

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082123\
 Data File : BG058794.D
 Acq On : 21 Aug 2023 15:10
 Operator : MA/JU
 Sample : 04086-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-PP09B

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-BG081823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058794.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.981	148	152	161	rVB3	8950	15791	1.14%	0.230%
2	5.385	381	391	403	rBV	314868	521627	37.62%	7.585%
3	6.789	626	630	635	rVB3	11478	16825	1.21%	0.245%
4	6.983	654	663	676	rBV	303061	546613	39.42%	7.949%
5	7.806	794	803	810	rBV	88282	154476	11.14%	2.246%
6	8.458	906	914	925	rVB6	10232	24783	1.79%	0.360%
7	8.911	986	991	995	rBV2	17724	26221	1.89%	0.381%
8	8.975	995	1002	1009	rBV	170995	316510	22.83%	4.603%
9	9.433	1076	1080	1085	rBV	10414	15289	1.10%	0.222%
10	9.856	1147	1152	1161	rVB5	6160	14161	1.02%	0.206%
11	10.009	1172	1178	1184	rBV4	14225	26576	1.92%	0.386%
12	10.609	1268	1280	1286	rBV	122939	250159	18.04%	3.638%
13	10.656	1286	1288	1295	rVB2	21908	36735	2.65%	0.534%
14	12.277	1557	1564	1577	rVB	36844	66194	4.77%	0.963%
15	12.500	1592	1602	1609	rBV	19541	35855	2.59%	0.521%
16	13.076	1693	1700	1713	rBV	474135	770839	55.60%	11.209%
17	14.457	1929	1935	1945	rBV	213307	338038	24.38%	4.916%
18	15.949	2182	2189	2205	rBV	368401	652305	47.05%	9.486%
19	17.201	2396	2402	2420	rBV	287489	468633	33.80%	6.815%
20	18.094	2548	2554	2561	rBV3	15862	30980	2.23%	0.450%
21	19.821	2842	2848	2859	rBV	1052889	1386475	100.00%	20.161%
22	21.096	3058	3065	3076	rBV	56571	109470	7.90%	1.592%
23	21.449	3118	3125	3139	rBV2	286570	510521	36.82%	7.424%
24	24.516	3636	3647	3664	rBV2	177687	541775	39.08%	7.878%

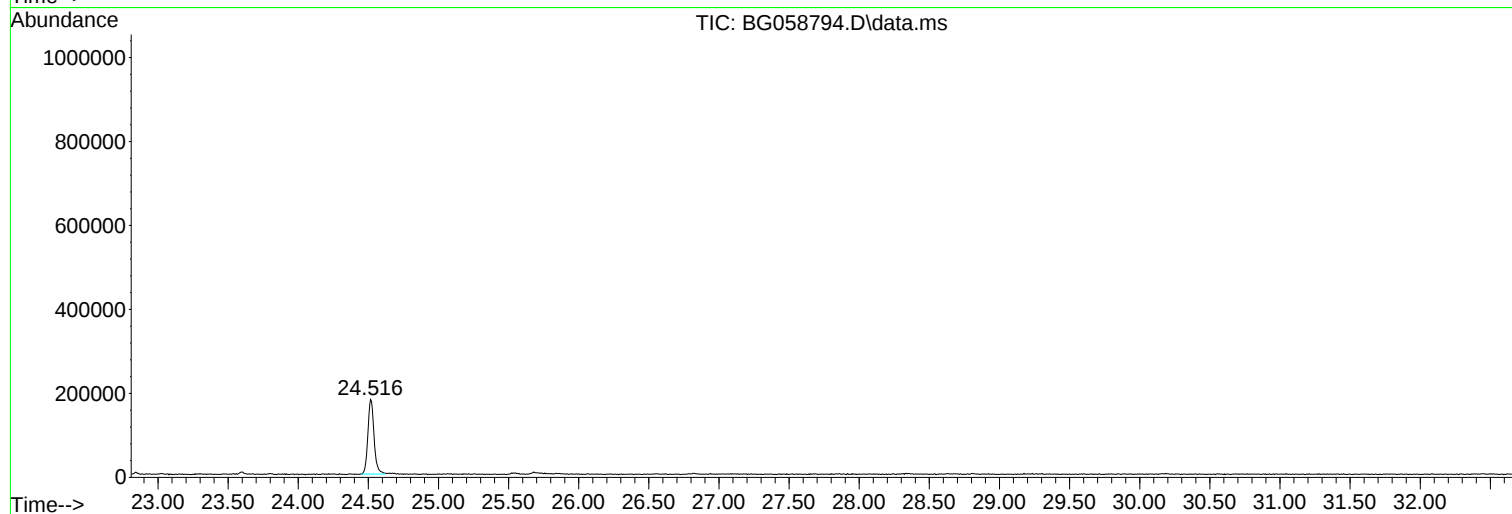
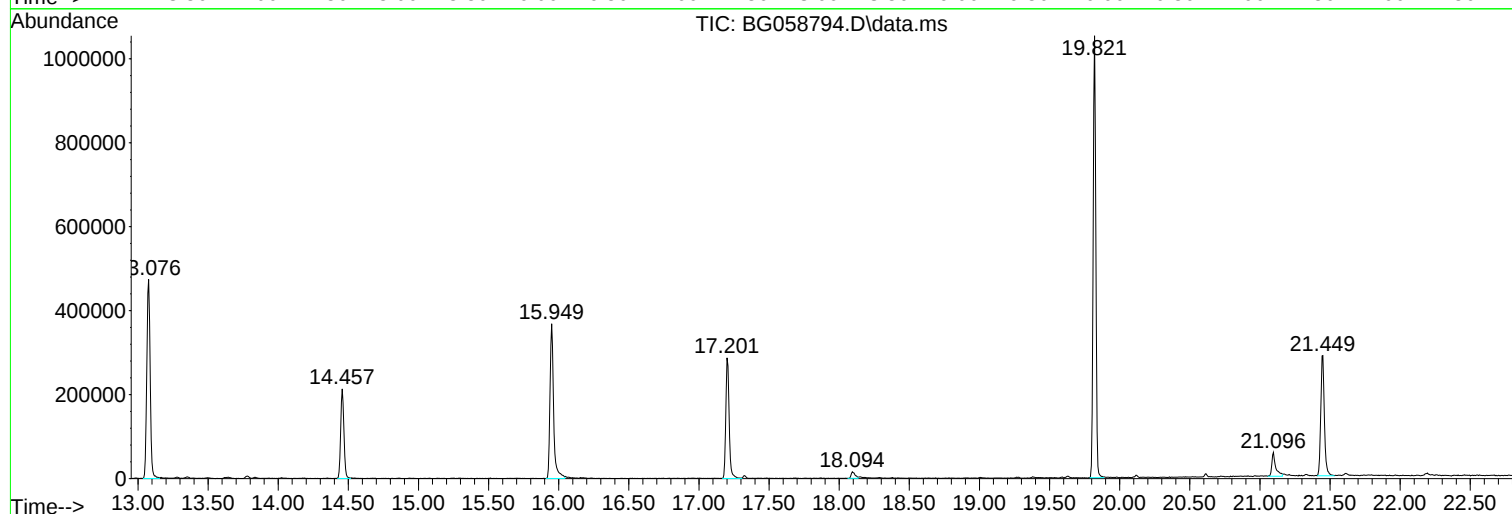
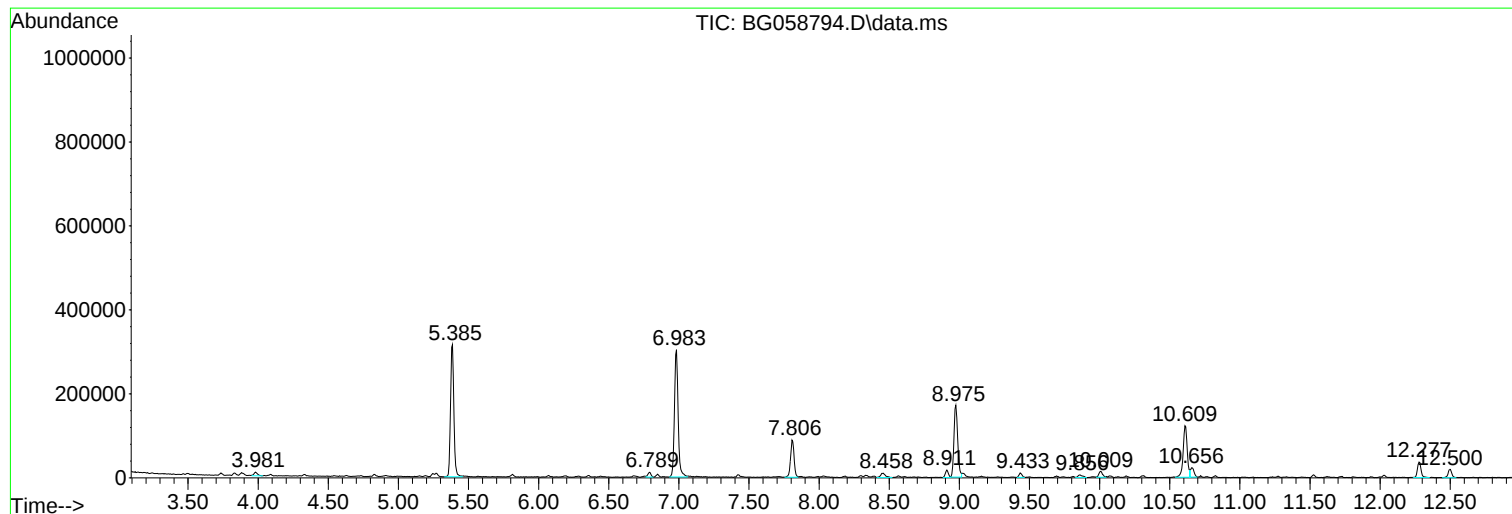
