

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
 Data File : BG048403.D
 Acq On : 17 Mar 2021 18:29
 Operator : CG/JU
 Sample : M1686-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SW-SUMMER-STREET

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-BG031621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.583	204	212	220	rBV	1126255	1652197	44.63%	9.043%
2	5.194	309	316	326	rBV	1014797	1523010	41.14%	8.336%
3	5.658	389	395	403	rBV	178824	280068	7.56%	1.533%
4	7.256	656	667	676	rBV	747172	1292942	34.92%	7.077%
5	8.114	805	813	822	rBV	227817	379507	10.25%	2.077%
6	8.761	916	923	932	rVB2	20017	41129	1.11%	0.225%
7	9.278	1004	1011	1019	rVB	573164	994897	26.87%	5.446%
8	10.934	1284	1293	1305	rBV2	302715	541225	14.62%	2.962%
9	13.379	1700	1709	1716	rBV	1507807	2338372	63.16%	12.799%
10	14.195	1843	1848	1858	rVB	61619	91448	2.47%	0.501%
11	14.754	1935	1943	1949	rBV	528725	798296	21.56%	4.369%
12	17.503	2404	2411	2416	rBV	659583	1008280	27.23%	5.519%
13	18.379	2556	2560	2565	rBV5	37244	53928	1.46%	0.295%
14	18.813	2628	2634	2638	rVB7	28125	38967	1.05%	0.213%
15	18.902	2641	2649	2655	rBV8	24133	60393	1.63%	0.331%
16	19.154	2688	2692	2697	rBV2	90973	111343	3.01%	0.609%
17	19.554	2755	2760	2766	rVB	101039	145243	3.92%	0.795%
18	19.912	2818	2821	2829	rVB	80722	115359	3.12%	0.631%
19	20.112	2849	2855	2861	rBV	2959369	3702211	100.00%	20.264%
20	21.017	3005	3009	3014	rVB3	31295	44948	1.21%	0.246%
21	21.375	3066	3070	3072	rBV2	39897	62475	1.69%	0.342%
22	21.422	3074	3078	3087	rVV2	277578	516529	13.95%	2.827%
23	21.510	3088	3093	3100	rVB	311823	459979	12.42%	2.518%
24	21.792	3135	3141	3147	rBV	602449	1032937	27.90%	5.654%
25	25.135	3701	3710	3719	rVB3	349500	984244	26.59%	5.387%

