

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041921\
 Data File : BG048779.D
 Acq On : 20 Apr 2021 1:41
 Operator : CG/JU
 Sample : M2079-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-06

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-BG041421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048779.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.623	381	389	397	rBV	243627	388338	17.40%	4.551%
2	6.545	540	546	556	rVB	29293	43426	1.95%	0.509%
3	7.039	623	630	637	rVB2	60193	92518	4.14%	1.084%
4	7.239	655	664	677	rVB2	171676	309963	13.89%	3.633%
5	8.073	800	806	813	rBV	72797	121149	5.43%	1.420%
6	8.449	865	870	880	rVB	45229	74202	3.32%	0.870%
7	8.567	884	890	894	rBV2	26702	43875	1.97%	0.514%
8	8.719	911	916	920	rBV3	15874	25698	1.15%	0.301%
9	9.189	989	996	1000	rBV2	50565	85934	3.85%	1.007%
10	9.248	1000	1006	1017	rVB	328163	611431	27.39%	7.166%
11	9.718	1080	1086	1090	rBV	27428	46931	2.10%	0.550%
12	10.905	1279	1288	1292	rBV	99720	172680	7.74%	2.024%
13	10.952	1292	1296	1302	rVB2	30990	56978	2.55%	0.668%
14	12.785	1599	1608	1613	rVB3	14433	23512	1.05%	0.276%
15	13.355	1697	1705	1713	rBV	886229	1363400	61.07%	15.978%
16	14.172	1839	1844	1851	rVB2	18132	30125	1.35%	0.353%
17	14.736	1932	1940	1946	rBV2	155897	259087	11.61%	3.036%
18	14.795	1946	1950	1956	rVB2	34479	54267	2.43%	0.636%
