

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040521\
 Data File : BG048590.D
 Acq On : 5 Apr 2021 19:19
 Operator : CG/JU
 Sample : M1897-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-1

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-BG033021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.166	306	311	316	rBV2	6867	11538	1.02%	0.168%
2	5.636	383	391	401	rBV	309059	489917	43.17%	7.142%
3	7.240	655	664	672	rBV	326075	553958	48.81%	8.076%
4	8.092	802	809	821	rVB	118071	189989	16.74%	2.770%
5	9.261	1000	1008	1017	rBV	198822	365532	32.21%	5.329%
6	10.918	1282	1290	1299	rBV	148510	257913	22.73%	3.760%
7	13.362	1700	1706	1714	rBV	564669	846474	74.59%	12.341%
8	13.532	1730	1735	1737	rBV5	7021	12206	1.08%	0.178%
9	13.626	1744	1751	1756	rBV	52611	85141	7.50%	1.241%
10	14.185	1840	1846	1850	rBV3	22520	37878	3.34%	0.552%
11	14.384	1877	1880	1885	rBV6	11525	20425	1.80%	0.298%
12	14.490	1893	1898	1902	rBV8	21014	45899	4.04%	0.669%
13	14.531	1902	1905	1908	rVV4	20317	30416	2.68%	0.443%
14	14.572	1908	1912	1917	rVB6	31387	50723	4.47%	0.739%
15	14.655	1917	1926	1929	rBV9	18431	45606	4.02%	0.665%
16	14.707	1931	1935	1936	rVV4	21655	27690	2.44%	0.404%