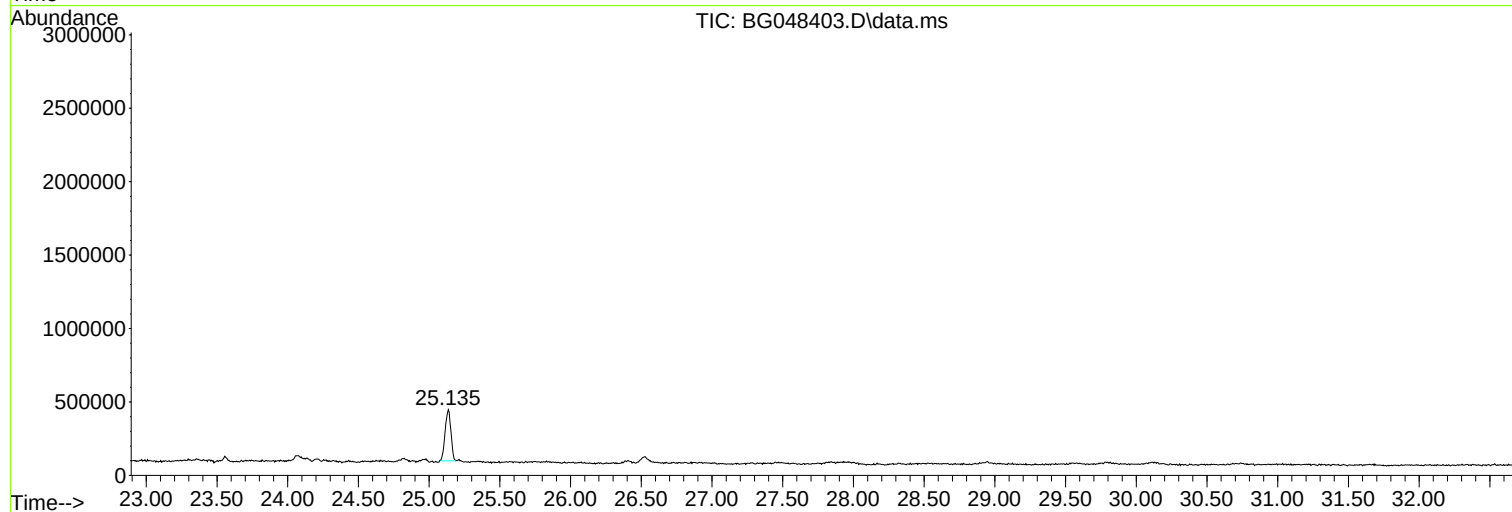
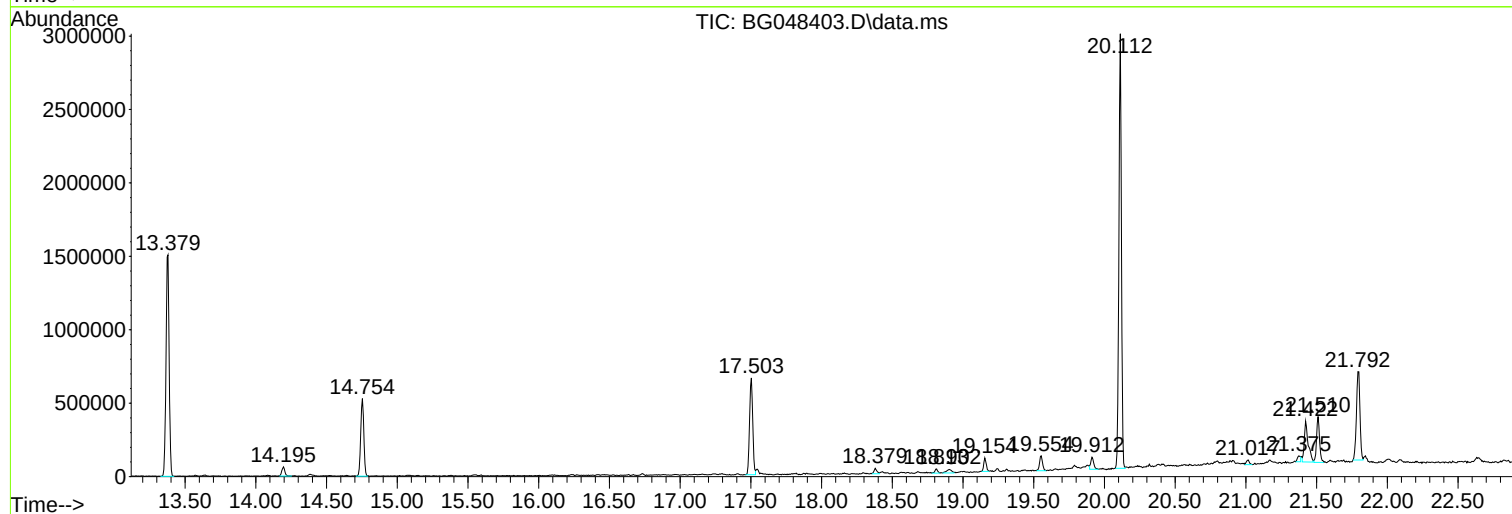
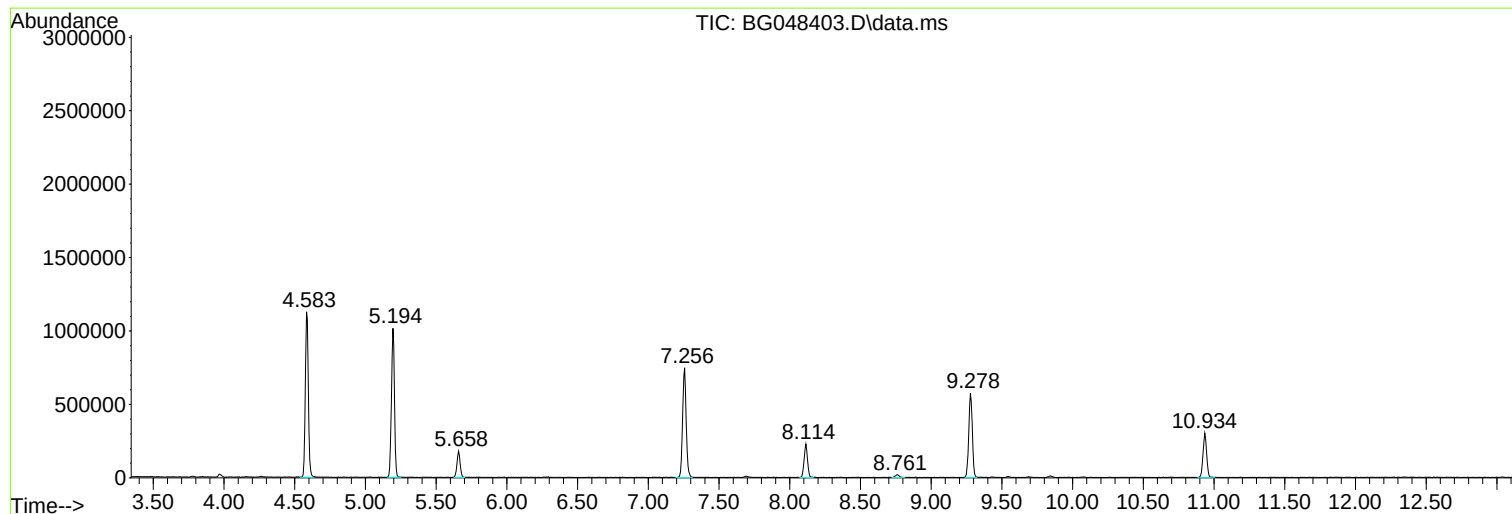
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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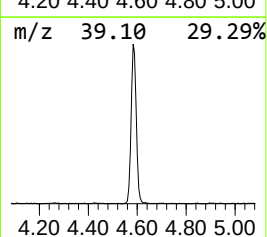
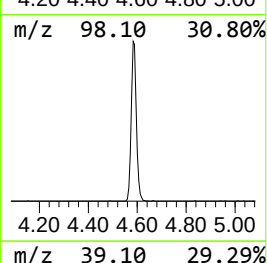
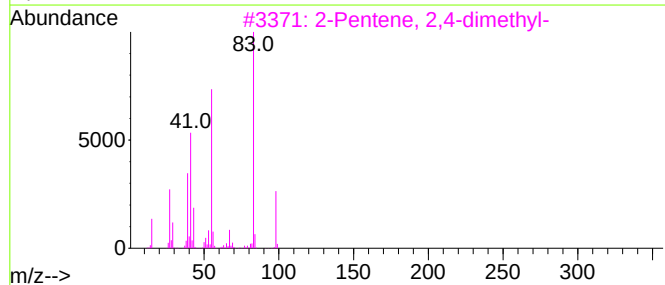
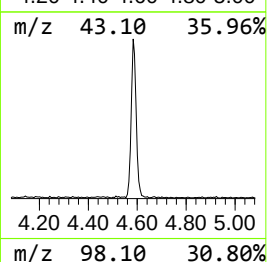
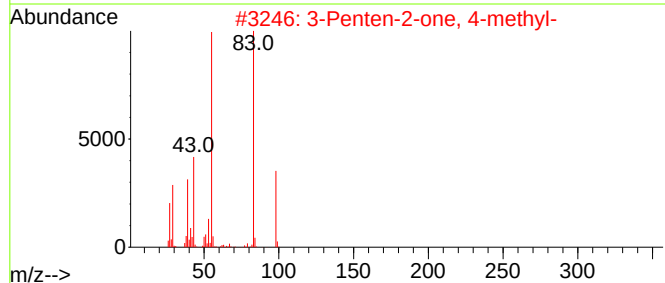
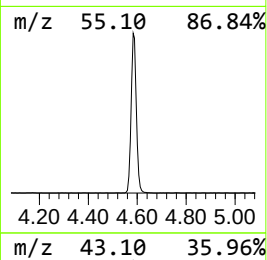
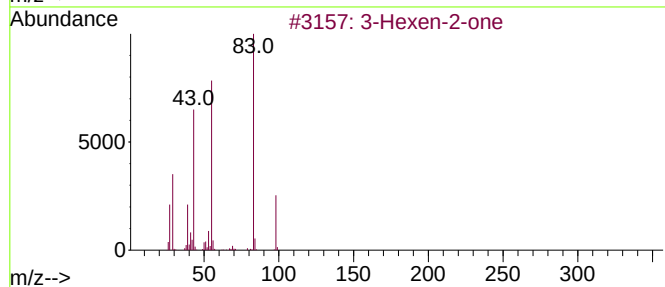
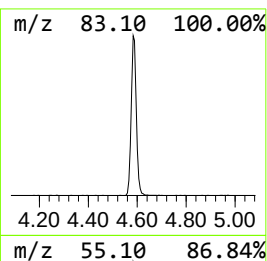
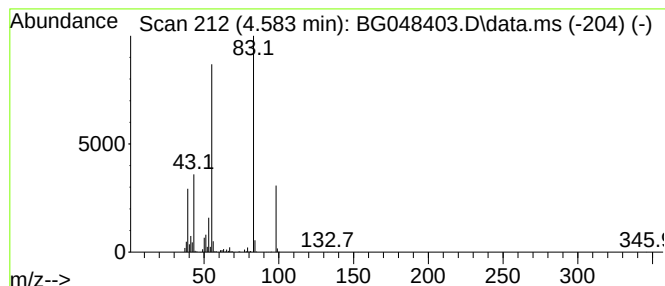
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.583	87.07 ng	1652200	1,4-Dichlorobenzene-d4	8.114

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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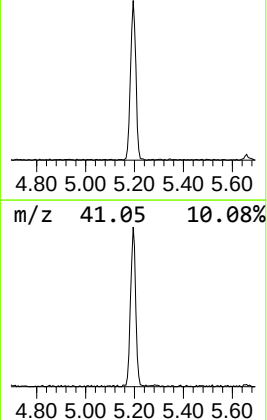