19	15.135	2002	2008	2012	rBV	19694	27921	1.25%	0.327%
20	16.228	2188	2194	2212	rBV	685299	1131521	50.69%	13.261%
21	17.491	2403	2409	2414	rBV	226916	339479	15.21%	3.978%
22	17.533	2414	2416	2422	rVB4	16476	23249	1.04%	0.272%
23	17.621	2424	2431	2436	rVB	17146	27996	1.25%	0.328%
24	19.542	2754	2758	2763	rBV	36128	54974	2.46%	0.644%
25	19.906	2817	2820	2826	rVB2	30281	38917	1.74%	0.456%
26	20.106	2847	2854	2859	rBV	1648393	2232347	100.00%	26.162%
27	21.405	3070	3075	3087	rBV2	64465	118183	5.29%	1.385%
28	21.786	3132	3140	3147	rBV2	215362	369089	16.53%	4.326%
29	25.130	3696	3709	3720	rVB3	122433	365662	16.38%	4.285%

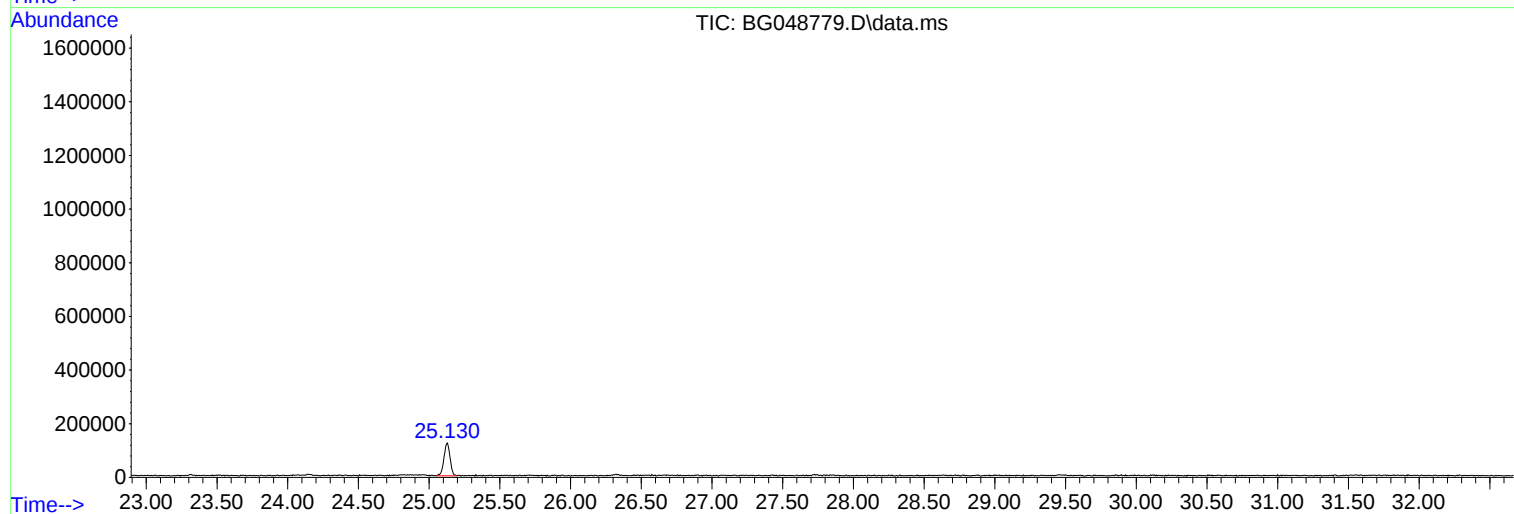
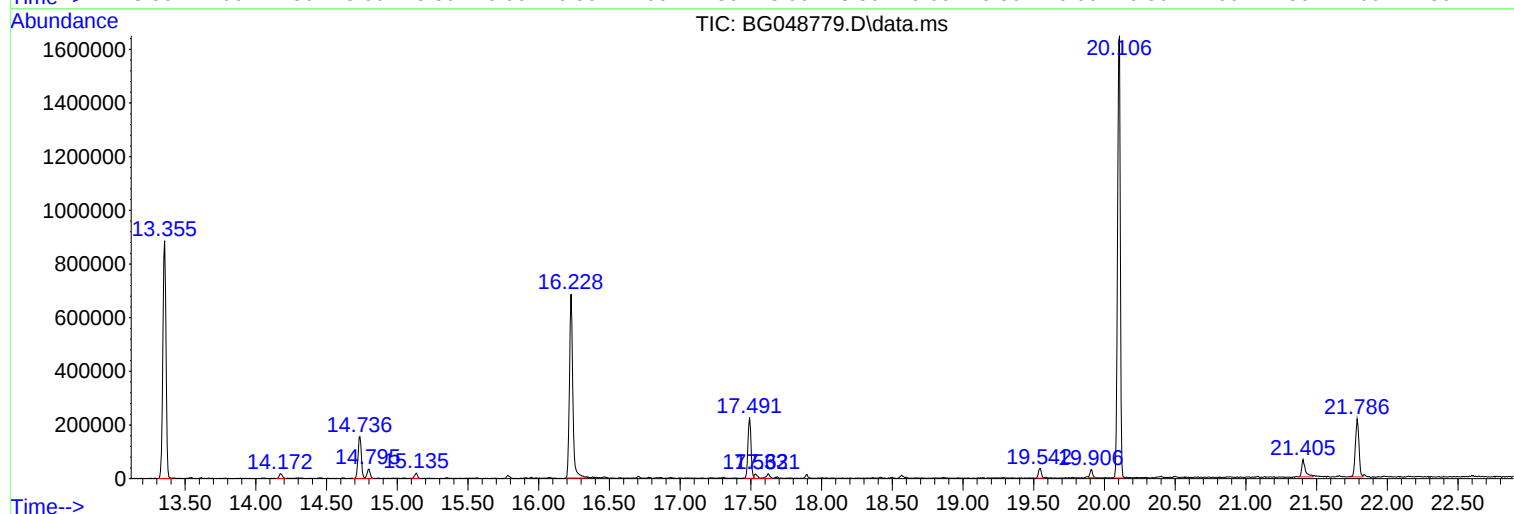
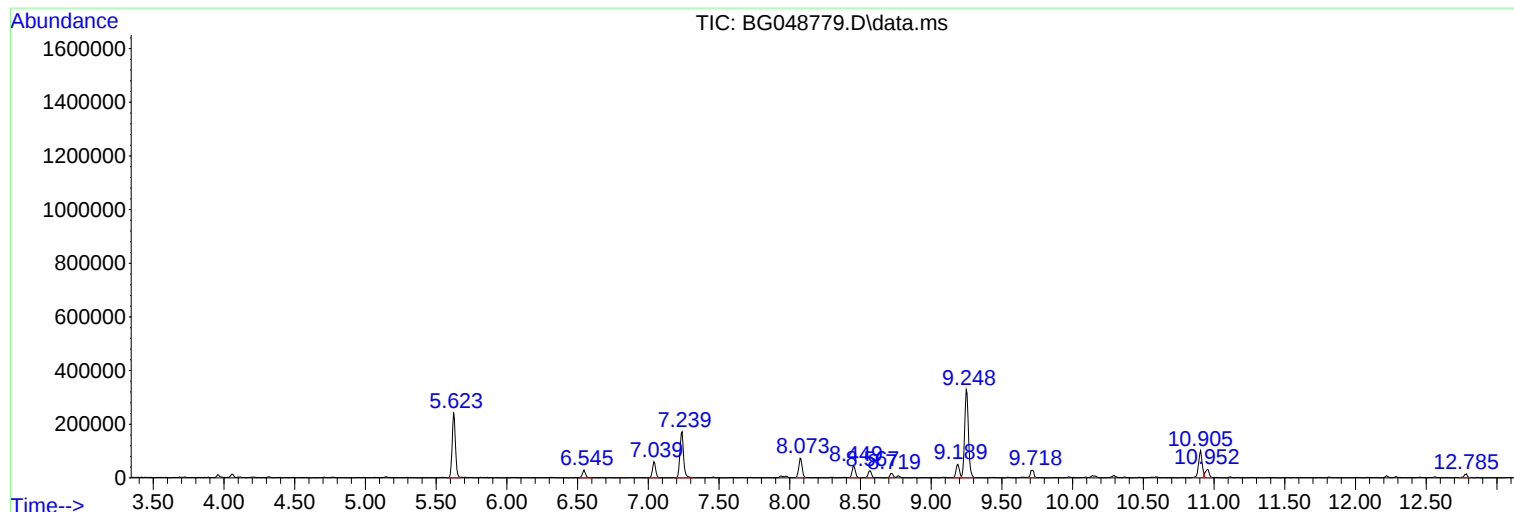
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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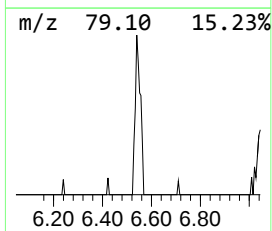
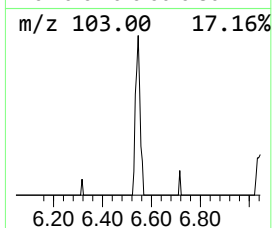
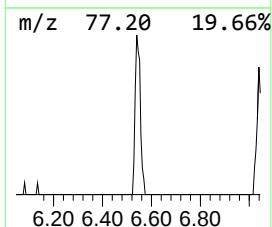
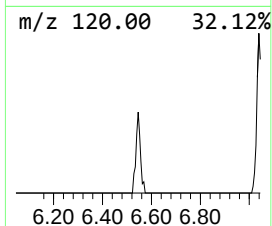
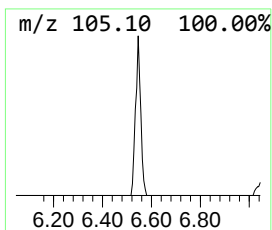
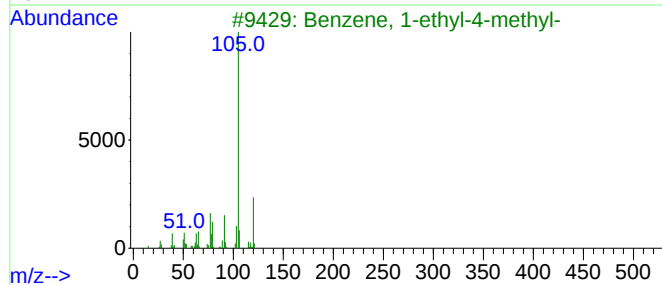
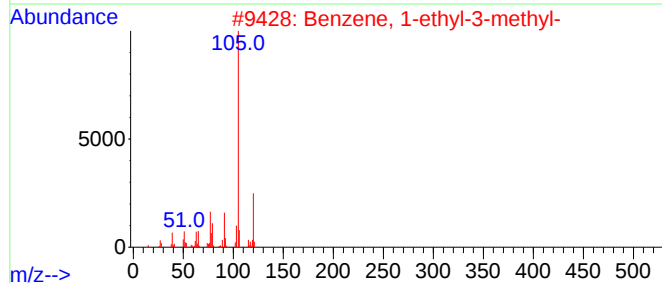
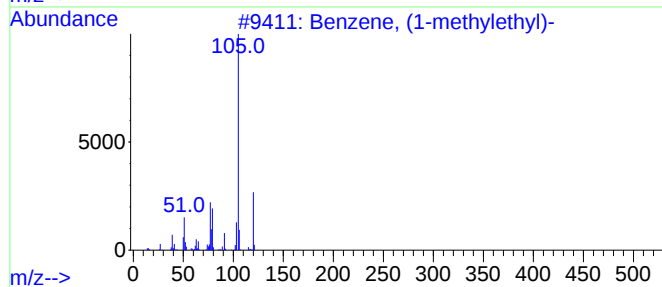
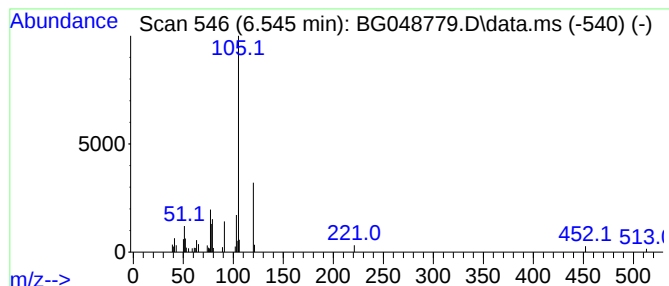
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzene, (1-methylethyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.545	7.17 ng	43426	1,4-Dichlorobenzene-d4	8.073

