

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
 Data File : BM033547.D
 Acq On : 20 Dec 2021 19:20
 Operator : CG/JU
 Sample : M5115-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-3

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_M\Methods\8270-BM121621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033547.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.025	298	304	313	rBV	93830	136865	7.14%	1.334%
2	5.484	376	382	392	rBV	401150	591958	30.87%	5.771%
3	6.107	482	488	496	rBV	28476	44251	2.31%	0.431%
4	7.090	649	655	669	rBV	205653	369524	19.27%	3.602%
5	7.919	788	796	805	rBV	145556	233783	12.19%	2.279%
6	9.095	988	996	1011	rBV	537746	927594	48.37%	9.043%
7	9.372	1037	1043	1051	rBV3	12538	22805	1.19%	0.222%
8	10.007	1140	1151	1155	rBV4	11607	21113	1.10%	0.206%
9	10.731	1267	1274	1279	rBV	173224	299094	15.60%	2.916%
10	10.778	1279	1282	1287	rVV3	33007	58098	3.03%	0.566%
11	10.842	1287	1293	1301	rVB	70689	120896	6.30%	1.179%
12	11.307	1366	1372	1381	rBV	16844	29983	1.56%	0.292%
13	13.189	1685	1692	1698	rBV	1242431	1868223	97.42%	18.213%
14	13.319	1706	1714	1719	rBV7	9596	22009	1.15%	0.215%
15	13.624	1761	1766	1774	rVB	39749	61613	3.21%	0.601%
16	13.907	1806	1814	1819	rBV10	18490	35890	1.87%	0.350%
17	14.566	1920	1926	1933	rBV	236003	375987	19.61%	3.665%
18	14.954	1988	1992	1998	rVB5	16614	25646	1.34%	0.250%
19	15.495	2080	2084	2090	rBV7	8344	20850	1.09%	0.203%
20	15.924	2151	2157	2166	rBV2	95783	159492	8.32%	1.555%
21	16.060	2174	2180	2192	rBV	868050	1320838	68.88%	12.877%