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ClientSampleId :
B-PP09B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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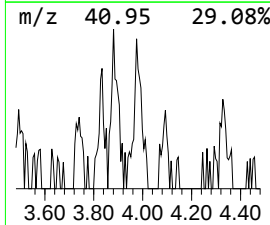
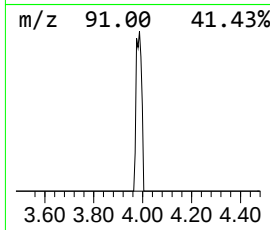
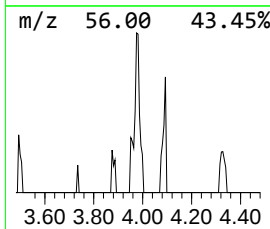
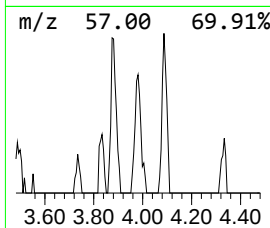
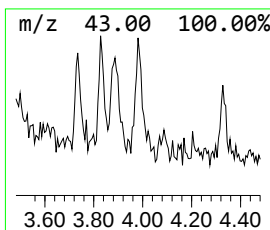
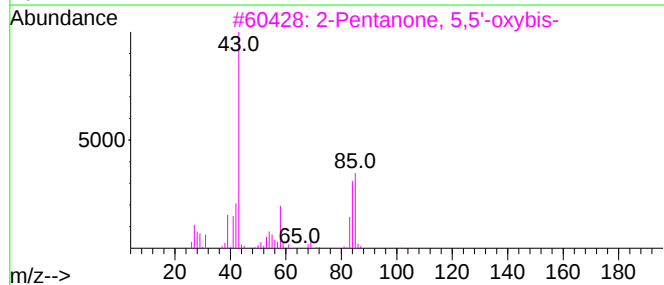
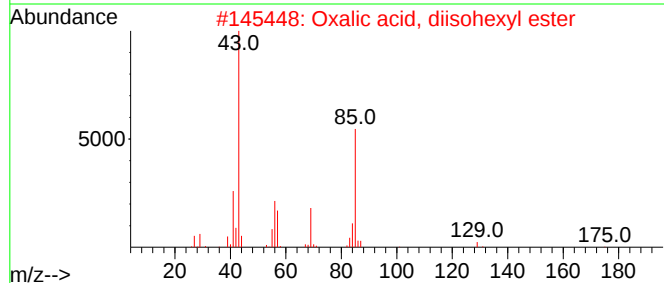
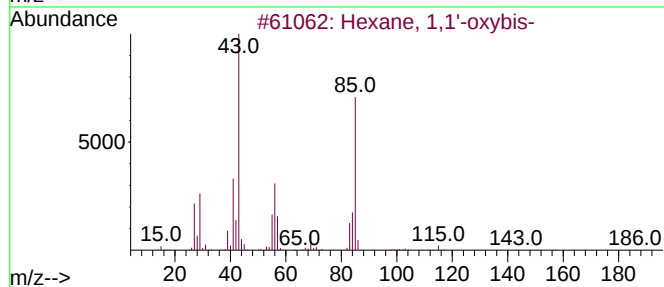
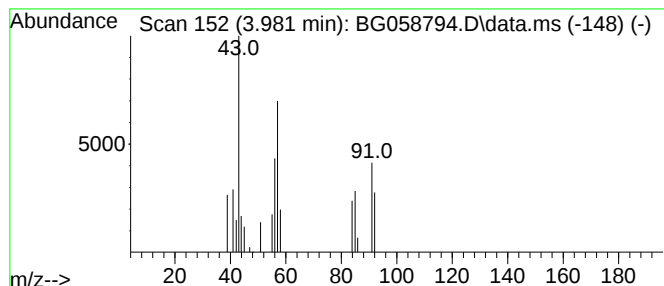
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.981 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.981	2.04 ng	15791	1,4-Dichlorobenzene-d4	7.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	17
2			Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	17
3			2-Pentanone, 5,5'-oxybis-	186	C10H18O3	093677-66-8	16
4			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	12