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	87
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	80
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	80
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	80
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	80



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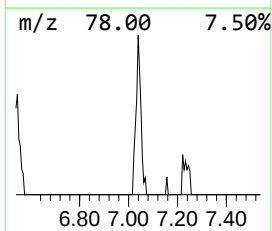
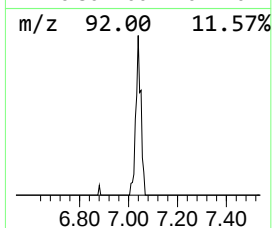
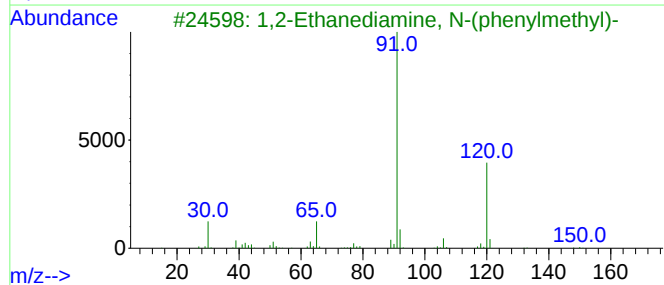
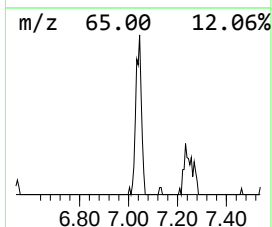
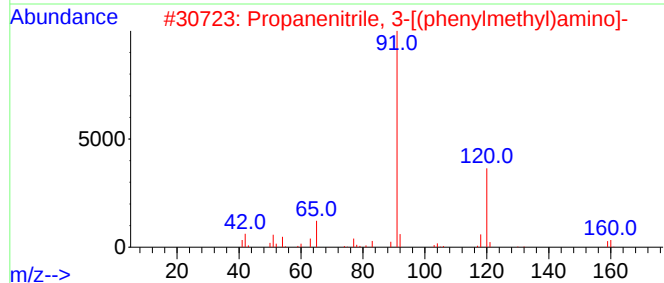
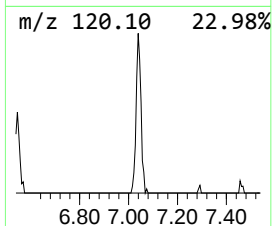
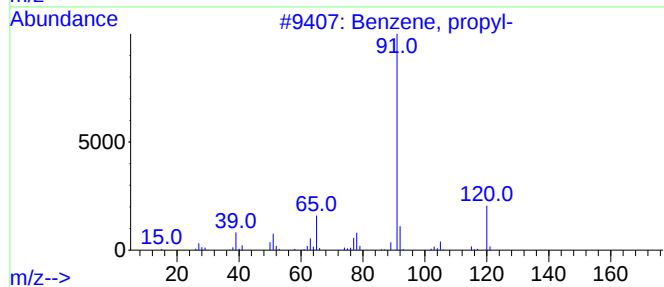
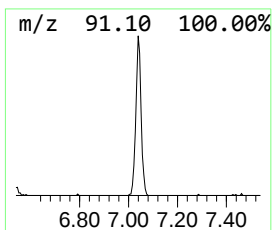
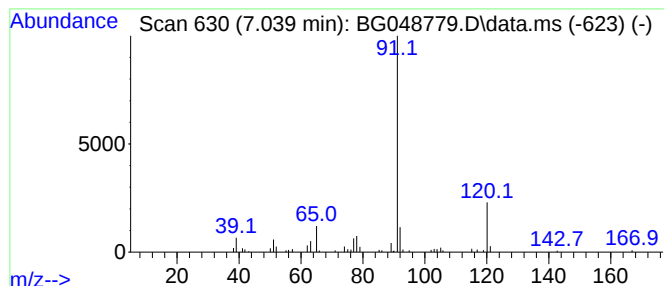
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Peak Number 2 Benzene, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.039	15.27 ng	92518	1,4-Dichlorobenzene-d4	8.073

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, propyl-	120	C9H12	000103-65-1	87
2		Propanenitrile, 3-[(phenylmethyl)amino]-	160	C10H12N2	000706-03-6	78
3		1,2-Ethanediamine, N-(phenylmethyl)-	150	C9H14N2	004152-09-4	72
4		N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	72
5		Phosphonous dichloride, (phenylmethyl)-	192	C7H7Cl2P	004545-85-1	47