22	17.312	2388	2393	2400	rBV	252427	378136	19.72%	3.686%
23	18.212	2541	2546	2551	rBV	158945	232189	12.11%	2.264%
24	19.483	2759	2762	2772	rVB	106553	150840	7.87%	1.471%
25	19.936	2834	2839	2846	rBV	1545165	1917722	100.00%	18.696%
26	21.195	3051	3053	3061	rVB3	52925	76752	4.00%	0.748%
27	21.495	3100	3104	3111	rVB	285079	361201	18.83%	3.521%
28	23.900	3507	3513	3526	rVB2	187490	394283	20.56%	3.844%

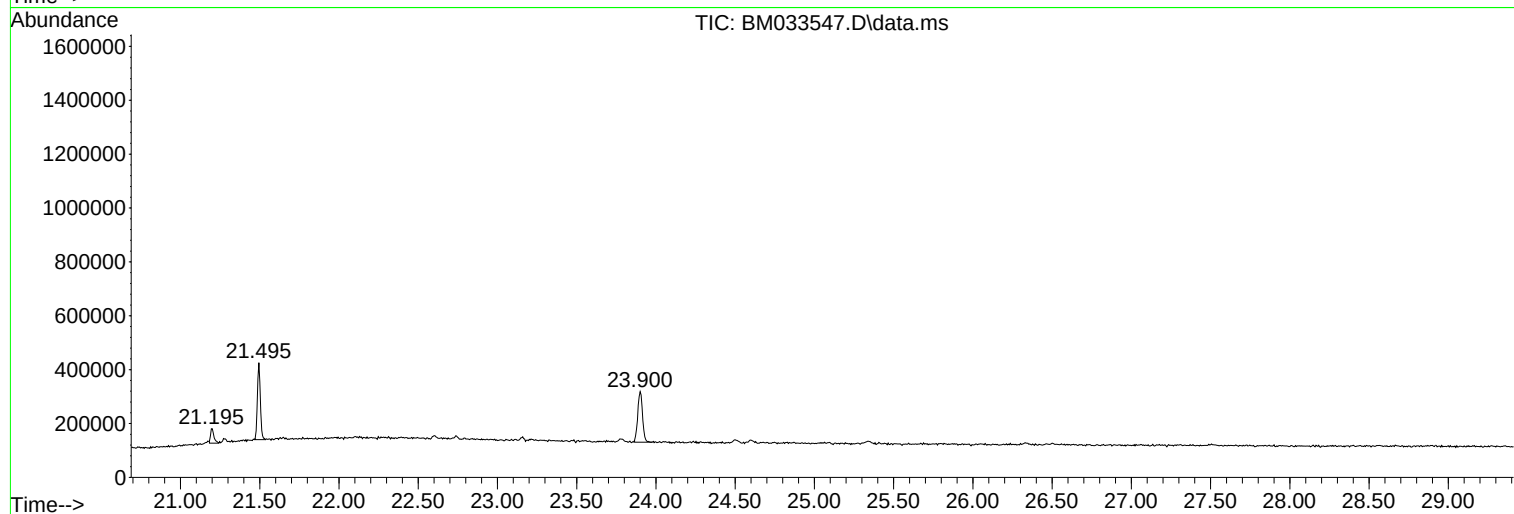
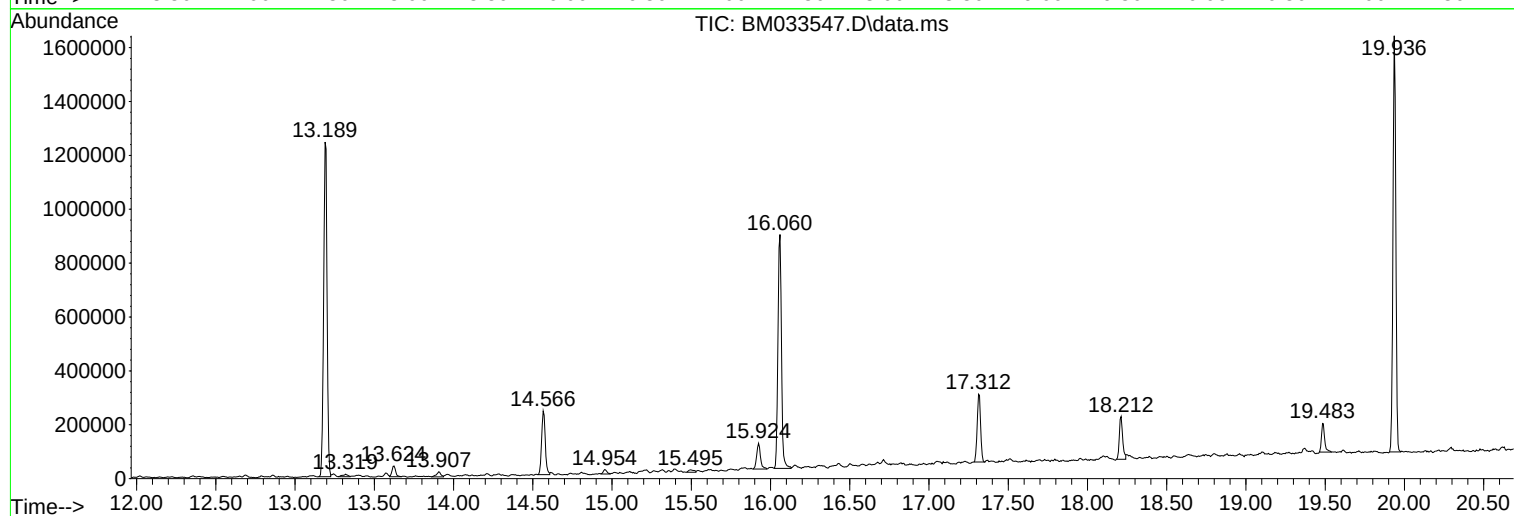
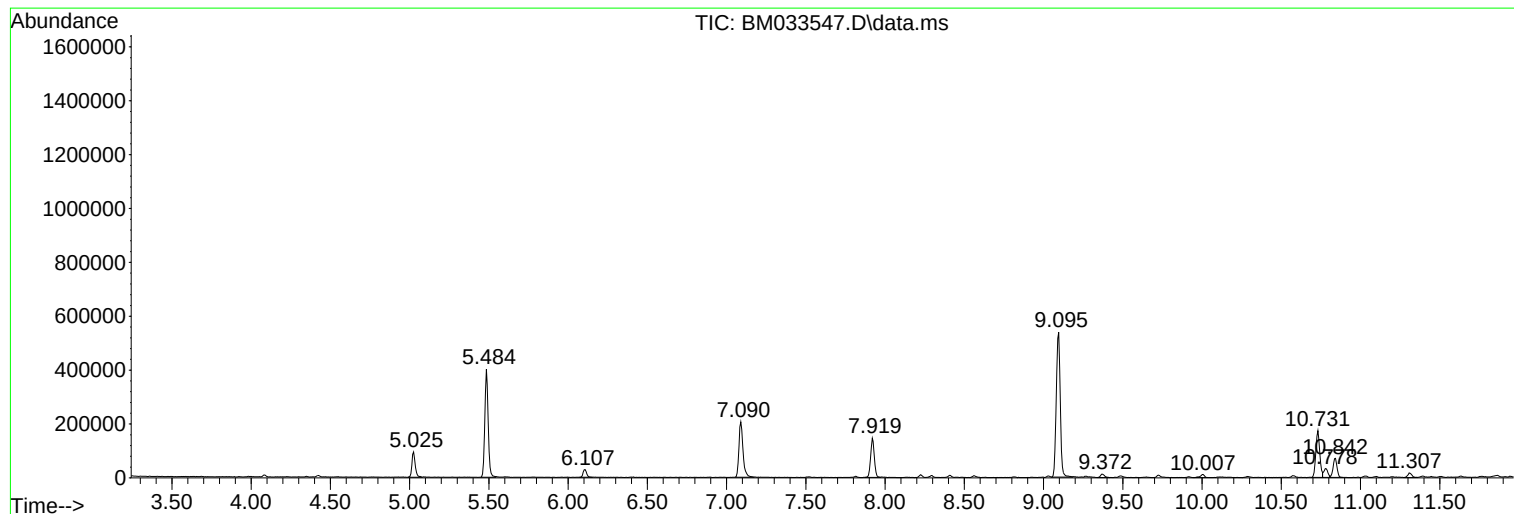
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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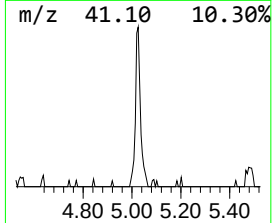
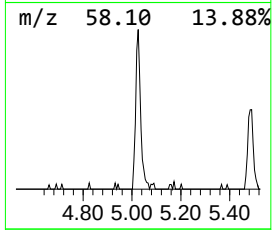