5			1,3-Dioxane-2-propanol, 2-methyl-	160	C8H16O3	036651-31-7	10



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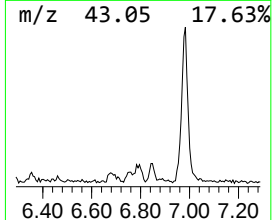
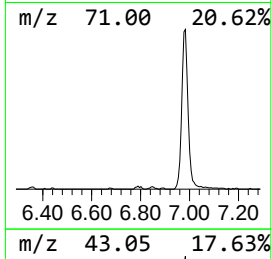
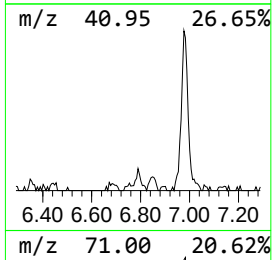
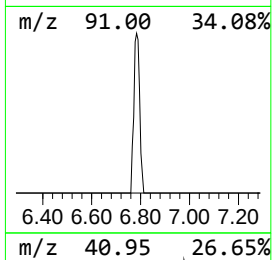
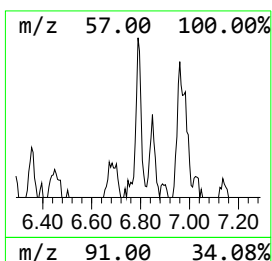
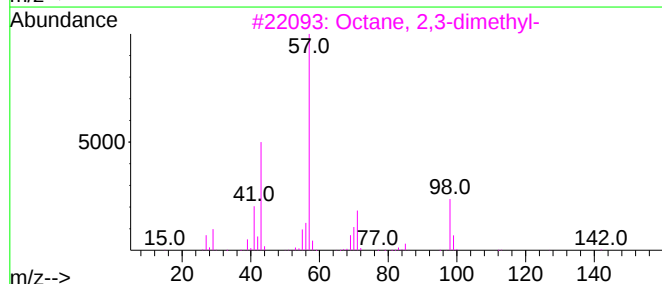
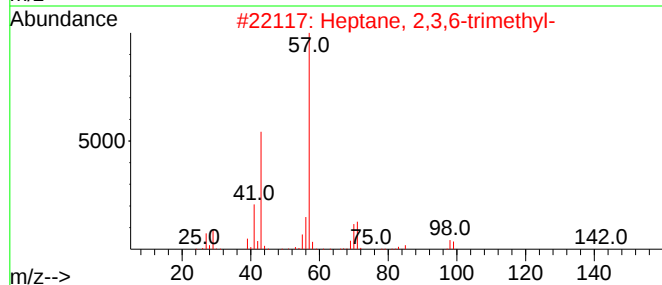
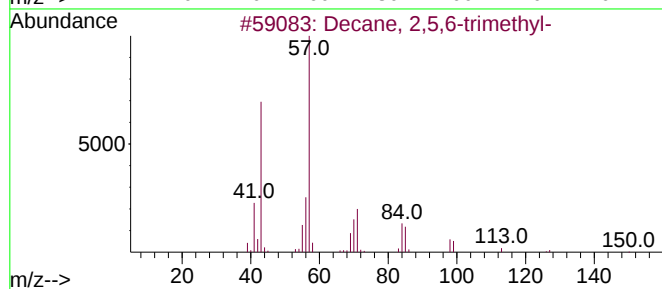
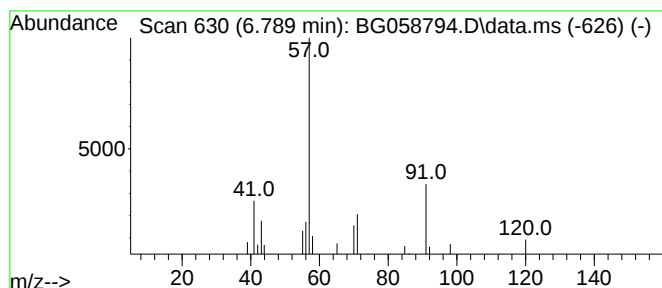
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Peak Number 2 unknown6.789 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.789	2.18 ng	16825	1,4-Dichlorobenzene-d4	7.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	40
2			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	36
3			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	36
4			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	33
