

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030321\
 Data File : BG048318.D
 Acq On : 3 Mar 2021 18:18
 Operator : CG/JU
 Sample : M1537-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BU-01-030221

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-BG021021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048318.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.580	205	211	218	rBV2	35047	54747	1.43%	0.311%
2	5.192	309	315	323	rBV	32121	54192	1.41%	0.308%
3	5.691	393	400	412	rBV	836543	1418619	36.95%	8.051%
4	7.313	666	676	693	rBV	857417	1600954	41.70%	9.086%
5	8.106	804	811	818	rBV	130207	223596	5.82%	1.269%
6	9.281	1001	1011	1023	rBV	522859	994120	25.89%	5.642%
7	10.926	1282	1291	1301	rBV	148035	309246	8.06%	1.755%
8	13.358	1697	1705	1719	rBV	1221202	2089998	54.44%	11.861%
9	14.187	1839	1846	1853	rBV2	25329	49684	1.29%	0.282%
10	14.739	1933	1940	1947	rBV	270937	462588	12.05%	2.625%
11	16.232	2187	2194	2211	rBV	1322244	2117956	55.17%	12.020%
12	17.483	2398	2407	2412	rBV	383293	642723	16.74%	3.648%
13	17.524	2412	2414	2421	rVV	86347	123443	3.22%	0.701%
14	17.612	2423	2429	2435	rVB	20102	44951	1.17%	0.255%
15	18.123	2512	2516	2522	rVB2	43903	56705	1.48%	0.322%
16	19.105	2677	2683	2689	rBV	69117	110186	2.87%	0.625%
17	19.257	2704	2709	2711	rBV	135051	178007	4.64%	1.010%
18	19.287	2711	2714	2723	rVB3	152579	228408	5.95%	1.296%
19	19.416	2730	2736	2741	rBV2	34104	50751	1.32%	0.288%
20	19.534	2749	2756	2763	rVB	164738	245199	6.39%	1.392%
21	19.892	2813	2817	2824	rVB	134333	198135	5.16%	1.124%
22	20.086	2843	2850	2857	rBV	2896603	3839043	100.00%	21.787%
23	21.343	3057	3064	3066	rBV3	60185	121870	3.17%	0.692%
24	21.408	3071	3075	3081	rVV	82805	167579	4.37%	0.951%
25	21.472	3081	3086	3093	rVB	202190	308601	8.04%	1.751%
26	21.766	3127	3136	3141	rBV2	455827	887432	23.12%	5.036%
27	21.813	3141	3144	3149	rVB	66622	102309	2.66%	0.581%
28	24.011	3513	3518	3522	rBV2	33146	82195	2.14%	0.466%
29	24.898	3664	3669	3675	rVB	42906	89134	2.32%	0.506%
30	25.062	3685	3697	3708	rBV	248709	768428	20.02%	4.361%