17	14.743	1936	1941	1948	rVB	237341	376454	33.17%	5.488%
18	14.837	1952	1957	1964	rBV	18401	52706	4.64%	0.768%
19	15.066	1992	1996	1997	rBV3	10489	14002	1.23%	0.204%
20	15.377	2045	2049	2050	rBV4	13341	19107	1.68%	0.279%
21	15.407	2050	2054	2058	rVB6	30423	47310	4.17%	0.690%
22	15.536	2072	2076	2080	rBV3	61776	86472	7.62%	1.261%
23	16.235	2189	2195	2205	rBV	408187	672473	59.25%	9.804%
24	17.498	2406	2410	2415	rVB	268195	401779	35.40%	5.858%
25	20.107	2849	2854	2860	rVB	876790	1134909	100.00%	16.546%
26	21.429	3075	3079	3091	rVB	39507	93078	8.20%	1.357%
27	21.793	3136	3141	3149	rVB2	269514	437497	38.55%	6.378%
28	24.179	3545	3547	3556	rVB8	7745	14509	1.28%	0.212%
29	25.131	3699	3709	3719	rBV	141948	422350	37.21%	6.157%
30	26.364	3913	3919	3922	rBV7	8953	15253	1.34%	0.222%

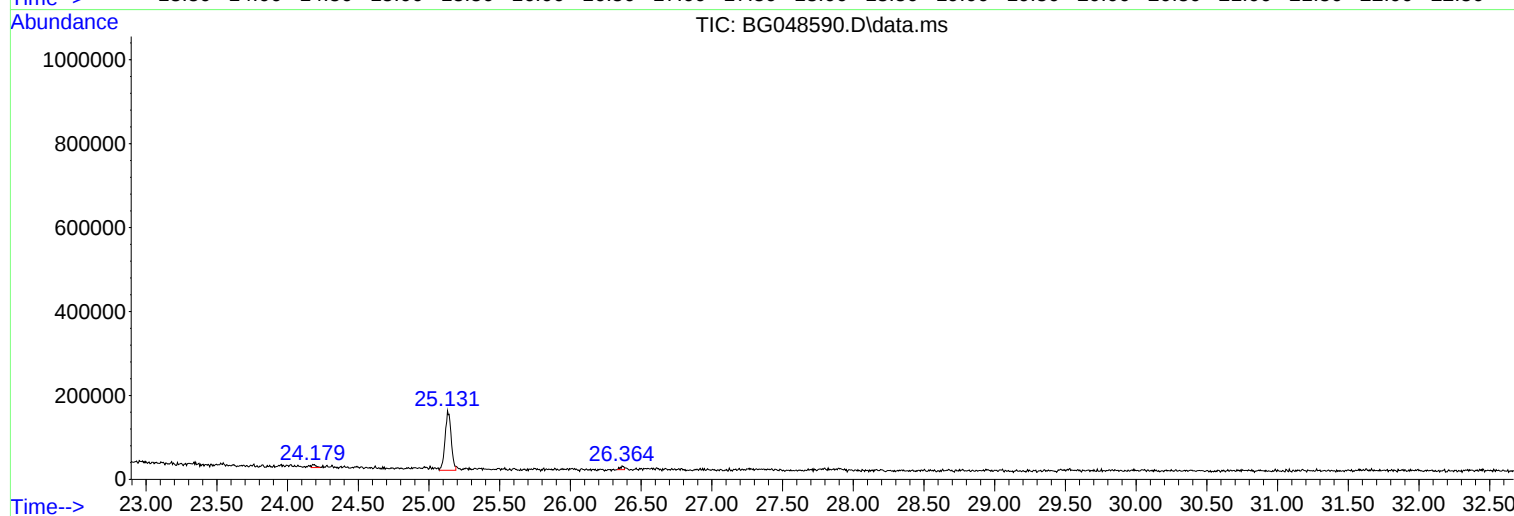
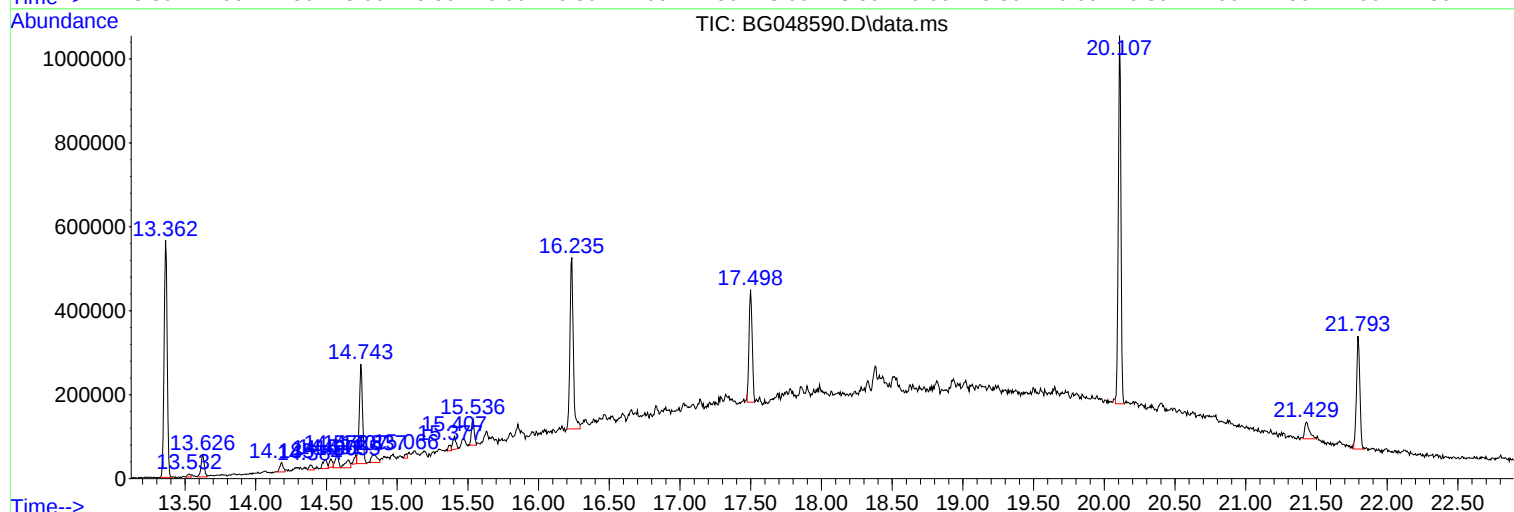
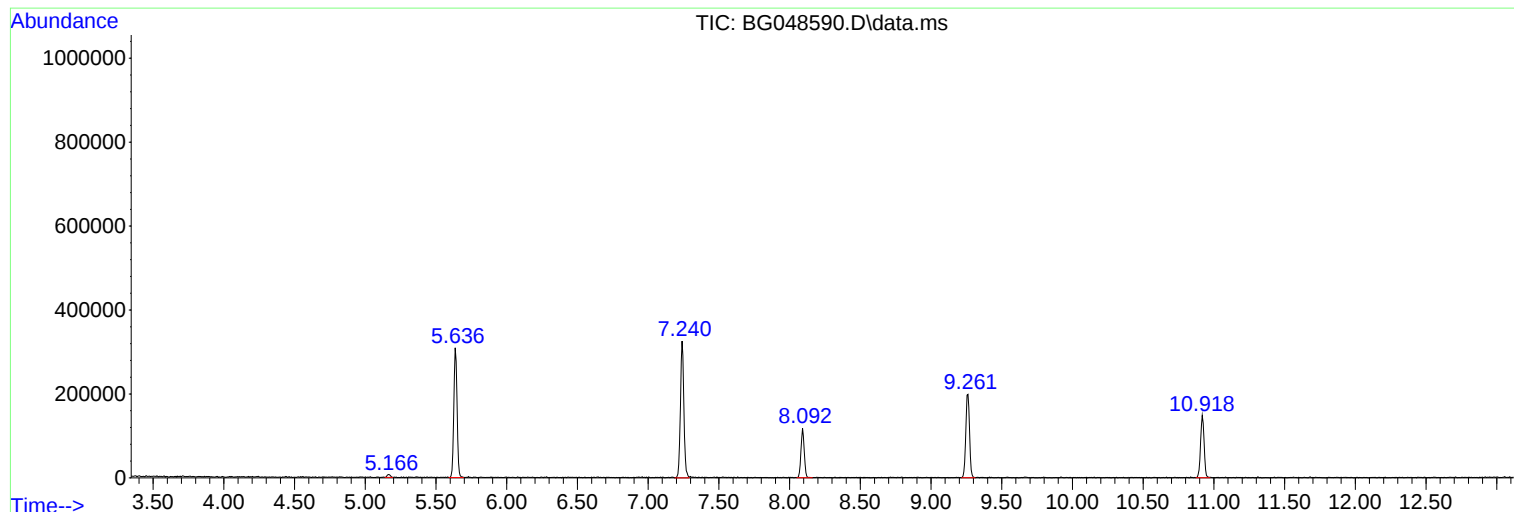
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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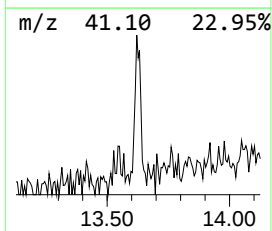
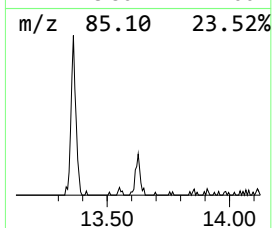
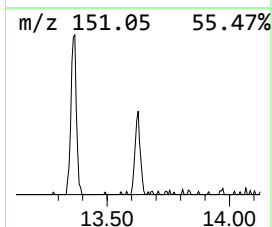
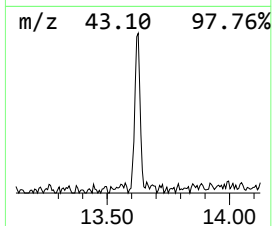