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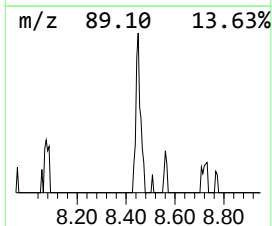
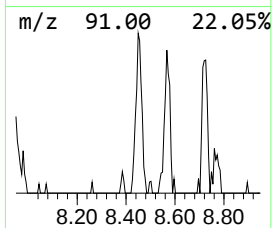
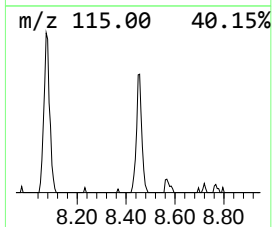
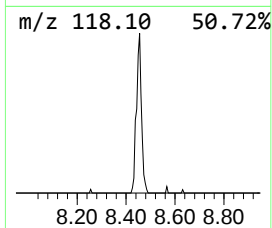
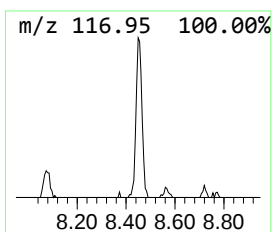
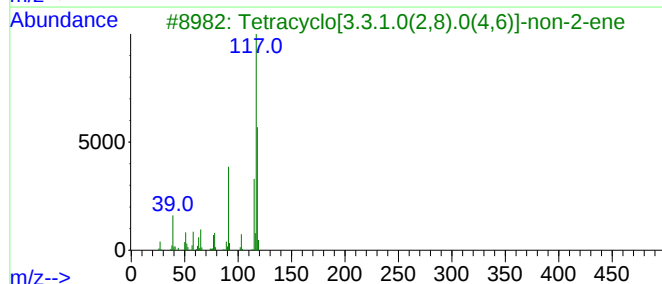
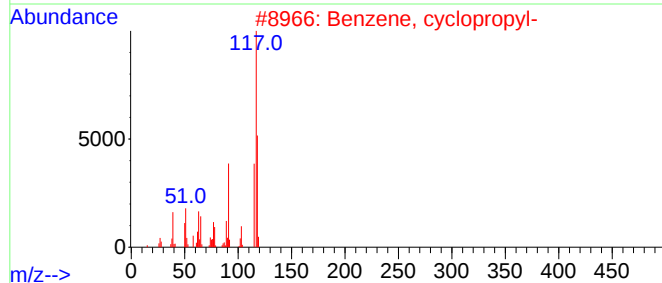
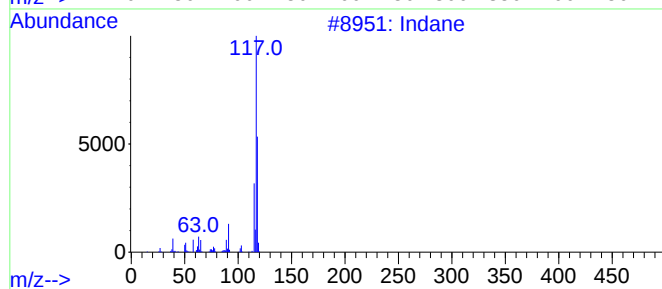
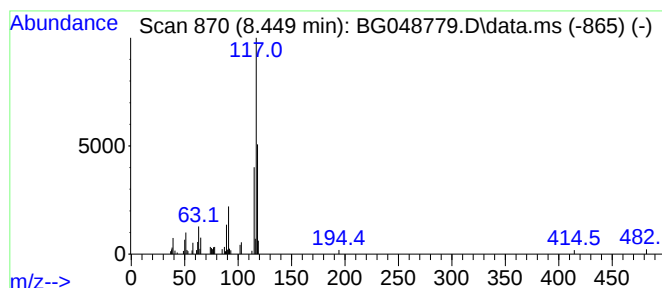
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.449	12.25 ng	74202	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	70
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	50
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50



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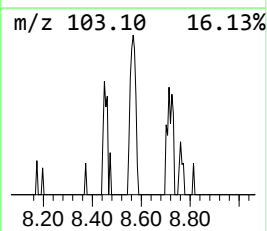
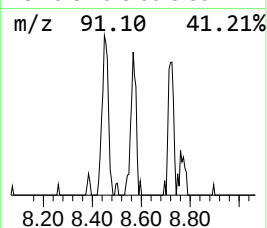
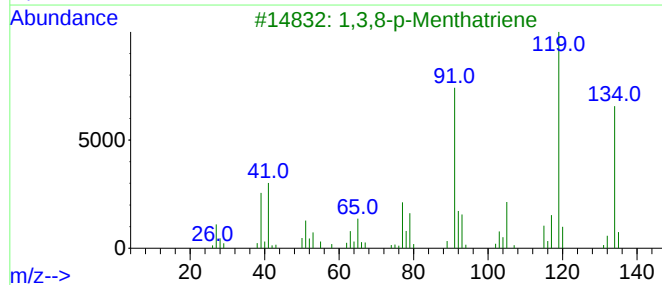
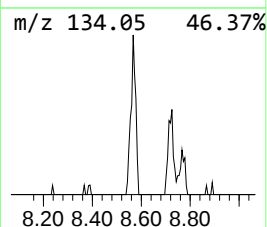
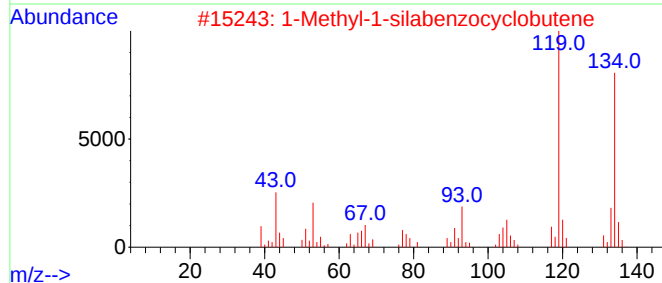
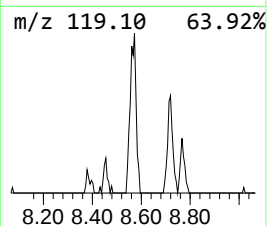
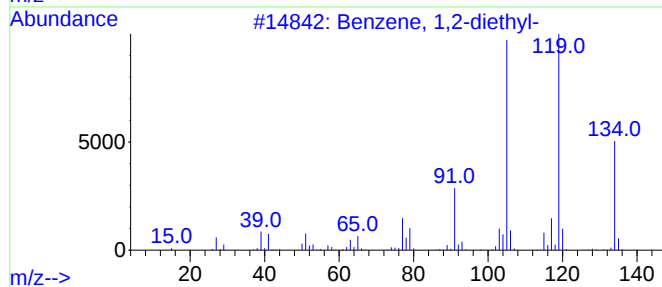
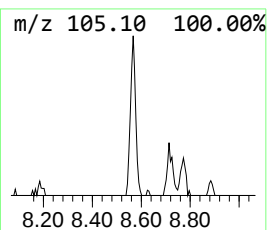
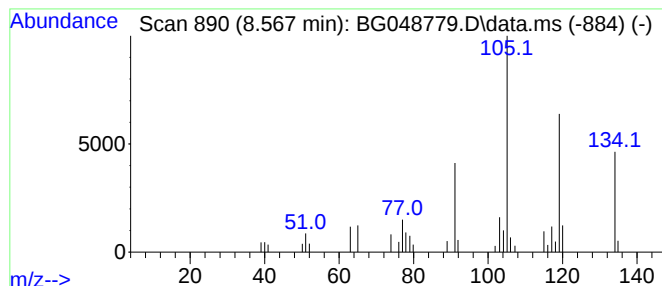
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Peak Number 4 Benzene, 1,2-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.567	7.24 ng	43875	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	90
2			1-Methyl-1-silabenzocyclobutene	134	C8H10Si	160841-06-5	80