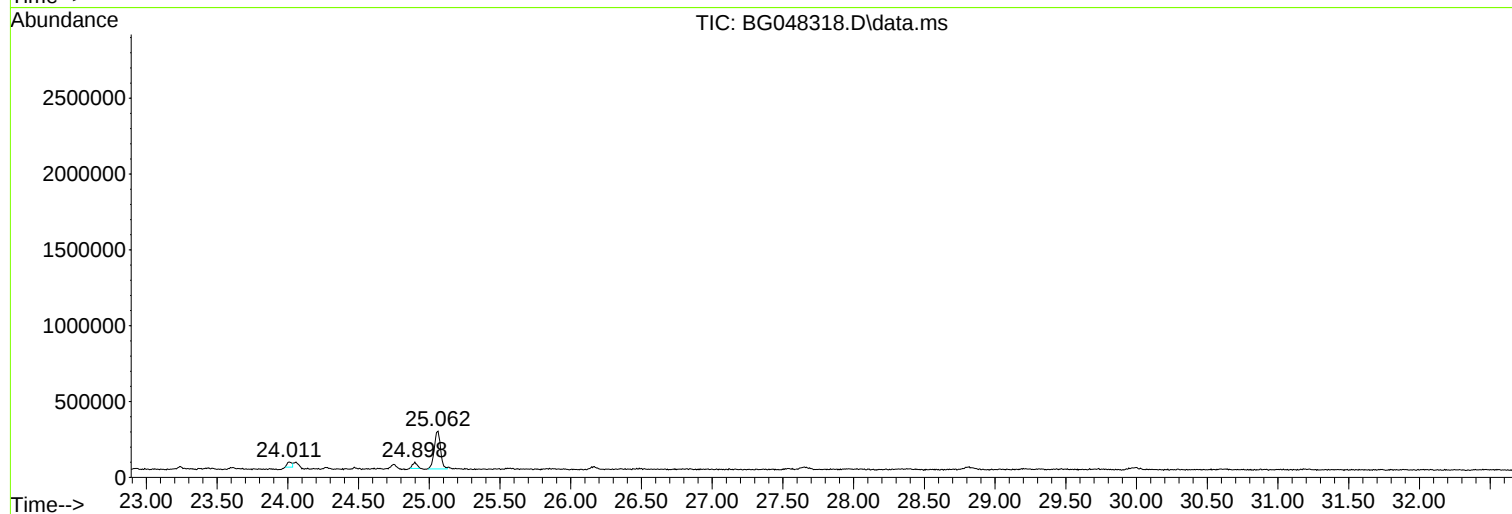
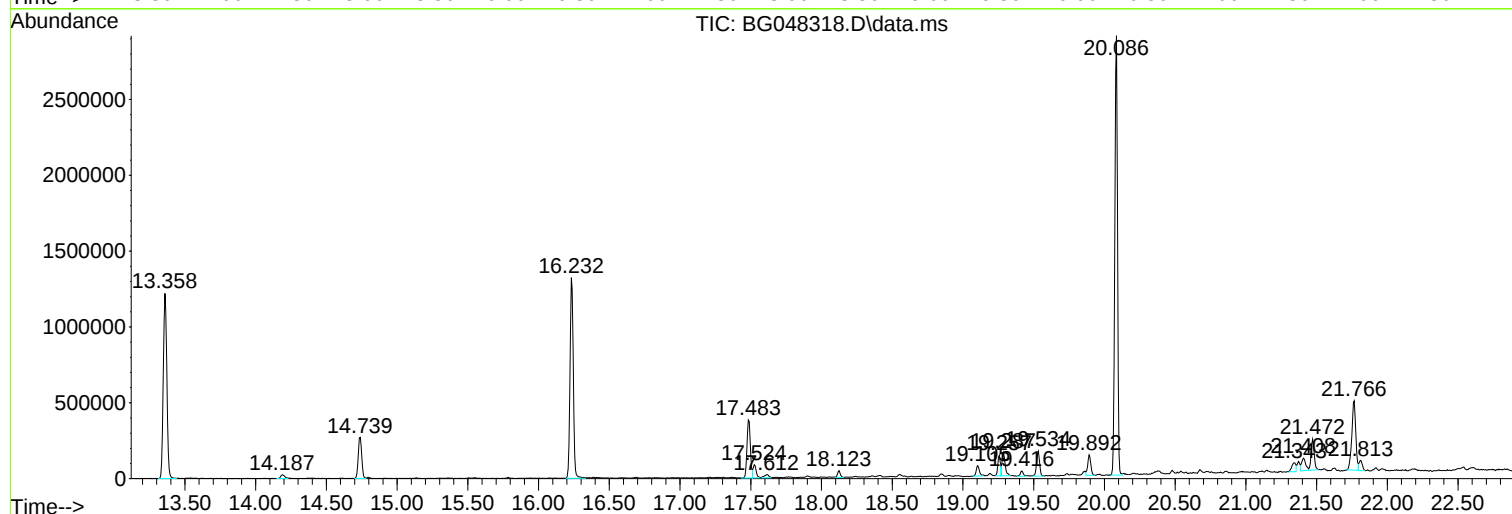
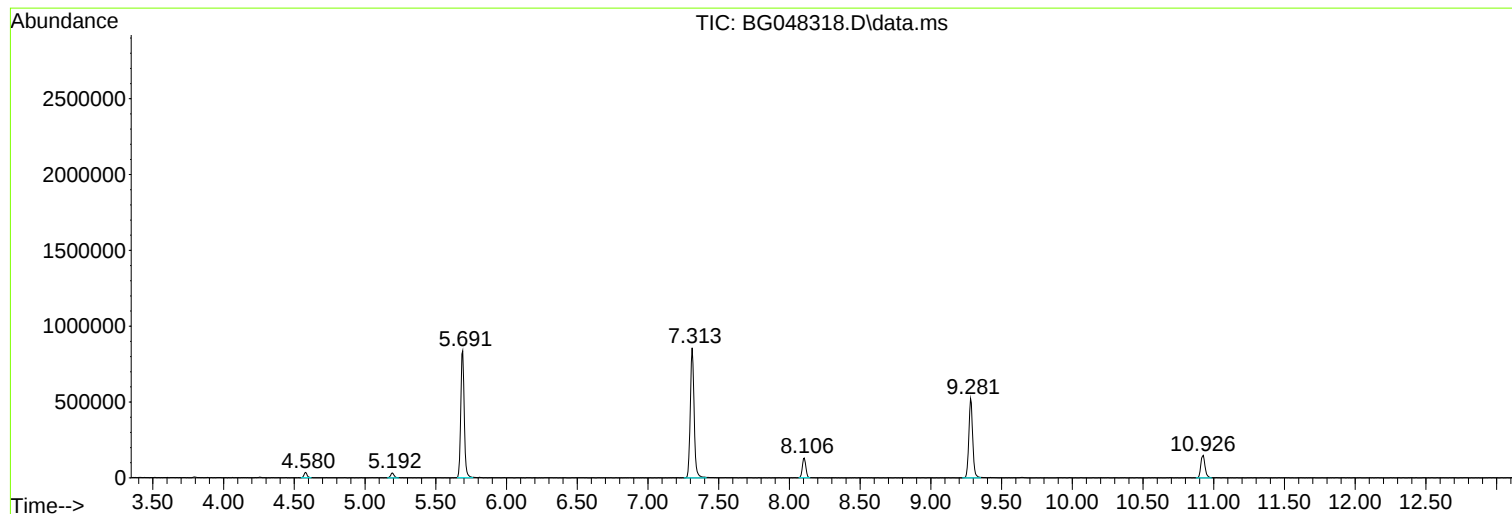
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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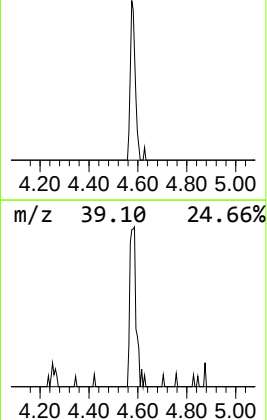
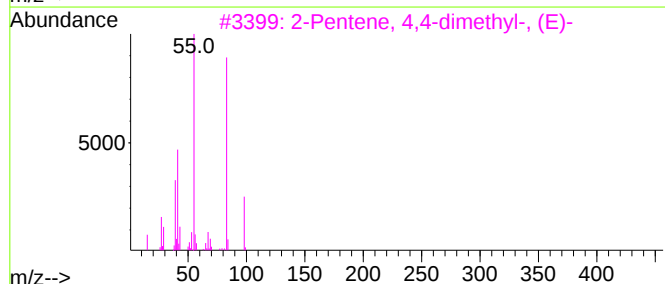
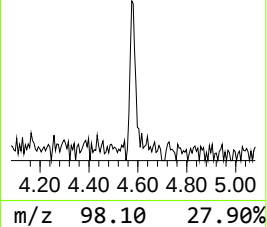
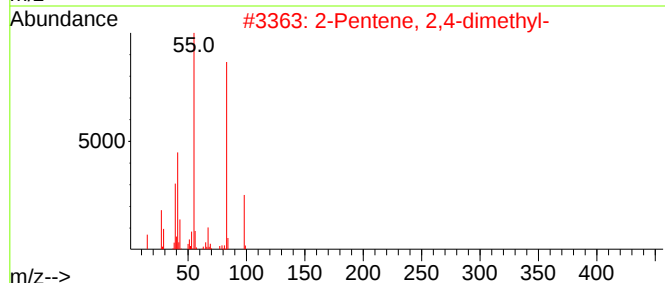
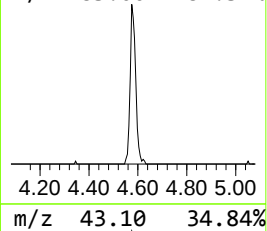
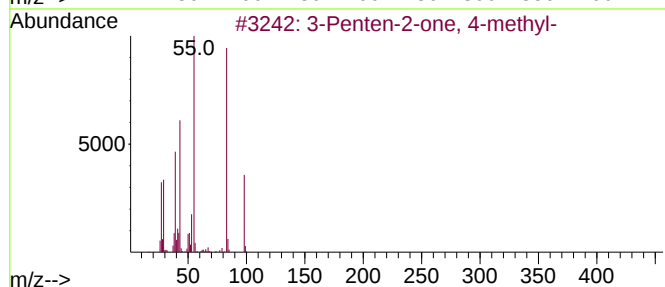
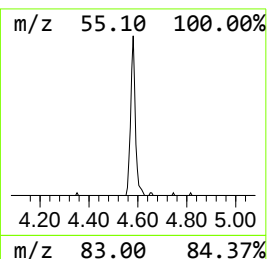
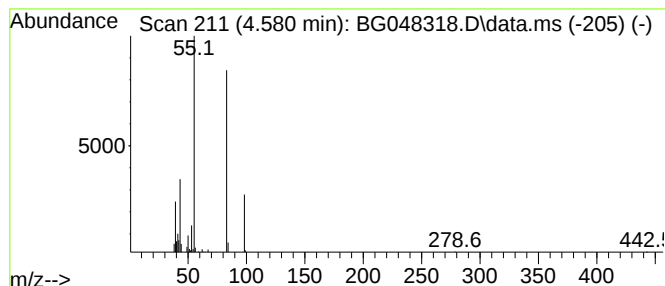
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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.580	4.90 ng	54747	1,4-Dichlorobenzene-d4	8.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
4			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80