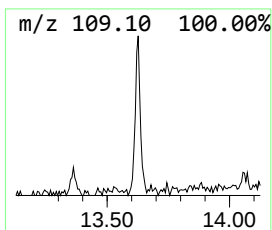
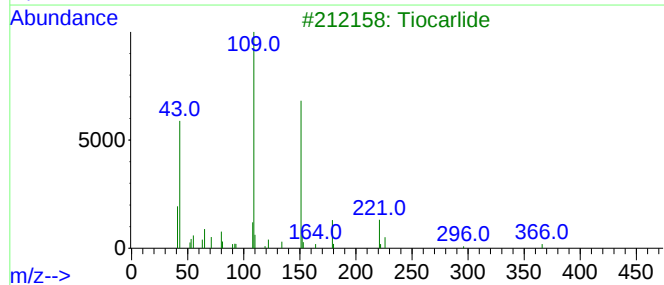
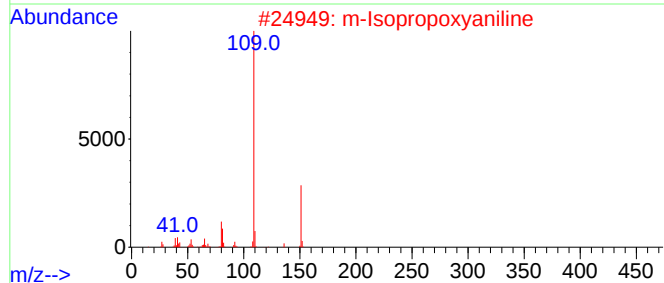
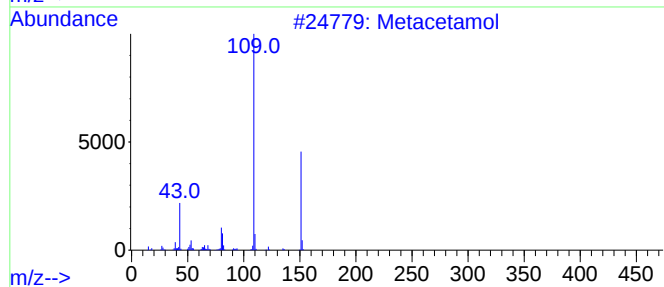
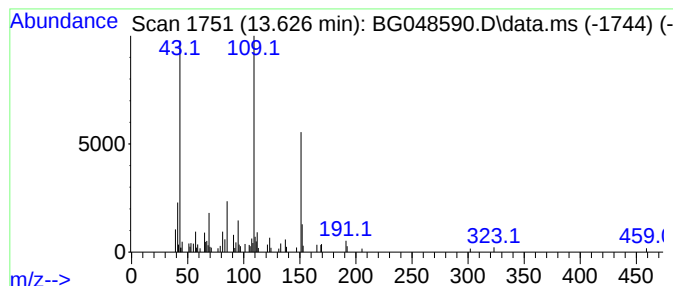
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Peak Number 1 Metacetamol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.626	4.52 ng	85141	Acenaphthene-d10	14.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Metacetamol	151	C8H9NO2	000621-42-1	58
2			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
3			Tiocarlide	400	C23H32N2O2S	000910-86-1	53
4			Hydroxy-.alpha.-terpenyl acetate	212	C12H20O3	1000293-00-9	43
5			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43



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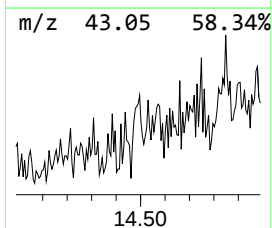
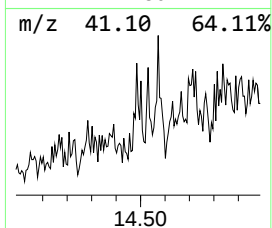
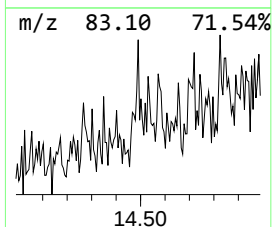
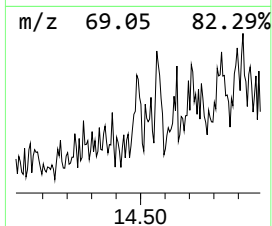
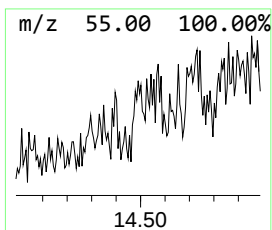
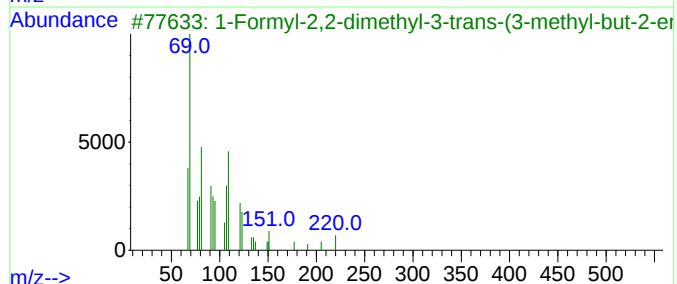
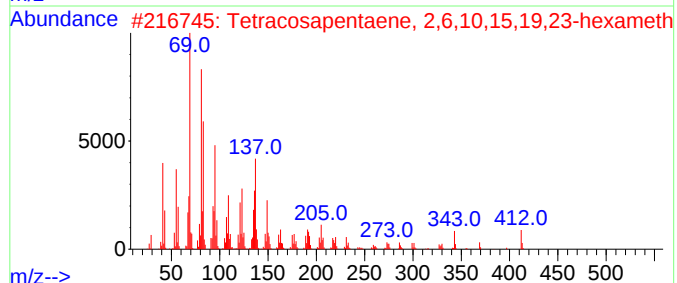
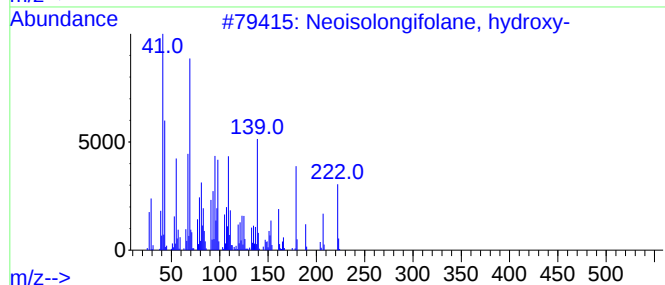
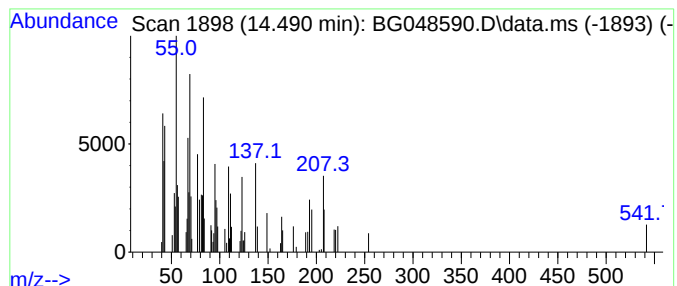