5			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	25



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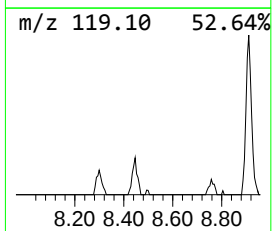
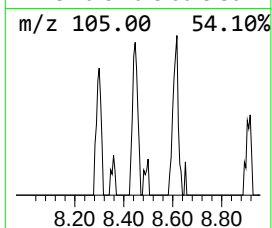
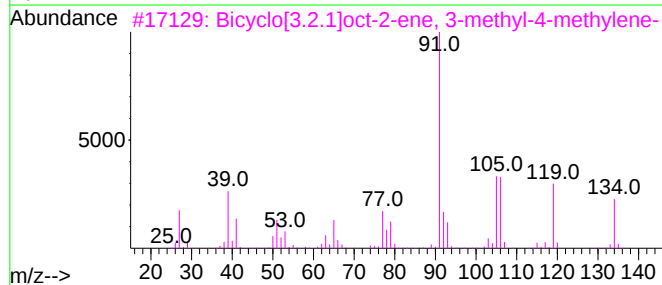
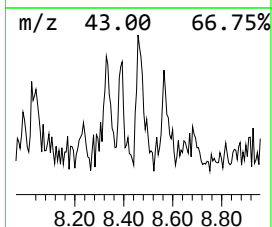
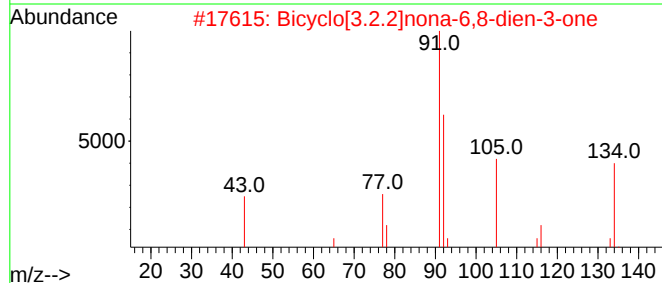
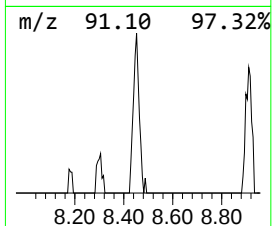
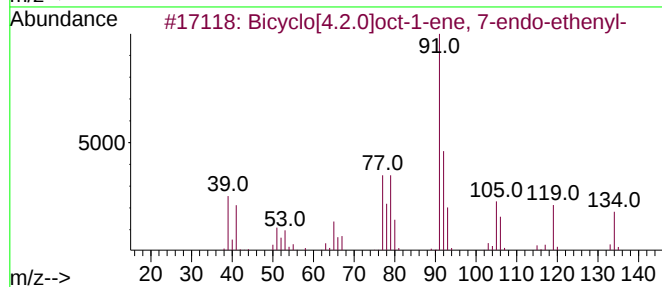
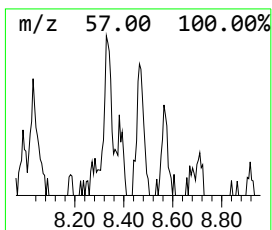
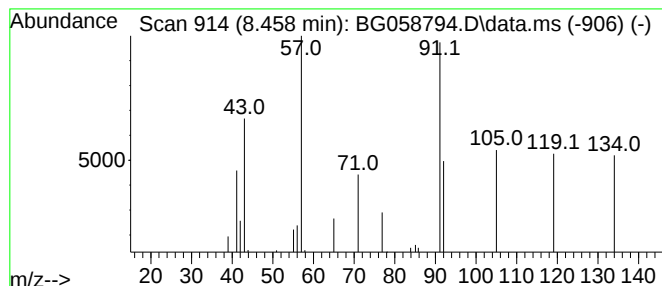
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.458 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.458	3.21 ng	24783	1,4-Dichlorobenzene-d4	7.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.2.0]oct-1-ene, 7-endo-...	134	C10H14	1000142-18-3	47
2			Bicyclo[3.2.2]nona-6,8-dien-3-one	134	C9H10O	026788-91-0	38
3			Bicyclo[3.2.1]oct-2-ene, 3-methy...	134	C10H14	049826-53-1	38