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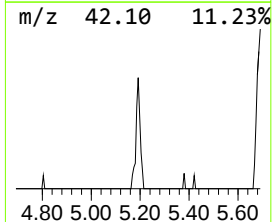
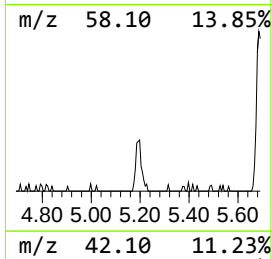
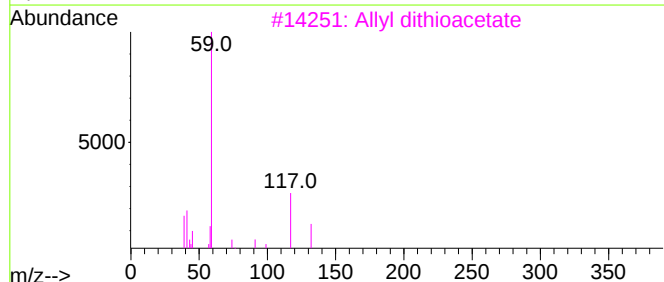
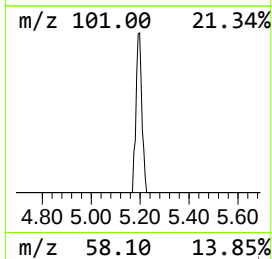
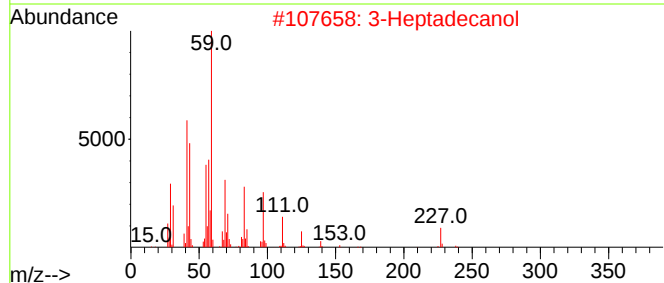
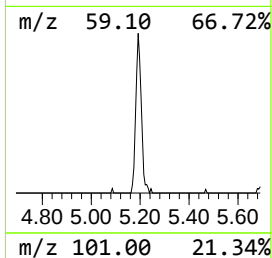
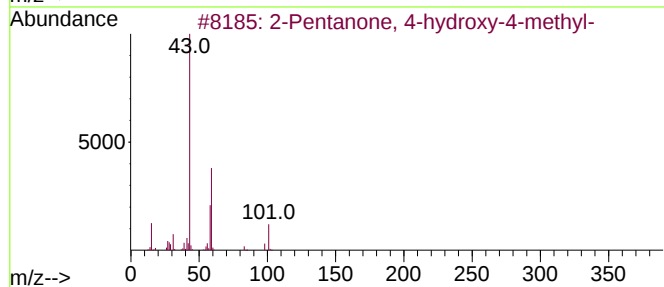
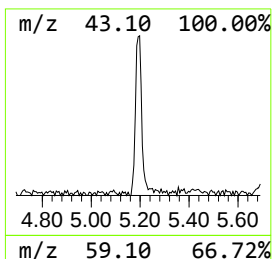
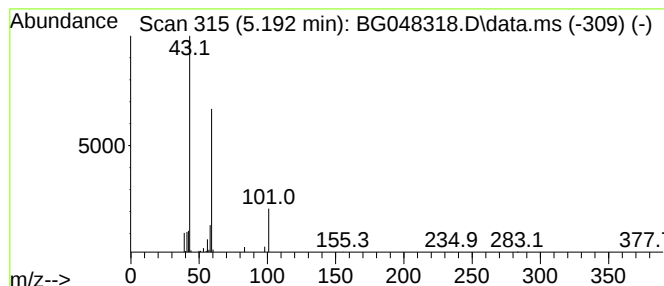
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	4.85 ng	54192	1,4-Dichlorobenzene-d4	8.106