3			1,3,8-p-Menthatriene	134	C10H14	018368-95-1	72
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	68
5			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	64



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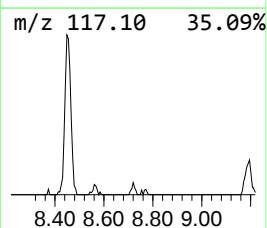
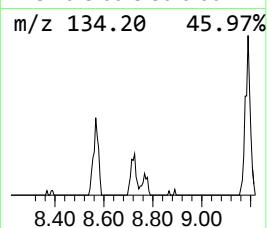
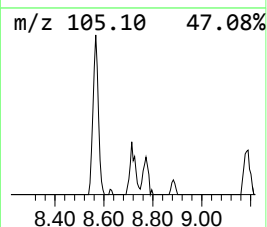
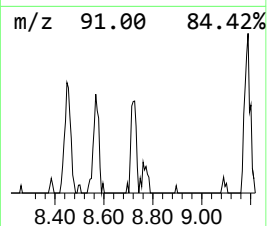
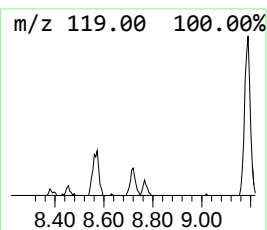
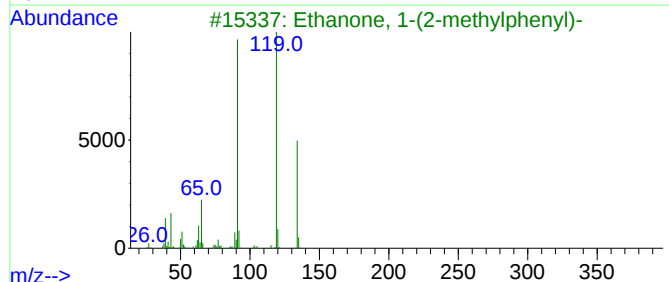
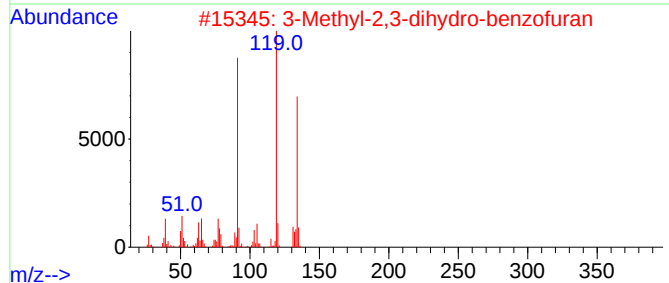
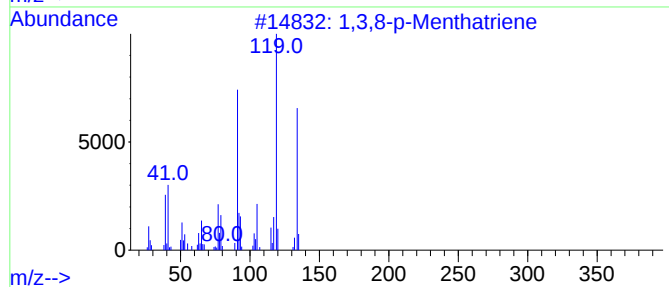
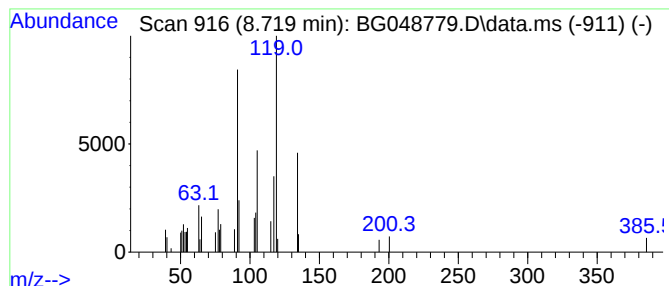
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 1,3,8-p-Menthatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.719	4.24 ng	25698	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,8-p-Menthatriene	134	C10H14	018368-95-1	83
2			3-Methyl-2,3-dihydro-benzofuran	134	C9H10O	013524-73-7	59
3			Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	52
4			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	50
5			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	50



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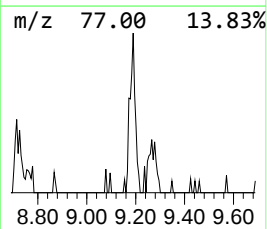
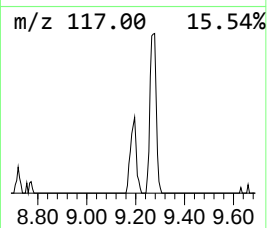
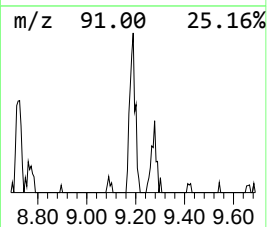
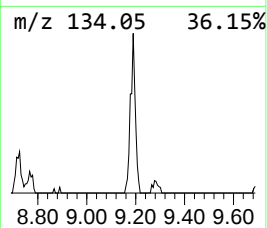