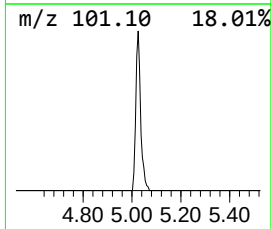
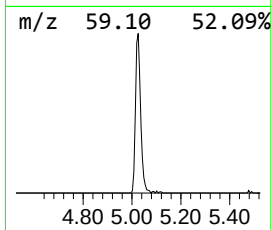
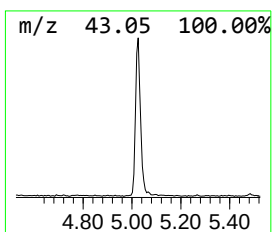
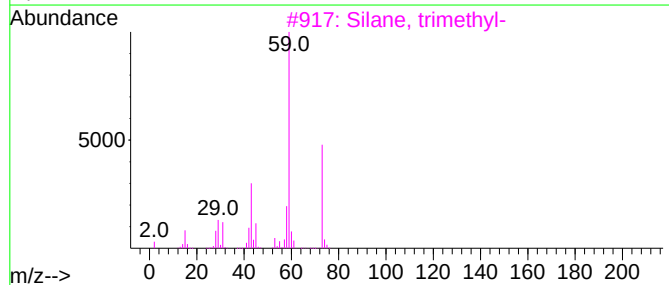
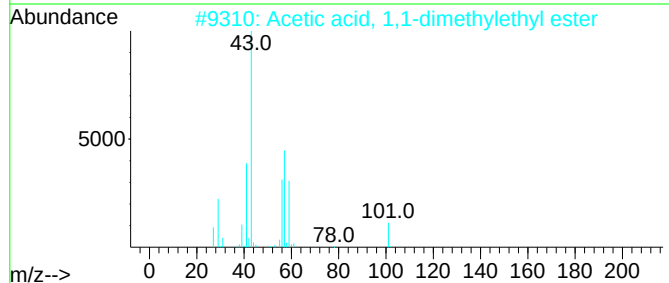
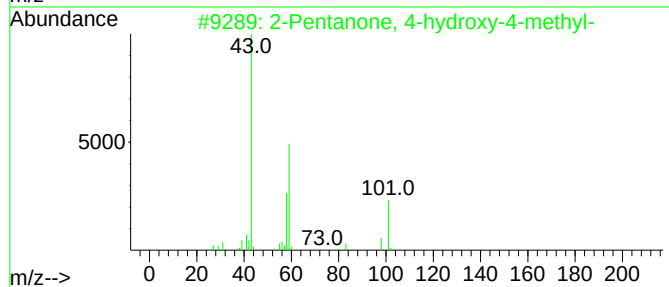
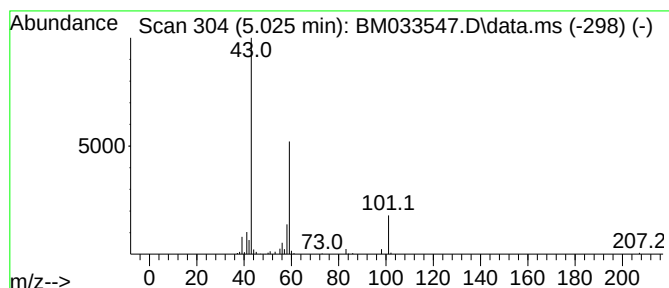
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.025	11.71 ng	136865	1,4-Dichlorobenzene-d4	7.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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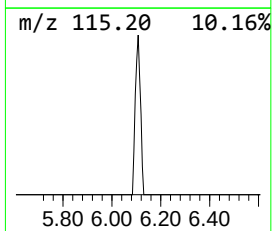
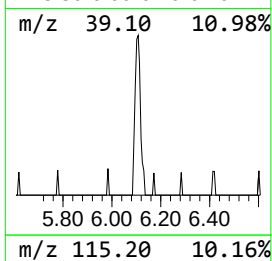
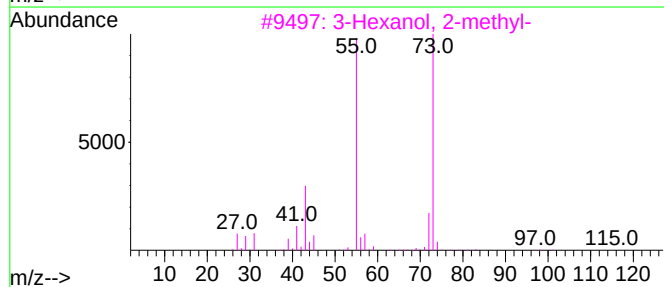
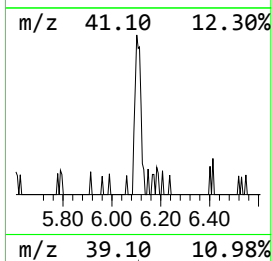
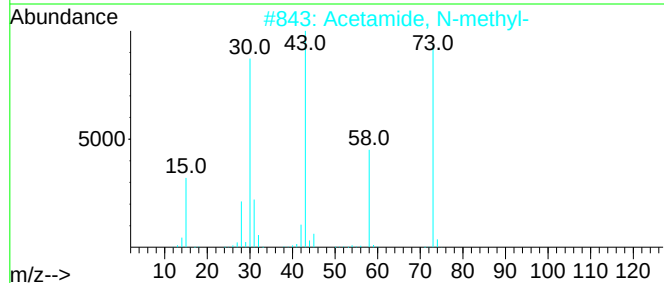
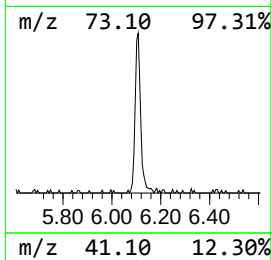
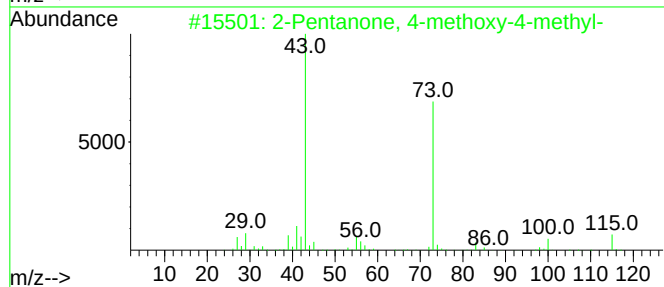