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		3-Heptadecanol	256	C17H36O	084534-30-5	23
3		Allyl dithioacetate	132	C5H8S2	027249-83-8	17
4		Butane	58	C4H10	000106-97-8	12
5		5-Hexen-2-one	98	C6H10O	000109-49-9	10



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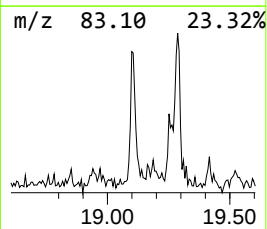
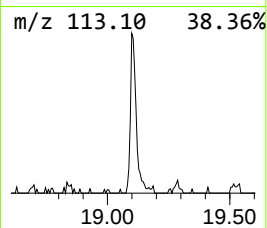
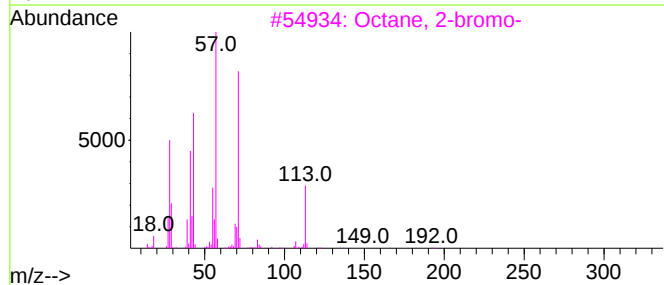
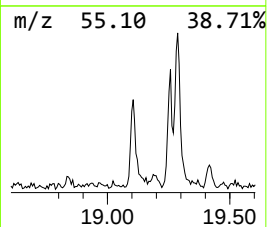
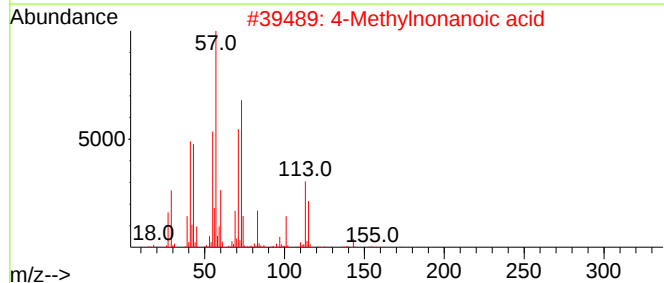
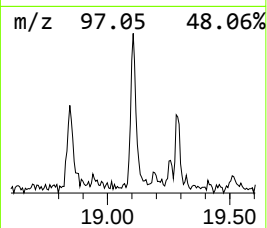
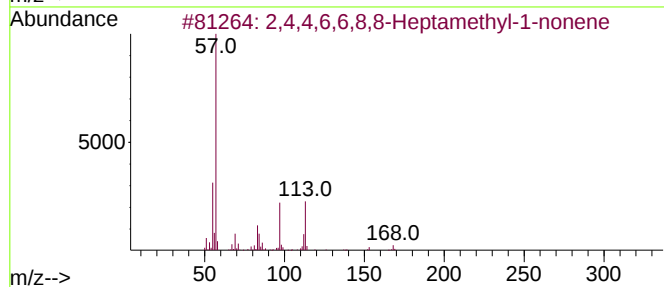
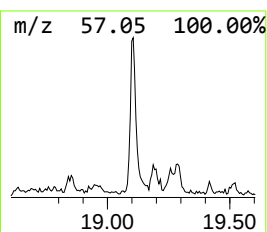
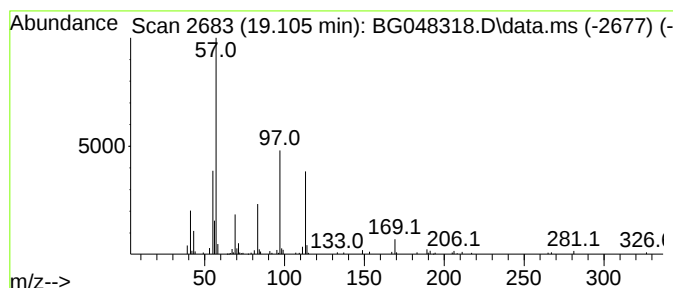
Instrument :
BNA_G
ClientSampleId :
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Peak Number 3 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.105	3.43 ng	110186	Phenanthrene-d10	17.483	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64
2	4-Methylnonanoic acid	172	C10H20O2	045019-28-1	33
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
4	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	25
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F502	1000365-51-0	16