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Peak Number 2 unknown14.490 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.490	2.44 ng	45899	Acenaphthene-d10	14.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neoisolongifolane, hydroxy-	222	C15H26O	1000159-37-9	47
2			Tetracosapentaene, 2,6,10,15,19,...	412	C30H52	026266-08-0	38
3			1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	32
4			Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-94-0	27
5			Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-95-1	27



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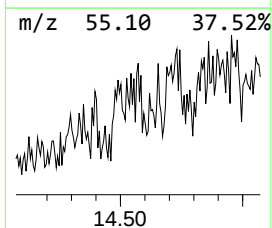
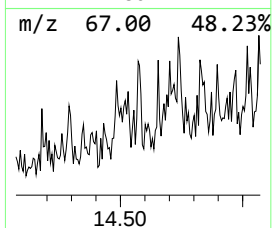
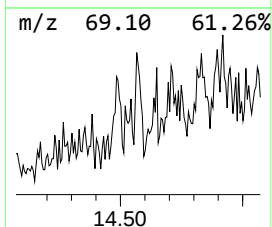
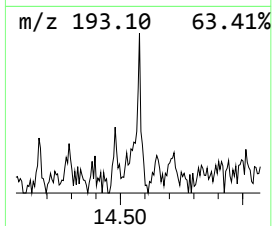
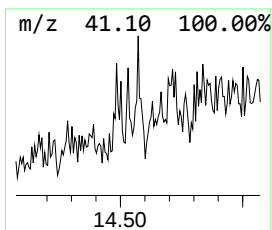
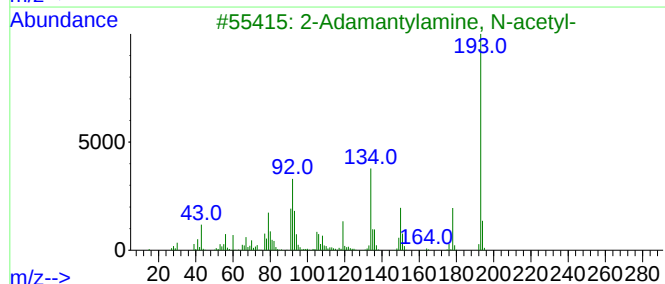
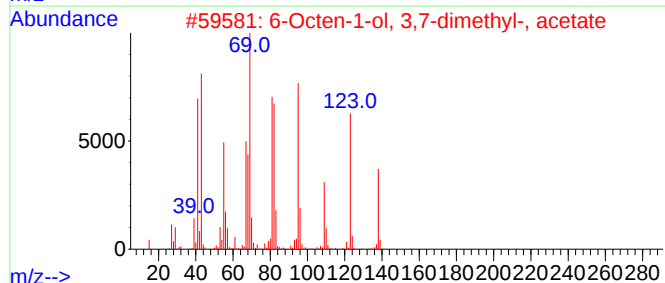
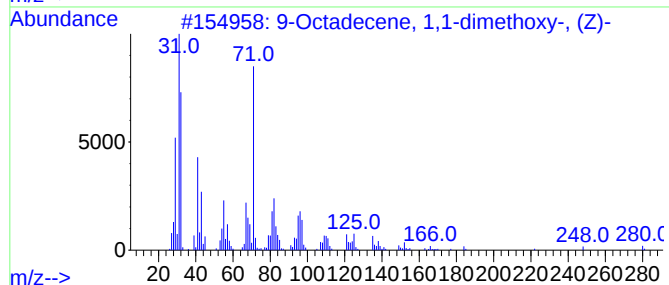
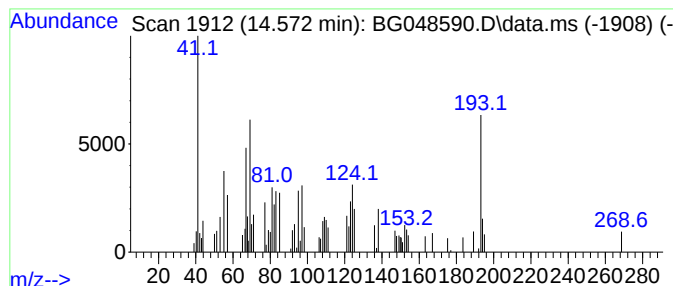
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Peak Number 3 unknown14.572 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.572	2.69 ng	50723	Acenaphthene-d10	14.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, 1,1-dimethoxy-, (Z)-	312	C20H40O2	015677-71-1	27		