4			Benzyl methyl ketone	134	C9H10O	000103-79-7	38
5			Aziridine, 1-phenyl-	119	C8H9N	000696-18-4	12



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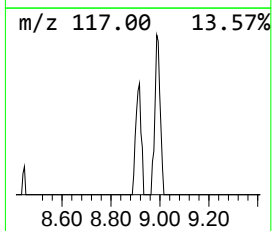
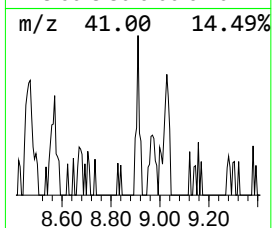
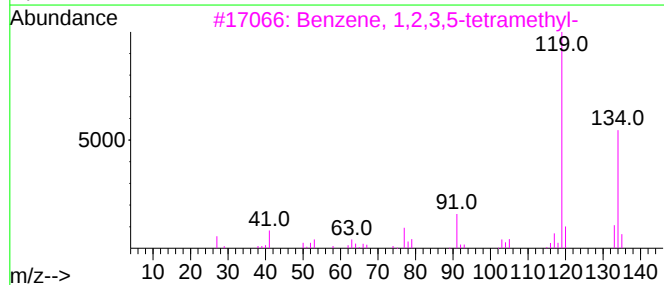
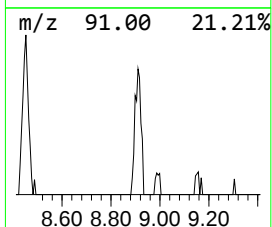
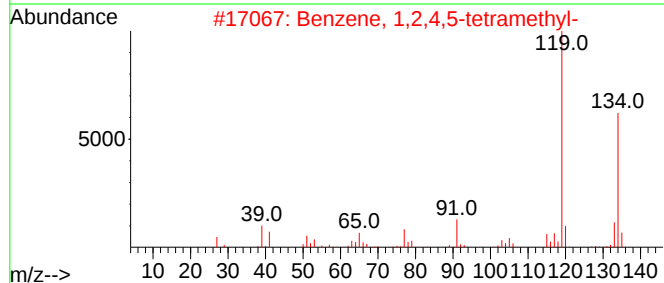
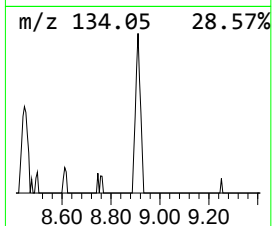
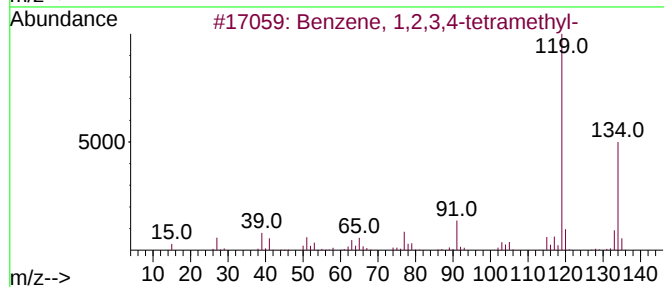
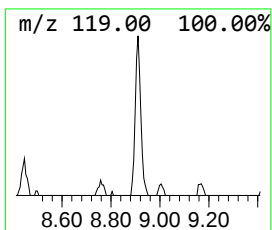
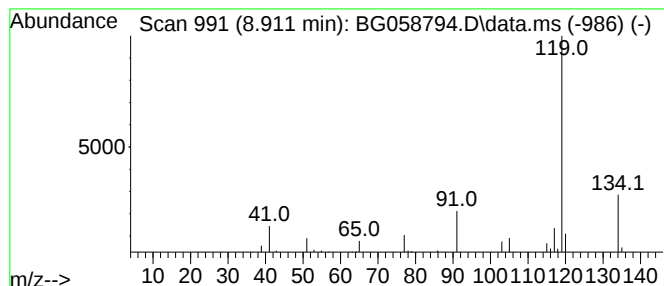
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Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.911	3.39 ng	26221	1,4-Dichlorobenzene-d4	7.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
4			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	91
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90



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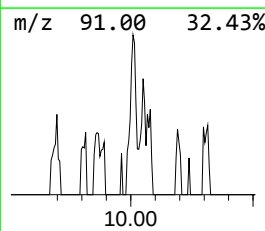