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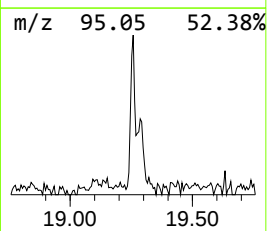
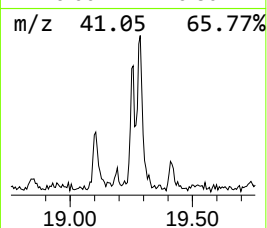
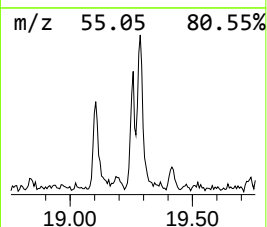
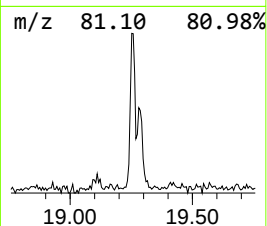
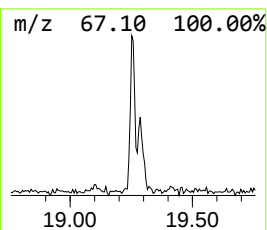
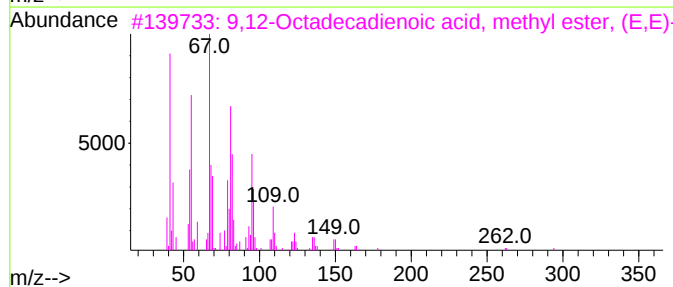
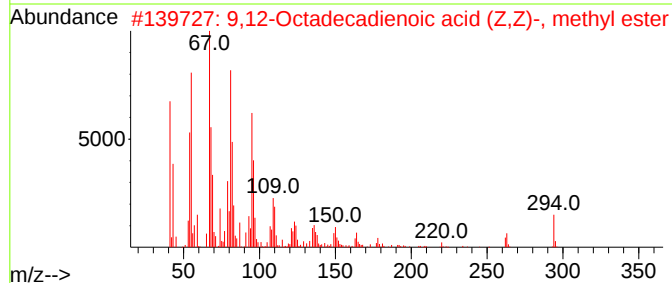
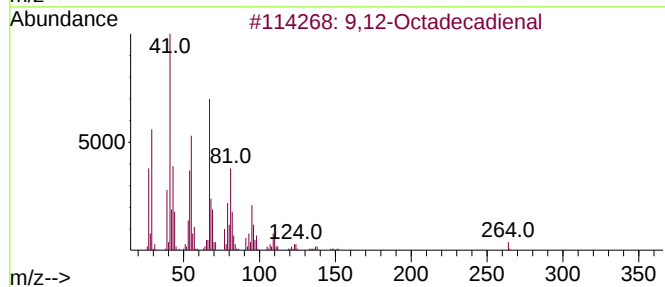
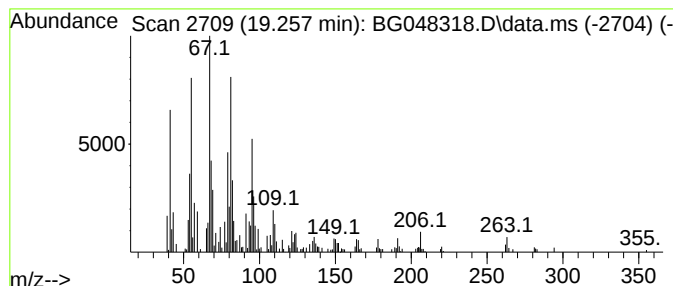
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Peak Number 4 9,12-Octadecadienal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.257	5.54 ng	178007	Phenanthrene-d10	17.483

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienal	264	C18H32O	026537-70-2	96
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
3		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95
4		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	95
5		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93