2	6-Octen-1-ol, 3,7-dimethyl-, ace...	198	C12H22O2	000150-84-5	22		
3	2-Adamantylamine, N-acetyl-	193	C12H19NO	052917-72-3	15		
4	Succinic acid, di(3,7-dimethyl-oc...	394	C24H42O4	1000353-35-2	14		
5	5-Hepten-1-ol, 2,6-dimethyl-	142	C9H18O	004234-93-9	14		



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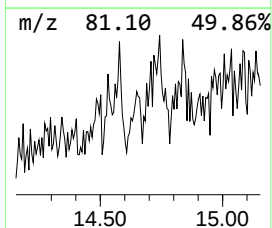
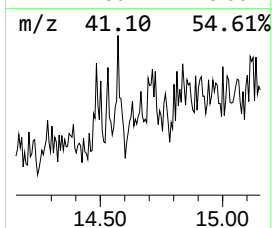
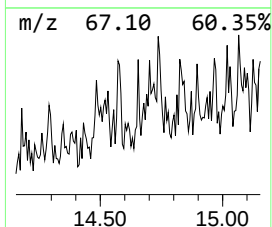
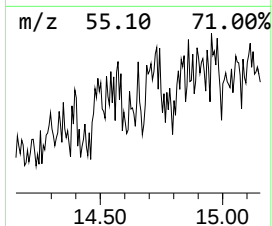
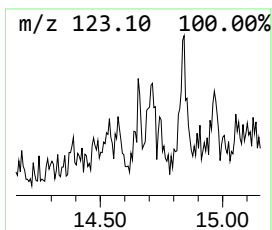
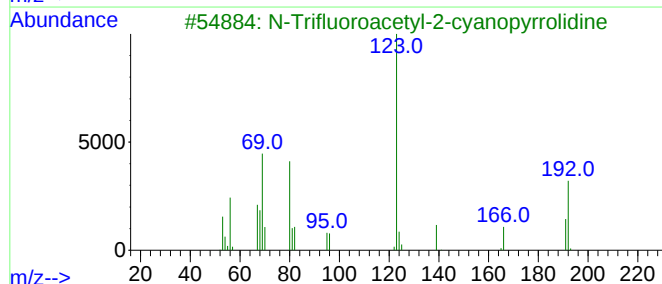
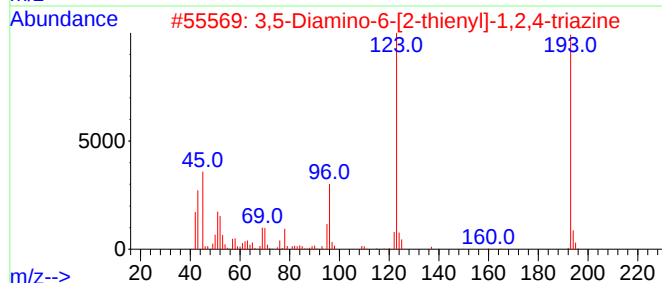
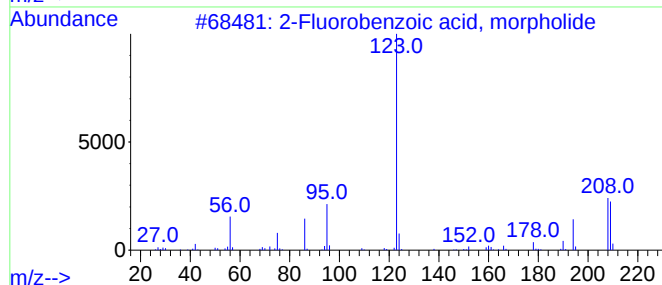
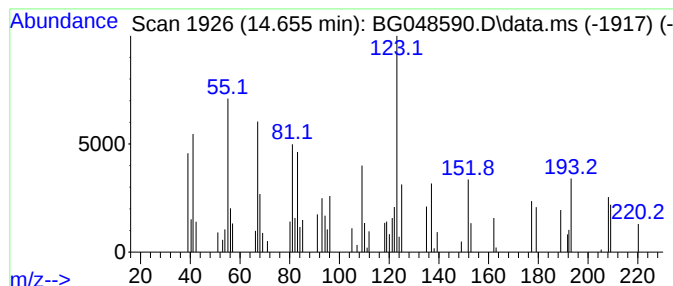
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Peak Number 4 unknown14.655 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.655	2.42 ng	45606	Acenaphthene-d10	14.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Fluorobenzoic acid, morpholide	209	C11H12FNO2	1000307-07-7	35
2			3,5-Diamino-6-[2-thienyl]-1,2,4-...	193	C7H7N5S	058848-66-1	22
3			N-Trifluoroacetyl-2-cyanopyrroli...	192	C7H7F3N2O	1000281-44-6	22
4			Benzenemethanol, 3-amino-	123	C7H9NO	001877-77-6	18
5			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	18