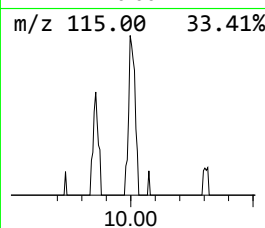
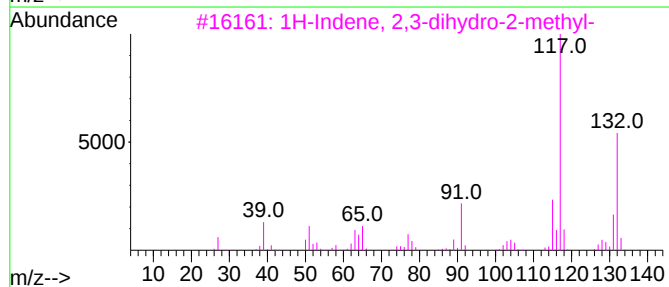
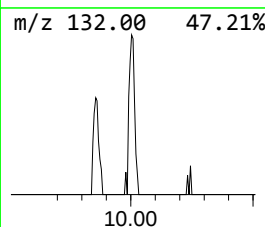
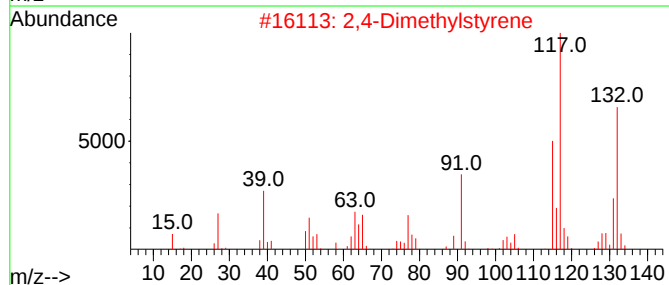
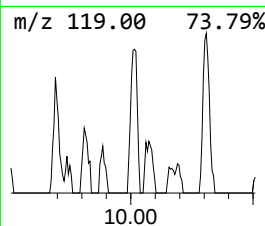
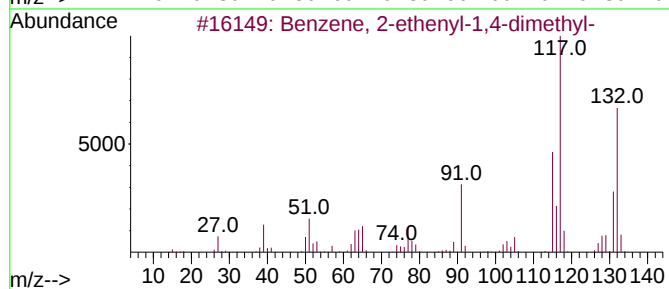
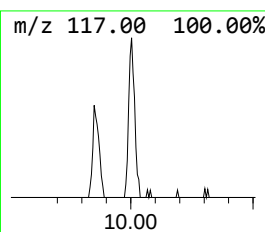
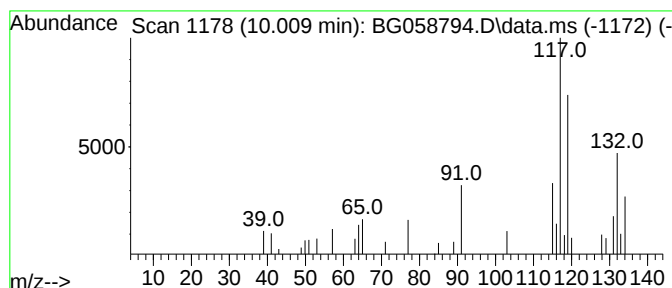
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Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.009	2.12 ng	26576	Naphthalene-d8	10.614

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	60
3			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	60
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	60
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	60



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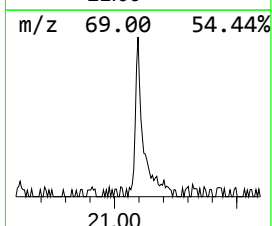
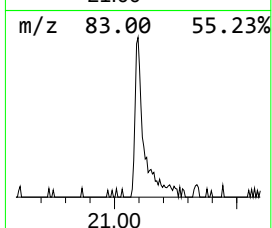
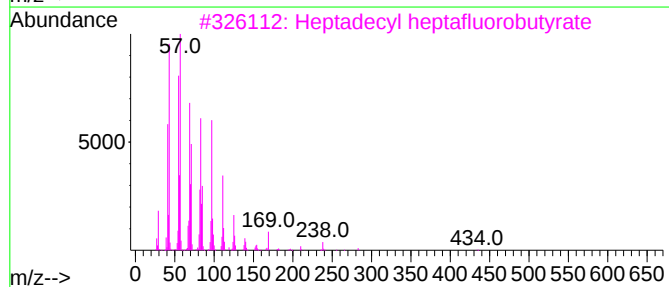