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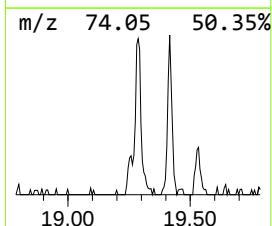
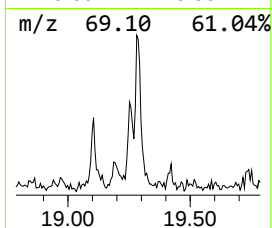
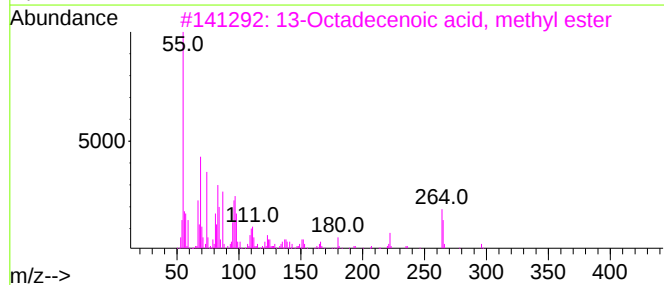
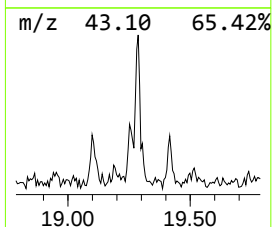
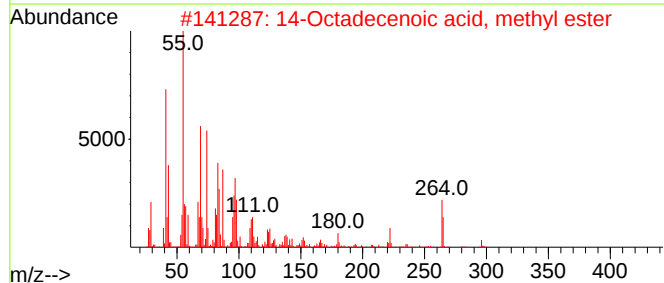
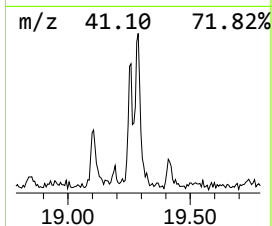
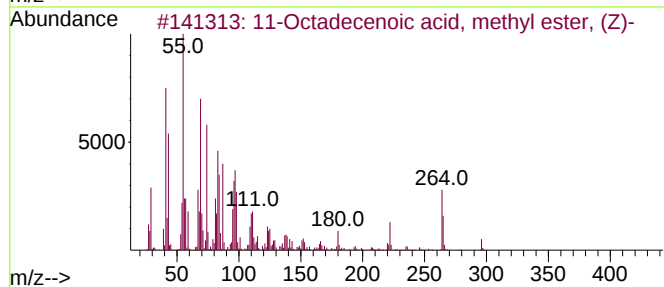
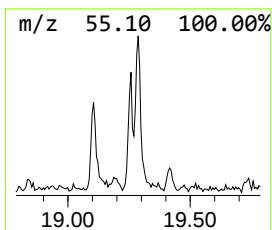
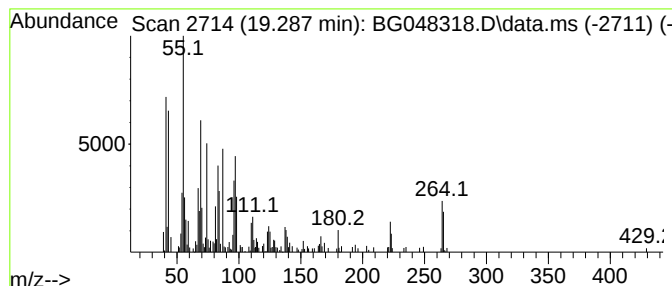
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Peak Number 5 11-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.287	7.11 ng	228408	Phenanthrene-d10	17.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	94
2			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	94
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	87
5			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87



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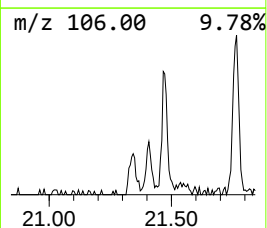
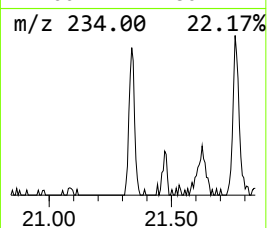
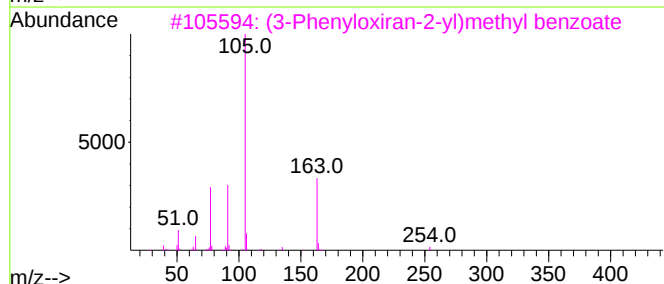
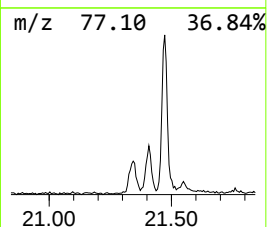
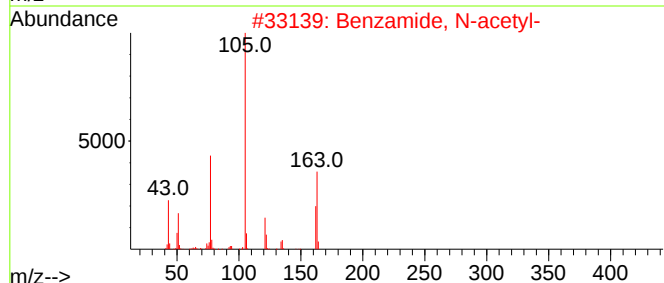
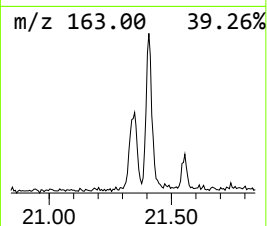
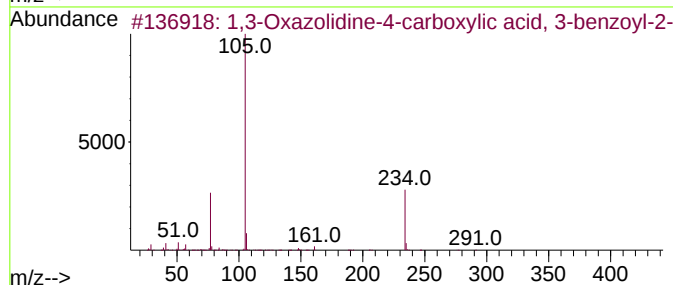
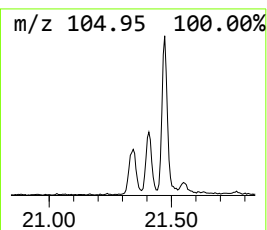
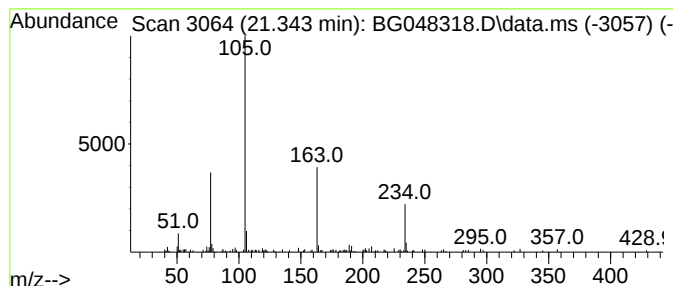
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.343 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.343	2.75 ng	121870	Chrysene-d12	21.766