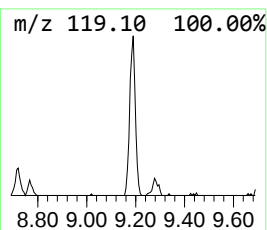
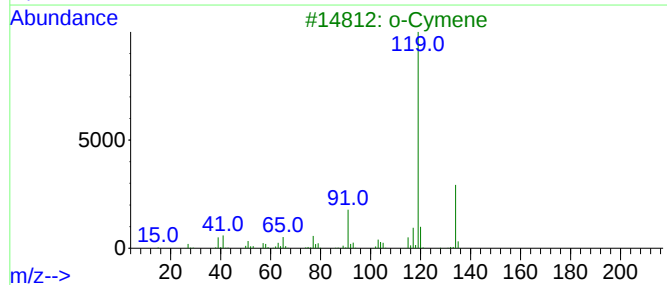
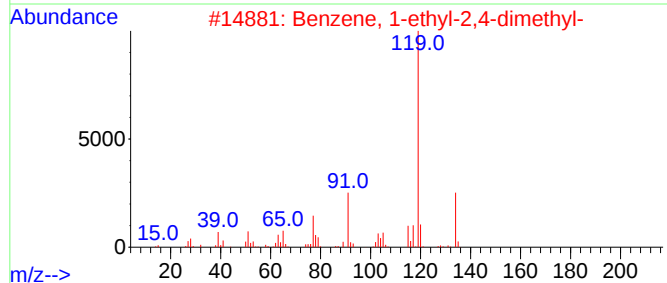
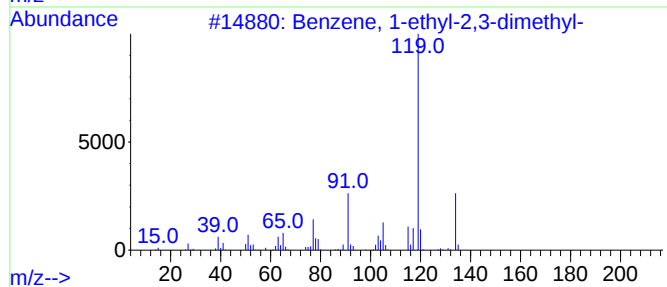
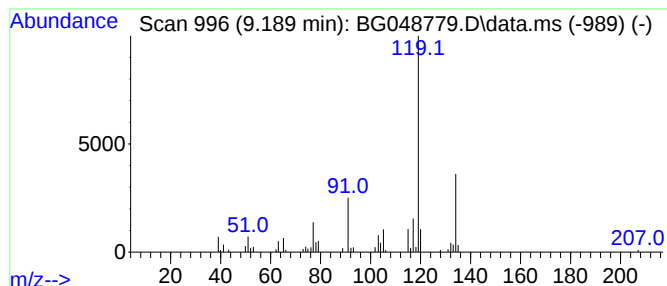
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.189	14.19 ng	85934	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
3			o-Cymene	134	C10H14	000527-84-4	93
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041921\
Data File : BG048779.D
Acq On : 20 Apr 2021 1:41
Operator : CG/JU
Sample : M2079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-06

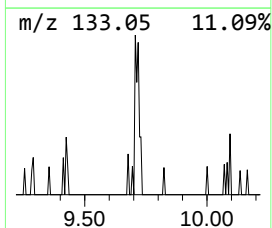
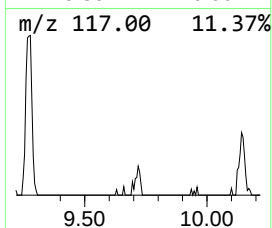
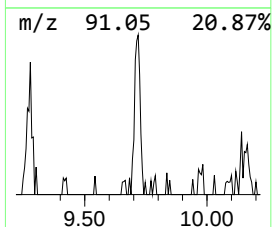
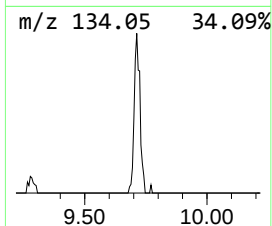
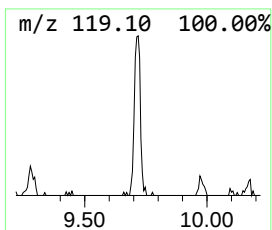
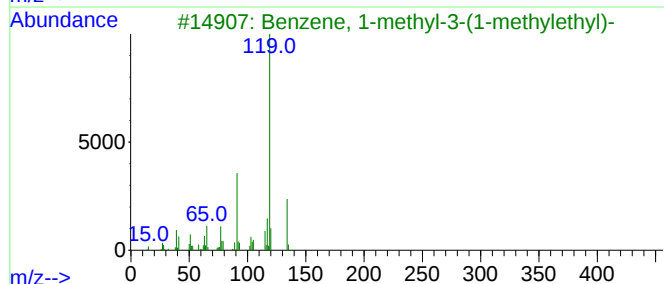
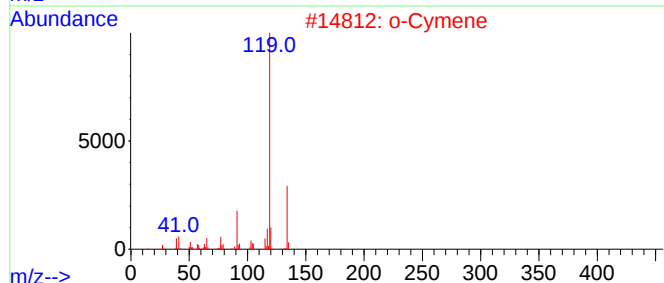
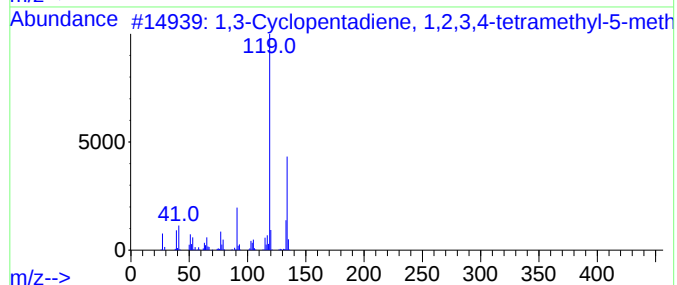
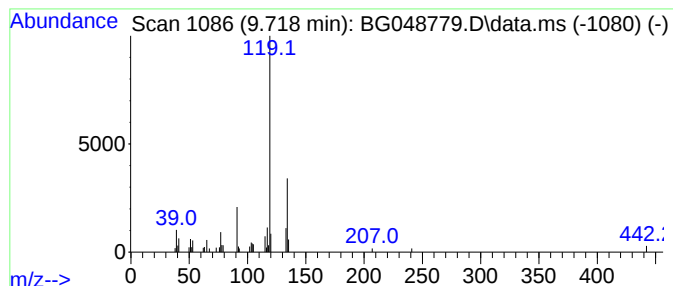
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3-Cyclopentadiene, 1,2,3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.718	5.44 ng	46931	Naphthalene-d8	10.905

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	93
2		o-Cymene	134	C10H14	000527-84-4	93
3		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93
4		p-Cymene	134	C10H14	000099-87-6	93
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041921\