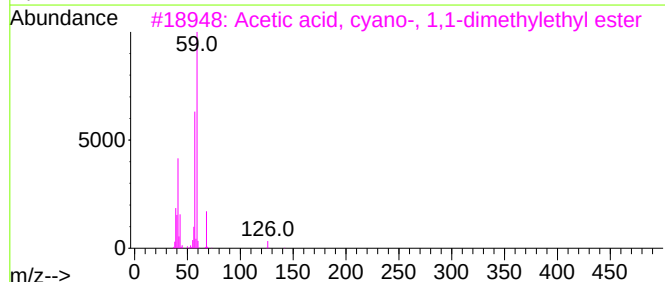
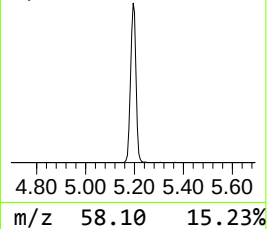
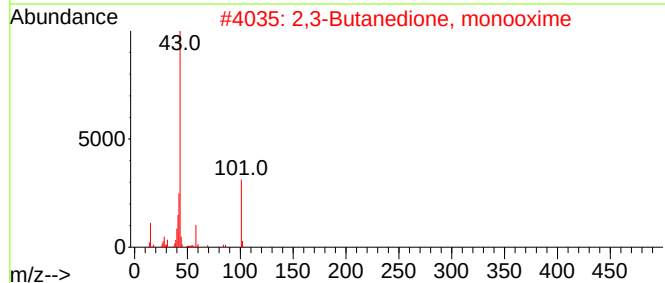
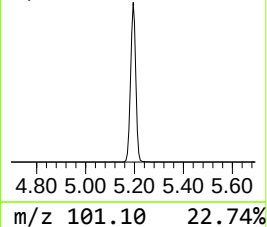
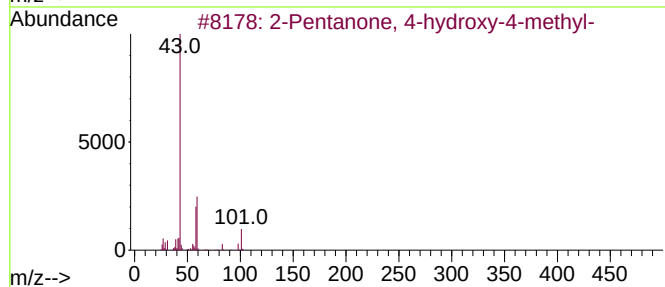
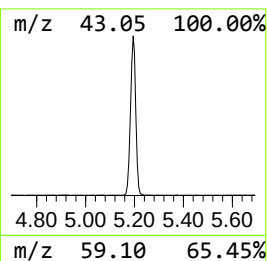
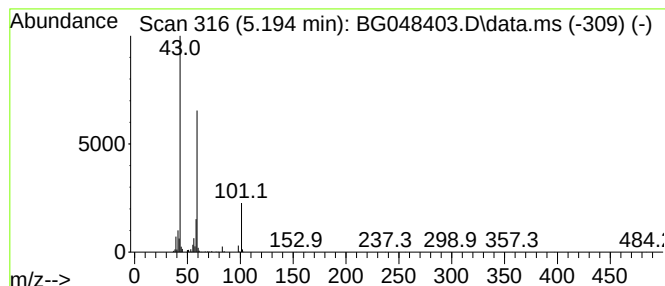
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	80.26 ng	1523010	1,4-Dichlorobenzene-d4	8.114

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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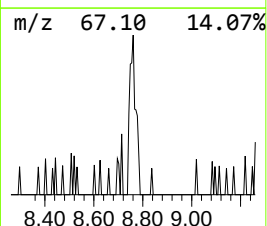
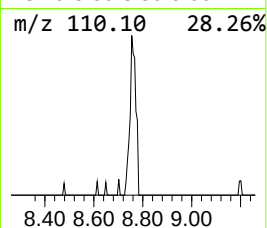
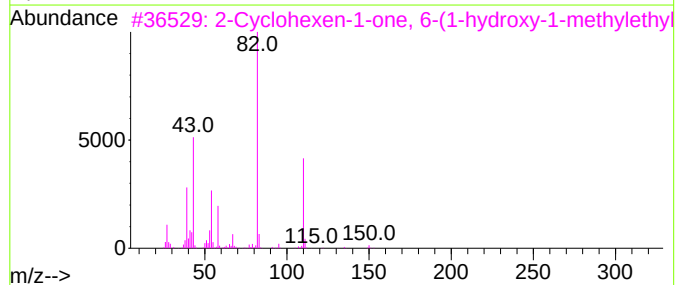
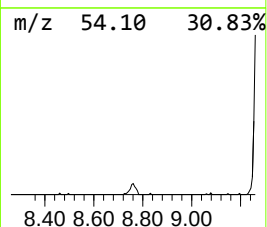
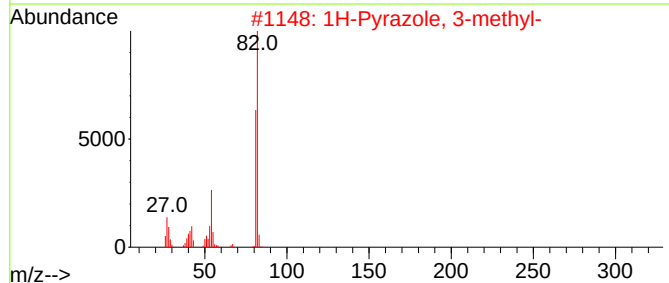
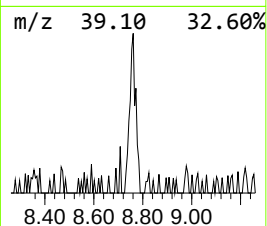
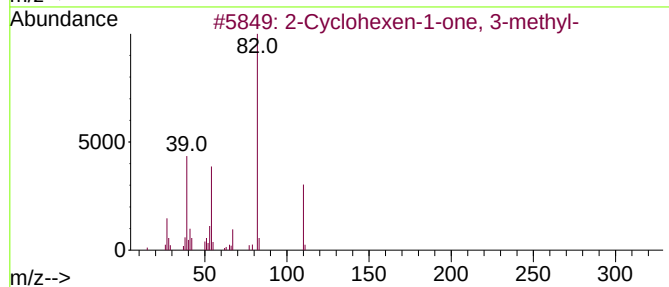
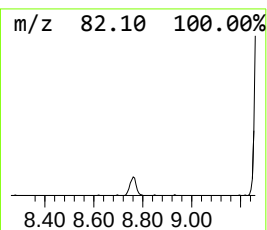