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Oxazolidine-4-carboxylic aci...	291	C16H21NO4	1000196-90-4	47
2			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	42
3			(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	42
4			Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	36
5			3-Benzoyl-5-(9'-methylidenanthra...	425	C25H15NO2S2	299929-16-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030321\
Data File : BG048318.D
Acq On : 3 Mar 2021 18:18
Operator : CG/JU
Sample : M1537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-01-030221

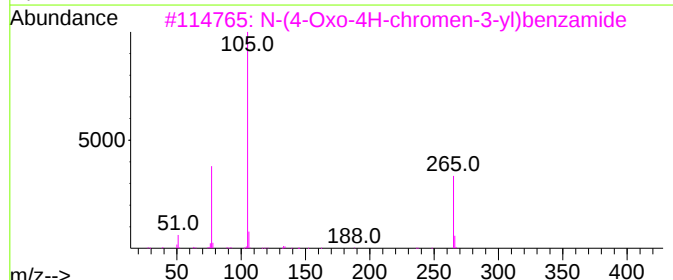
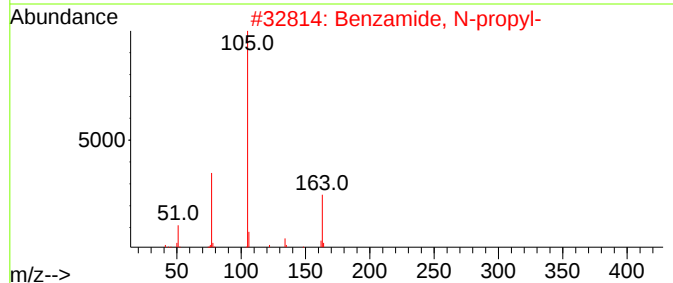
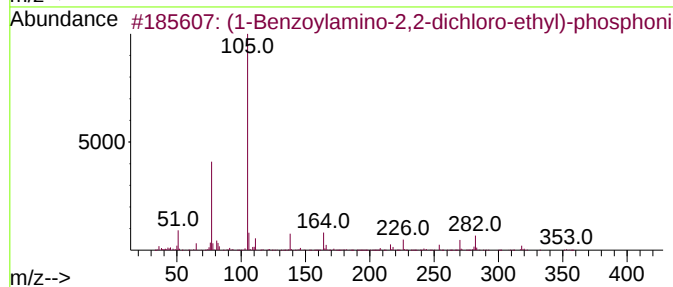
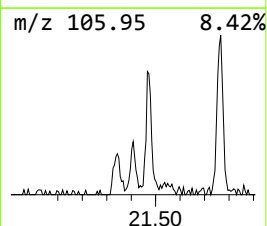
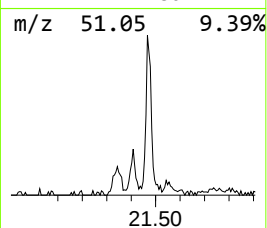
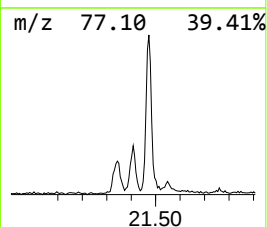
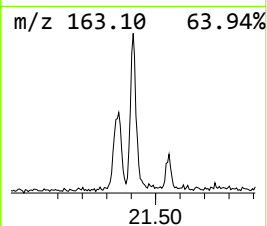
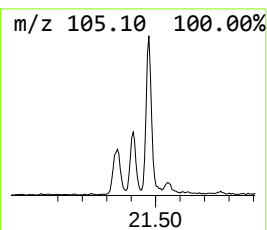
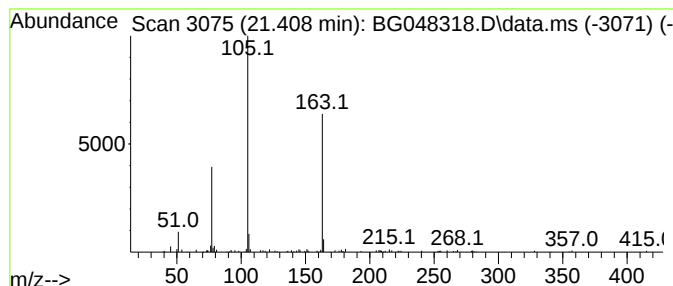
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.408 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.408	3.78 ng	167579	Chrysene-d12	21.766