Data File : BG048779.D
Acq On : 20 Apr 2021 1:41
Operator : CG/JU
Sample : M2079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-06

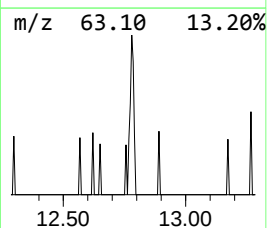
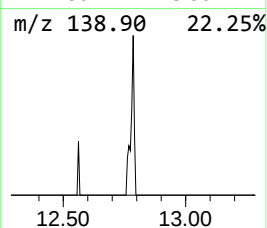
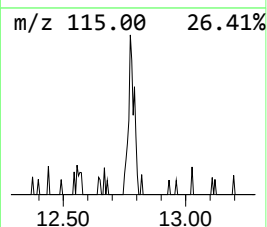
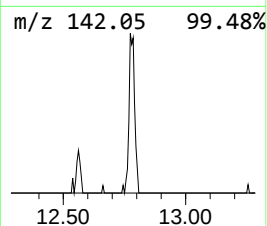
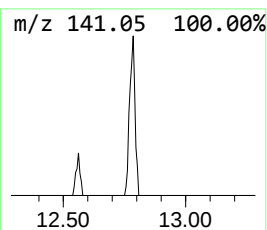
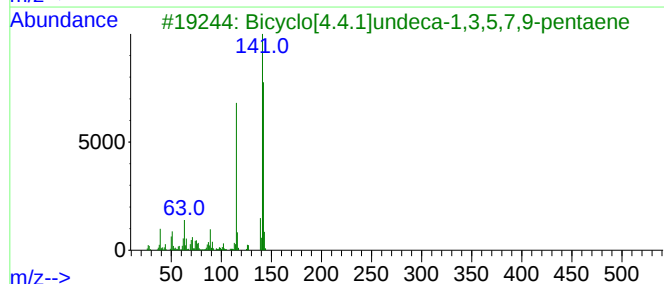
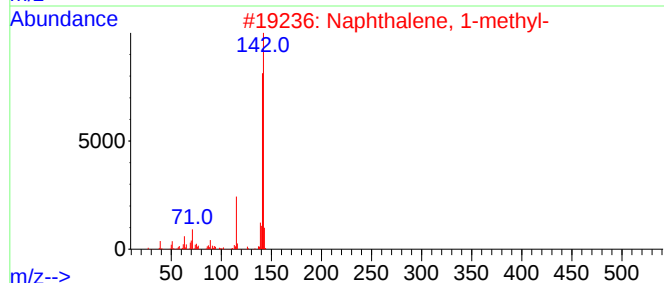
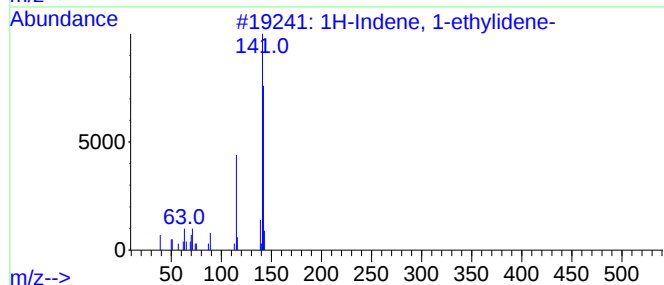
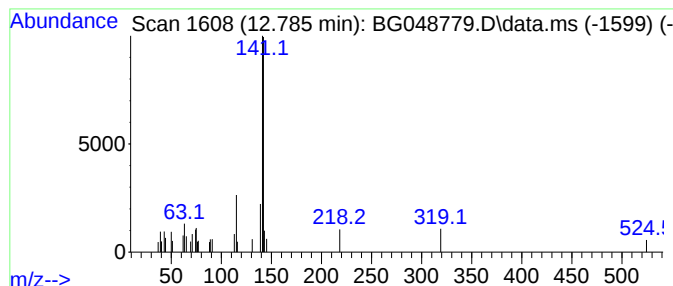
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Indene, 1-ethylidene- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.785	2.72 ng	23512	Naphthalene-d8	10.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	74
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	72
3			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	64
5			Benzocycloheptatriene	142	C11H10	000264-09-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041921\
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Sample : M2079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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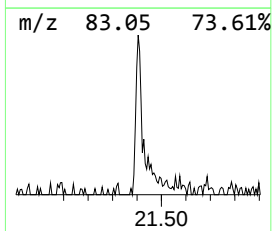
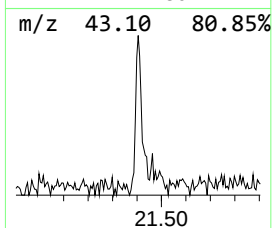
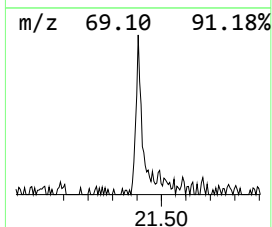
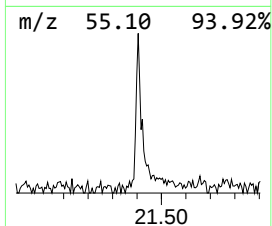
