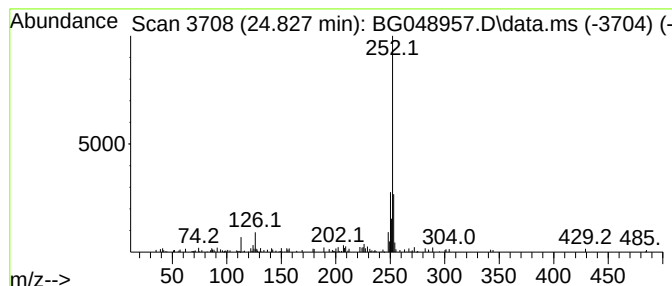
Instrument :
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ClientSampleId :
0241-AMND-COMP-F(CL-05)

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 9 1-Phenyl-3-(4-methoxyphenyl)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.827	5.51 ng	177407	Perylene-d12	25.144	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	68
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	68
3	1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	64
4	1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	62
5	Perylene	252	C20H12	000198-55-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
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Acq On : 14 Jun 2021 20:14
Operator : CG/JU
Sample : M2678-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0241-AMND-COMP-F(CL-05)

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-chlor...	3.164	29.3	ng	391778	1	8.117	267016	20.0
unknown3.287	3.287	12.7	ng	168874	1	8.117	267016	20.0
3-Penten-2-one,...	4.591	11.2	ng	150036	1	8.117	267016	20.0
unknown5.244	5.244	948.2	ng	12659200	1	8.117	267016	20.0
Ethanol, 2-(2-b...	10.708	41.3	ng	771326	2	10.943	373393	20.0
2-Propanol, 1-c...	17.259	4.3	ng	134846	4	17.512	626414	20.0
15-Octadecenoic...	19.339	5.1	ng	160049	4	17.512	626414	20.0
11H-Benzo[b]flu...	20.408	3.4	ng	174702	5	21.807	1025280	20.0
1-Phenyl-3-(4-m...	24.827	5.5	ng	177407	6	25.144	643775	20.0