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1-Benzoylamino-2,2-dichloro-eth...	353	C13H18Cl2NO4P	1000278-05-7	47
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	47
3			N-(4-Oxo-4H-chromen-3-yl)benzamide	265	C16H11NO3	1000243-49-5	46
4			3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	46
5			4,5-Bis(benzoylthio)-1,2-dithiol...	406	C17H10O2S5	082504-65-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030321\
Data File : BG048318.D
Acq On : 3 Mar 2021 18:18
Operator : CG/JU
Sample : M1537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-01-030221

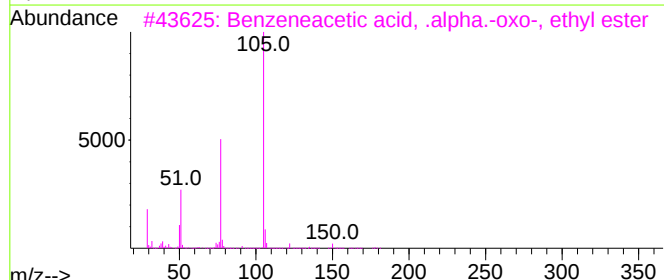
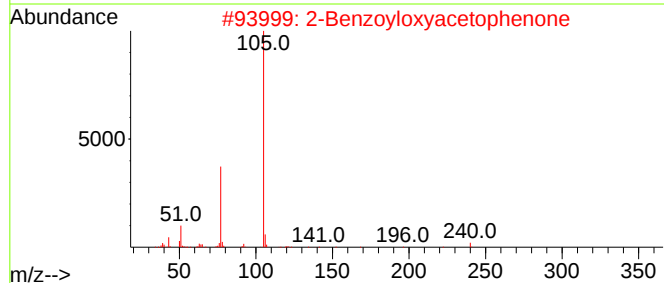
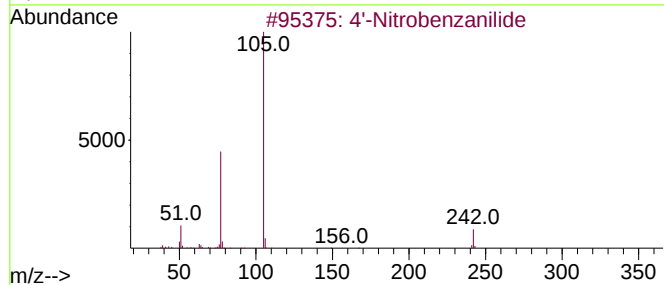
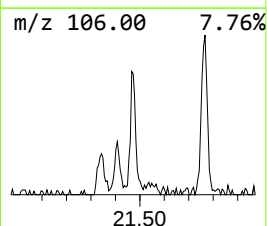
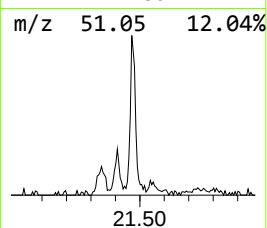
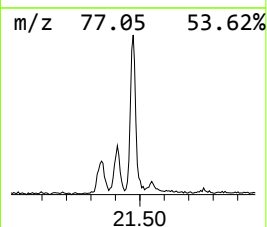
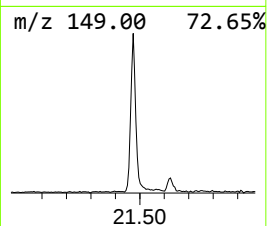
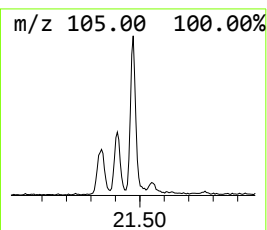
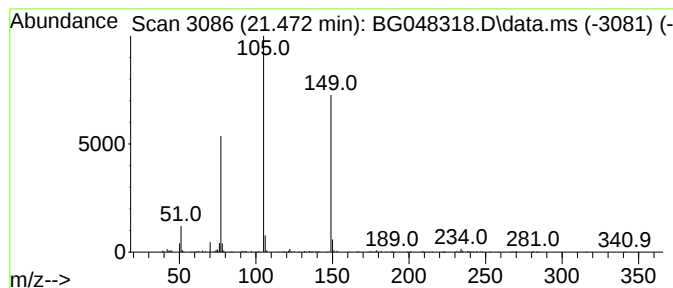
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown21.473 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.473	6.95 ng	308601	Chrysene-d12	21.766

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	49
2			2-Benzoyloxyacetophenone	240	C15H12O3	004010-33-7	47
3			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
4			N-[1-(3-Benzoyl-4-methyl-5-oxo-o...	350	C20H18N2O4	1000296-93-4	47
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030321\
Data File : BG048318.D
Acq On : 3 Mar 2021 18:18
Operator : CG/JU
Sample : M1537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-01-030221

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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
3-Penten-2-one,...	4.580	4.9	ng	54747	1	8.106	223596	20.0
2-Pentanone, 4-...	5.192	4.8	ng	54192	1	8.106	223596	20.0
2,4,4,6,6,8,8-H...	19.105	3.4	ng	110186	4	17.483	642723	20.0
9,12-Octadecadi...	19.257	5.5	ng	178007	4	17.483	642723	20.0
11-Octadecenoic...	19.287	7.1	ng	228408	4	17.483	642723	20.0
unknown21.343	21.343	2.8	ng	121870	5	21.766	887432	20.0
unknown21.408	21.408	3.8	ng	167579	5	21.766	887432	20.0
unknown21.473	21.473	7.0	ng	308601	5	21.766	887432	20.0