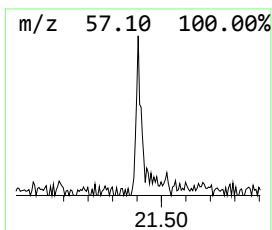
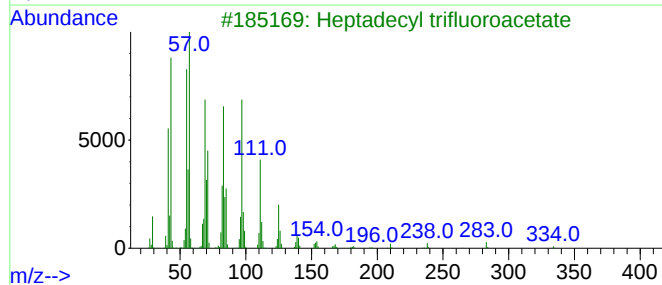
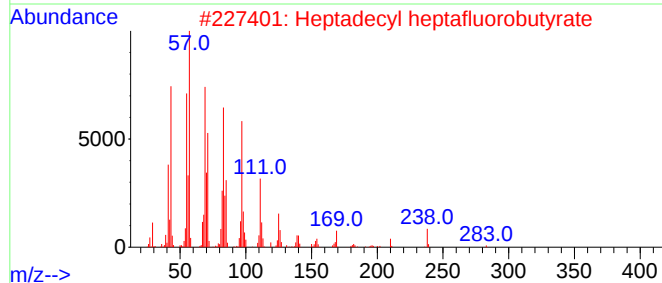
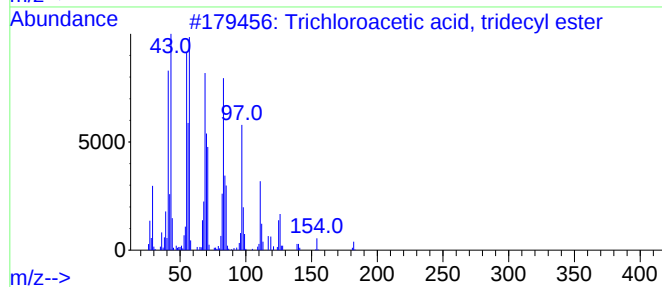
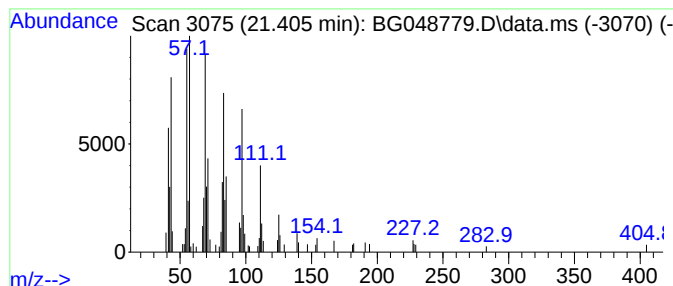
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, tride... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	6.40 ng	118183	Chrysene-d12	21.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	90
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	86
4			Octacosyl acetate	452	C30H60O2	018206-97-8	70
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041921\
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Operator : CG/JU
Sample : M2079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-06

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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
Benzene, (1-met...	6.545	7.2	ng	43426	1	8.073	121149	20.0
Benzene, propyl-	7.039	15.3	ng	92518	1	8.073	121149	20.0
Indane	8.449	12.3	ng	74202	1	8.073	121149	20.0
Benzene, 1,2-di...	8.567	7.2	ng	43875	1	8.073	121149	20.0
1,3,8-p-Menthat...	8.719	4.2	ng	25698	1	8.073	121149	20.0
Benzene, 1-ethy...	9.189	14.2	ng	85934	1	8.073	121149	20.0
1,3-Cyclopentad...	9.718	5.4	ng	46931	2	10.905	172680	20.0
1H-Indene, 1-et...	12.785	2.7	ng	23512	2	10.905	172680	20.0
Trichloroacetic...	21.404	6.4	ng	118183	5	21.786	369089	20.0