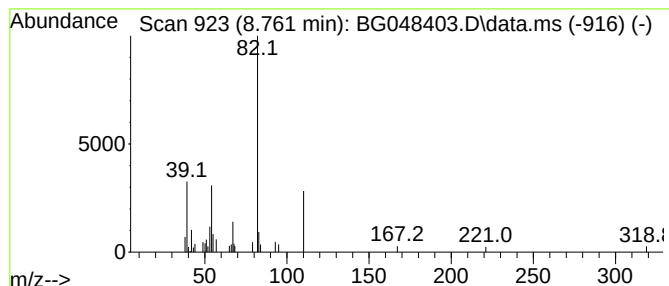
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Peak Number 3 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.761	2.17 ng	41129	1,4-Dichlorobenzene-d4	8.114

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	83
2			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	58
3			2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
4			1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	52
5			2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	42



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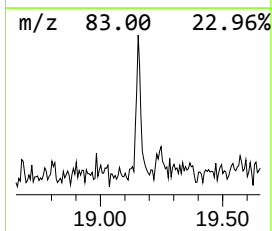
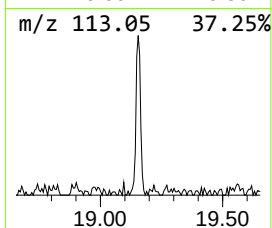
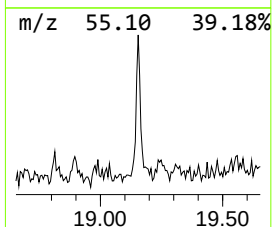
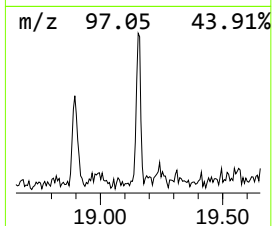
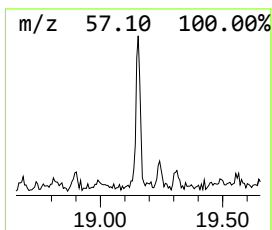
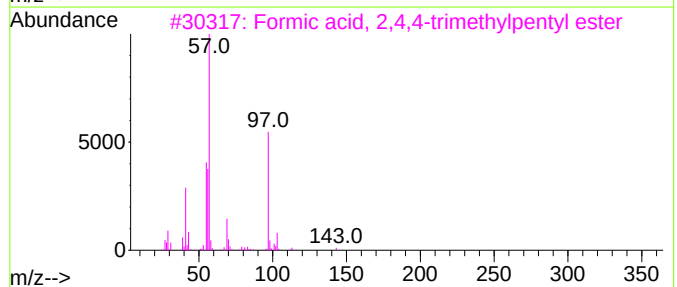
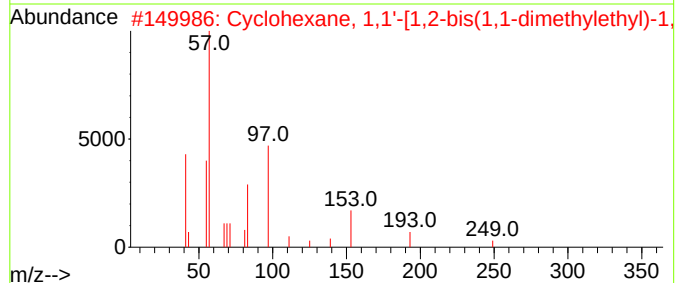