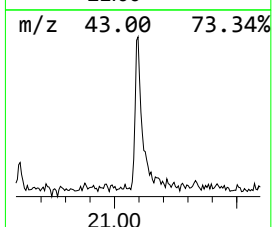
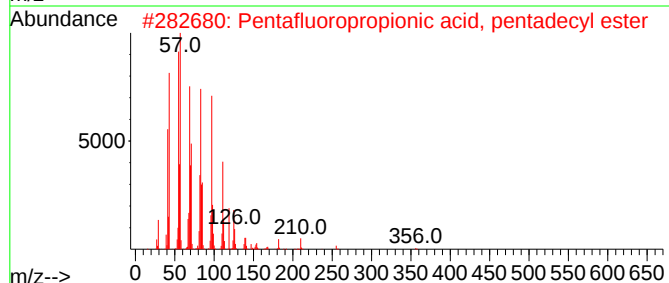
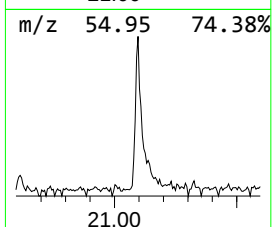
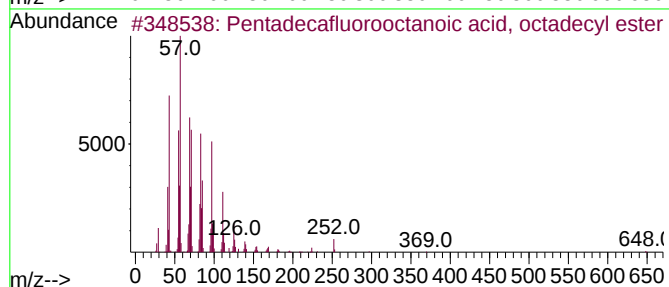
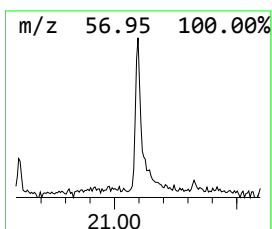
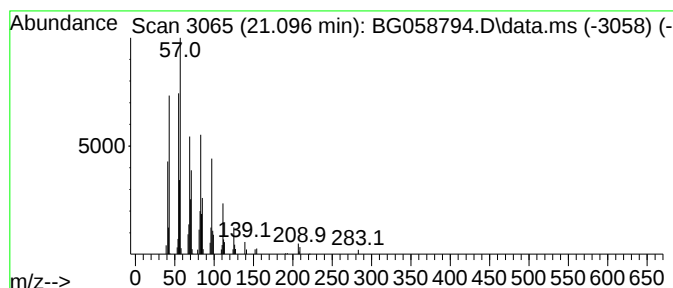
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.096	4.29 ng	109470	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082123\
Data File : BG058794.D
Acq On : 21 Aug 2023 15:10
Operator : MA/JU
Sample : 04086-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-PP09B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.981	3.981	2.0	ng	15791	1	7.806	154476	20.0
unknown6.789	6.789	2.2	ng	16825	1	7.806	154476	20.0
unknown8.458	8.458	3.2	ng	24783	1	7.806	154476	20.0
Benzene, 1,2,3,...	8.911	3.4	ng	26221	1	7.806	154476	20.0
Benzene, 2-ethe...	10.009	2.1	ng	26576	2	10.614	250159	20.0
Pentadecafluoro...	21.096	4.3	ng	109470	5	21.443	510521	20.0