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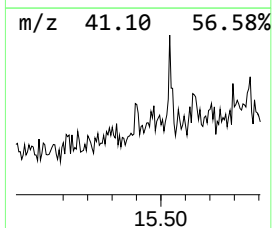
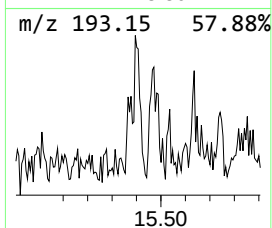
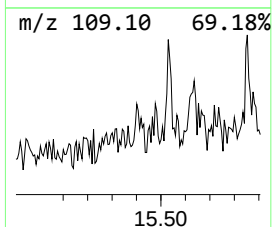
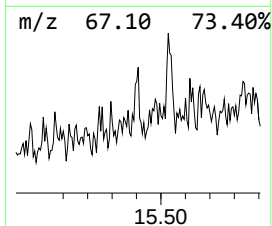
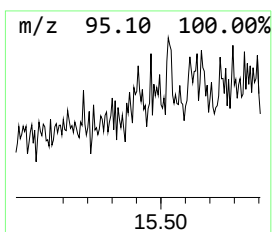
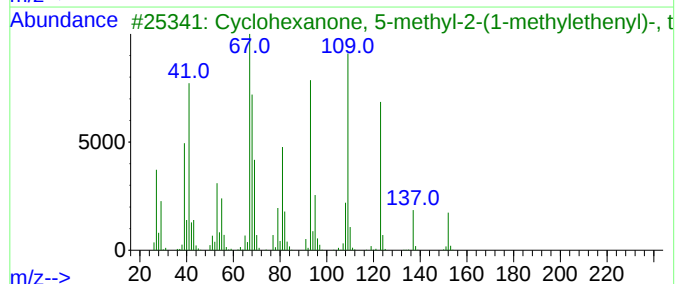
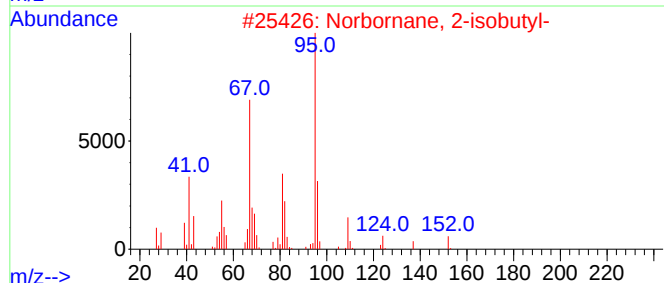
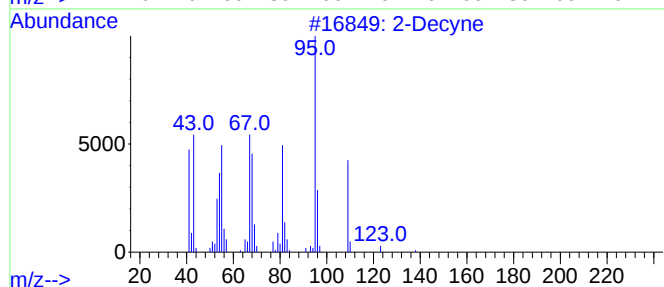
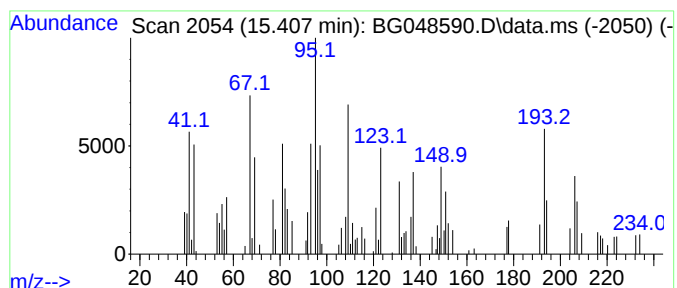
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown15.407 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.407	2.51 ng	47310	Acenaphthene-d10	14.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decyne	138	C10H18	002384-70-5	37
2			Norbornane, 2-isobutyl-	152	C11H20	018127-14-5	35
3			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	029606-79-9	30
4			(Cyclopropyl)trivinyisilane	150	C9H14Si	1000109-93-8	25
5			Cyclopropane, (2,2-dimethylpropy...	110	C8H14	039647-71-7	22



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TP-1

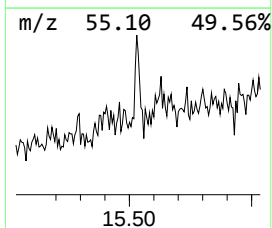
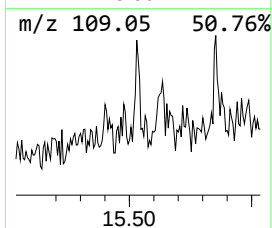
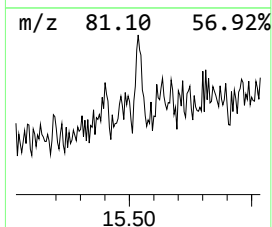
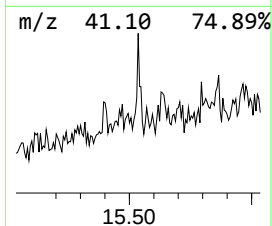