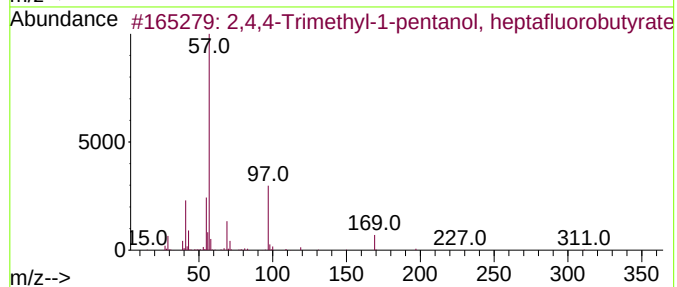
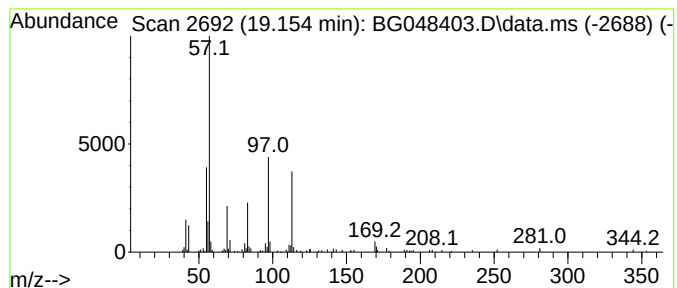
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Peak Number 4 unknown19.154 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.154	2.21 ng	111343	Phenanthrene-d10	17.503

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F702	1000365-01-4	37		
2	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	33		
3	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	32		
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	22		
5	2,2-Dimethyl-3-pentanol, heptafl...	312	C11H15F702	1000364-14-4	22		



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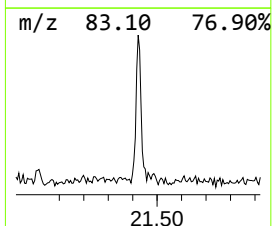
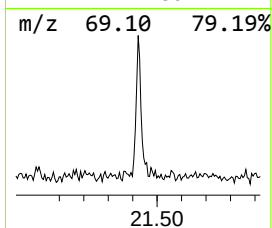
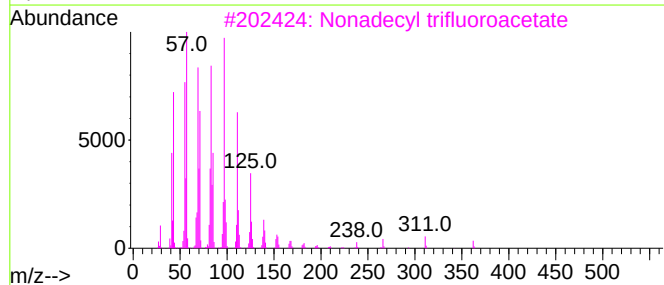
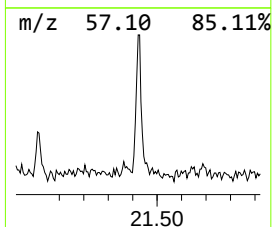
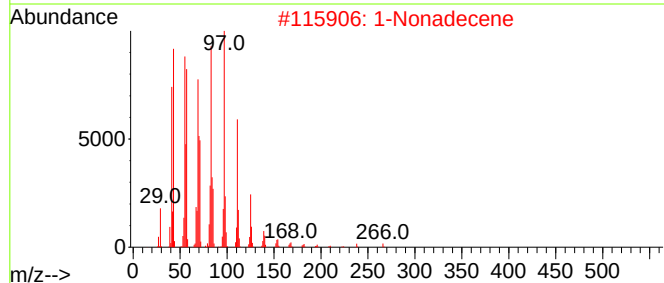