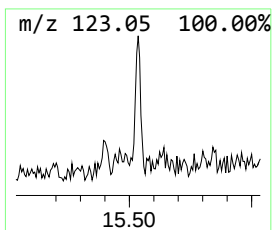
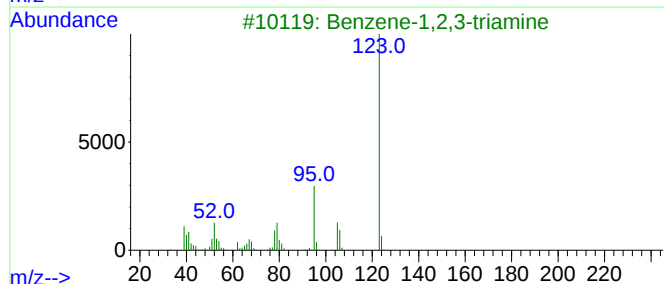
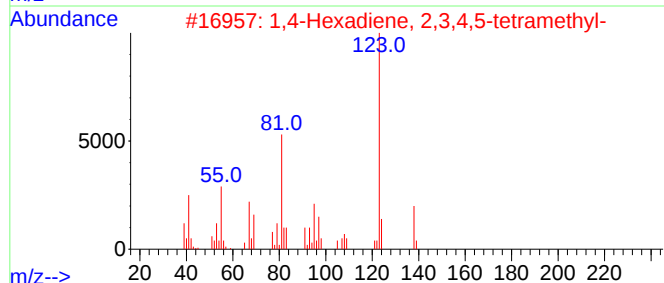
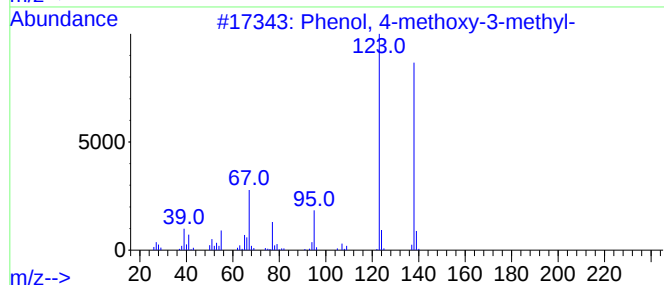
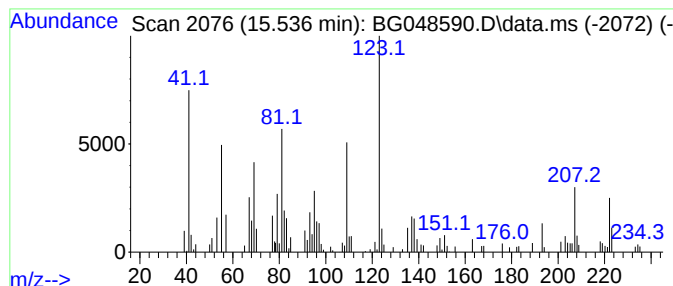
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.536 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	4.59 ng	86472	Acenaphthene-d10	14.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-methoxy-3-methyl-	138	C8H10O2	014786-82-4	38
2			1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	38
3			Benzene-1,2,3-triamine	123	C6H9N3	1000316-45-3	38
4			1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	38
5			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040521\
Data File : BG048590.D
Acq On : 5 Apr 2021 19:19
Operator : CG/JU
Sample : M1897-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
TP-1

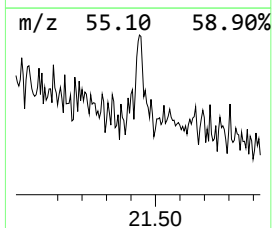
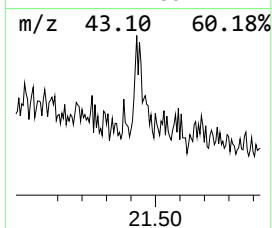
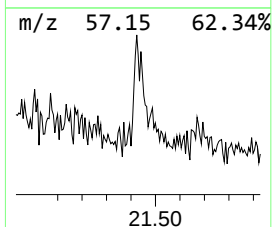
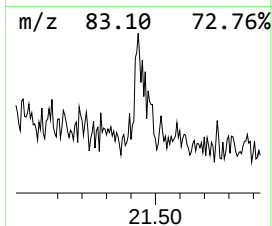
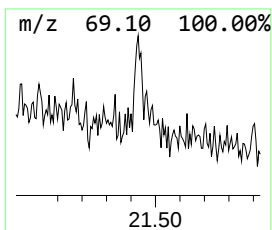
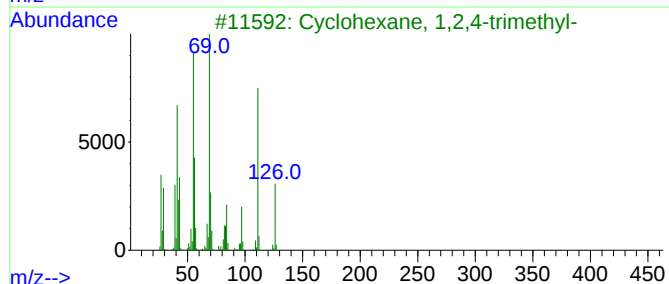
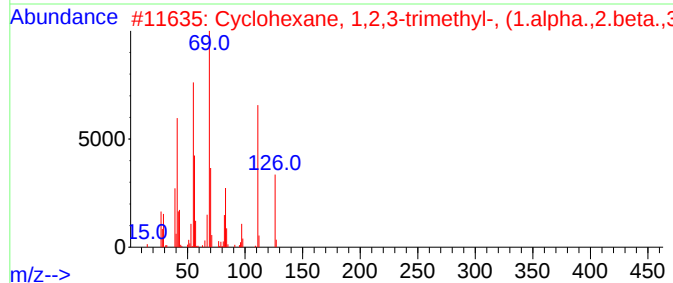
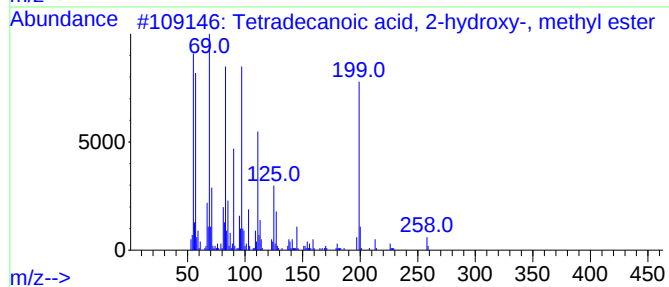
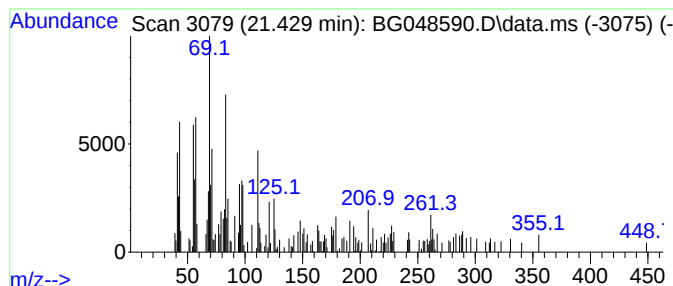
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid, 2-hydro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.429	4.26 ng	93078	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid, 2-hydroxy-, ...	258	C15H30O3	056009-40-6	64
2			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001678-81-5	49
3			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	46
4			Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	45
5			Cyclopentane, 1-butyl-2-ethyl-	154	C11H22	072993-32-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040521\
Data File : BG048590.D
Acq On : 5 Apr 2021 19:19
Operator : CG/JU
Sample : M1897-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.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
Metacetamol	13.626	4.5	ng	85141	3	14.743	376454	20.0
unknown14.490	14.490	2.4	ng	45899	3	14.743	376454	20.0
unknown14.572	14.572	2.7	ng	50723	3	14.743	376454	20.0
unknown14.655	14.655	2.4	ng	45606	3	14.743	376454	20.0
unknown14.837	14.837	2.8	ng	52706	3	14.743	376454	20.0
unknown15.407	15.407	2.5	ng	47310	3	14.743	376454	20.0
unknown15.536	15.536	4.6	ng	86472	3	14.743	376454	20.0
Tetradecanoic a...	21.429	4.3	ng	93078	5	21.793	437497	20.0