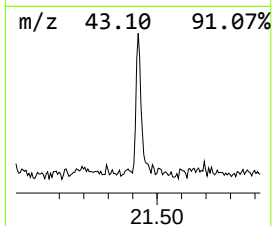
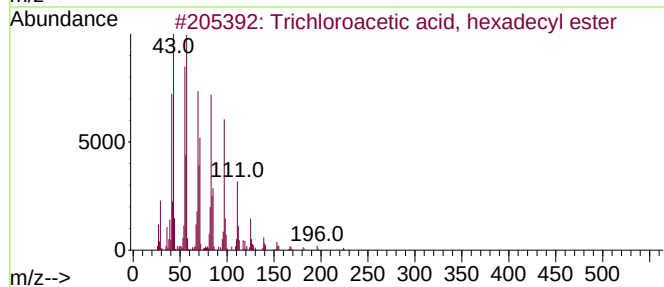
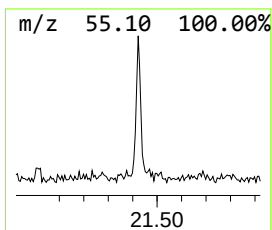
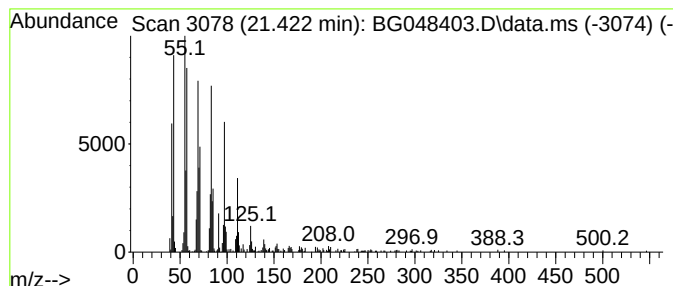
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	10.00 ng	516529	Chrysene-d12	21.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			1-Nonadecene	266	C19H38	018435-45-5	91
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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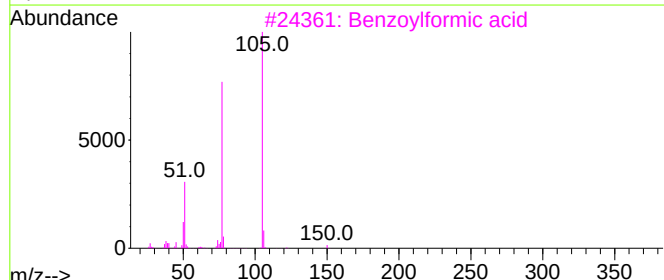
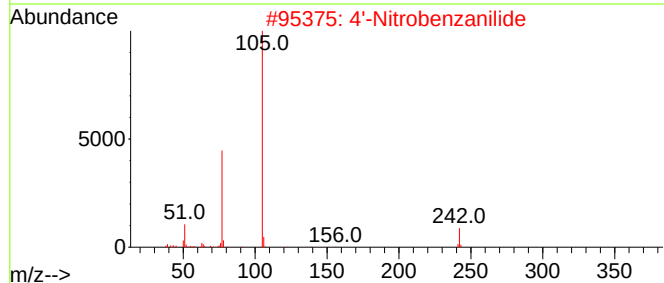
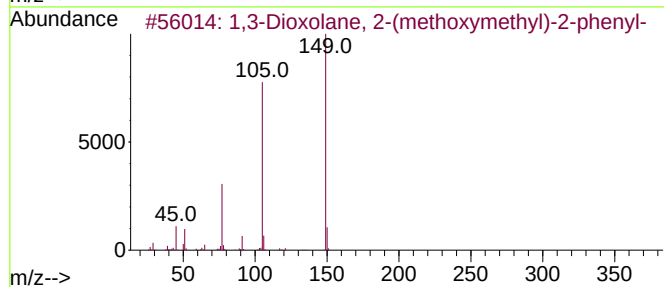
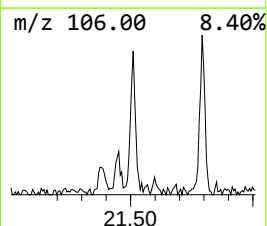
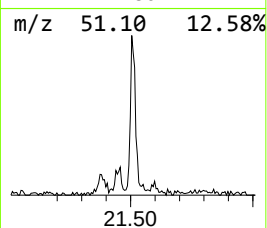
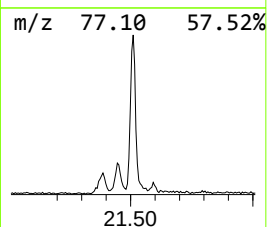
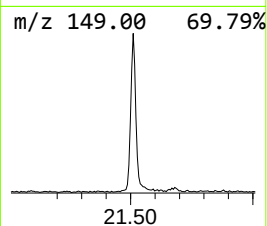
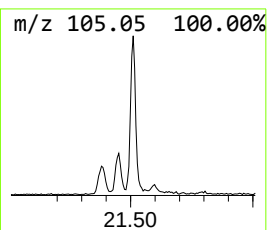
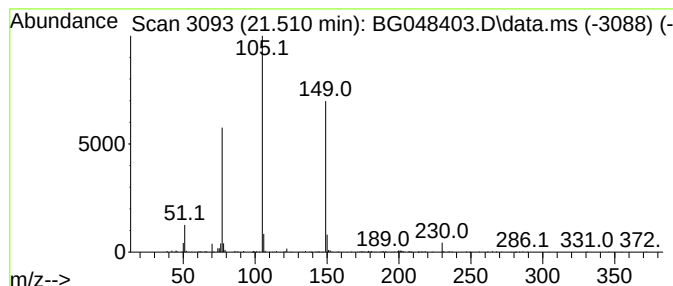
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.510	8.91 ng	459979	Chrysene-d12	21.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
2			4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	47
3			Benzoylformic acid	150	C8H6O3	000611-73-4	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048403.D
Acq On : 17 Mar 2021 18:29
Operator : CG/JU
Sample : M1686-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-SUMMER-STREET

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.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-Hexen-2-one	4.583	87.1	ng	1652200	1	8.114	379507	20.0
2-Pentanone, 4-...	5.194	80.3	ng	1523010	1	8.114	379507	20.0
2-Cyclohexen-1-...	8.761	2.2	ng	41129	1	8.114	379507	20.0
unknown19.154	19.154	2.2	ng	111343	4	17.503	1008280	20.0
Trichloroacetic...	21.422	10.0	ng	516529	5	21.798	1032940	20.0
1,3-Dioxolane, ...	21.510	8.9	ng	459979	5	21.798	1032940	20.0