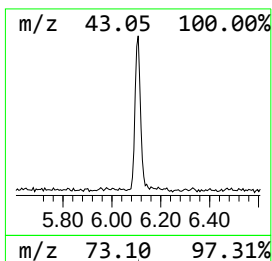
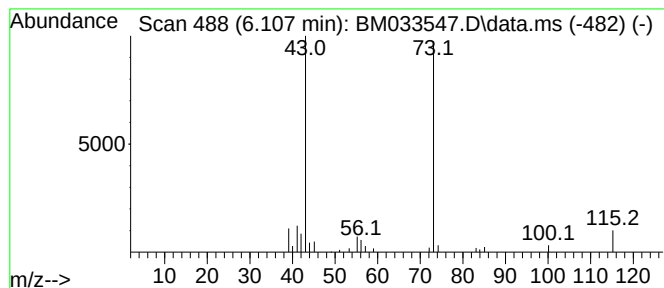
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.107	3.79 ng	44251	1,4-Dichlorobenzene-d4	7.919

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4		Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5		1,2-Dimethoxy-2-methylpropan-1-a...	133	C6H15NO2	1000445-17-2	12



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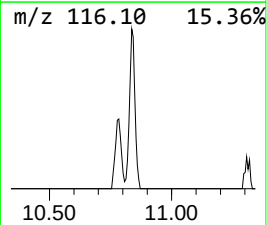
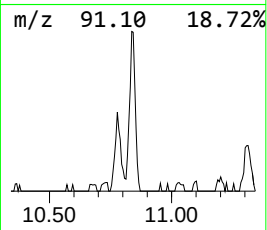
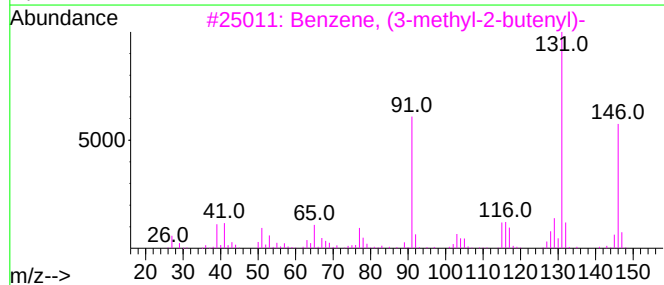
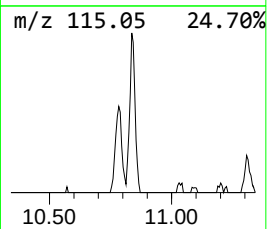
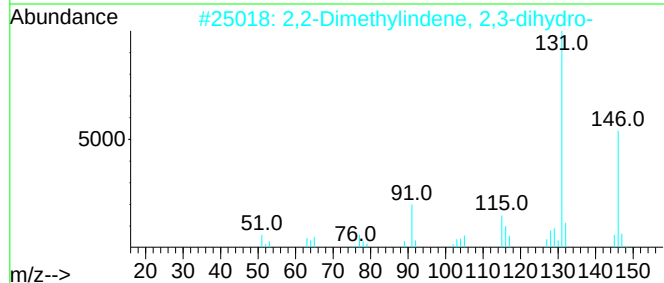
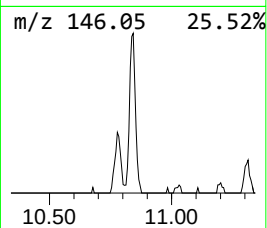
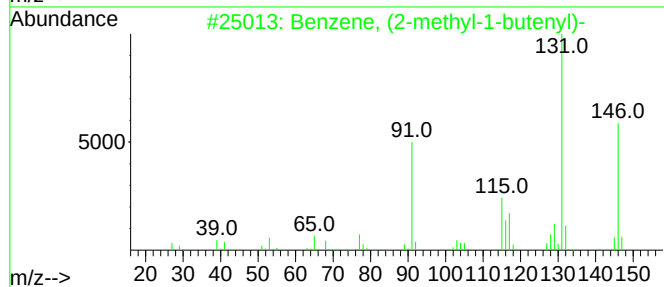
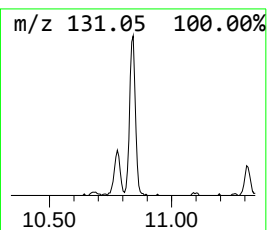
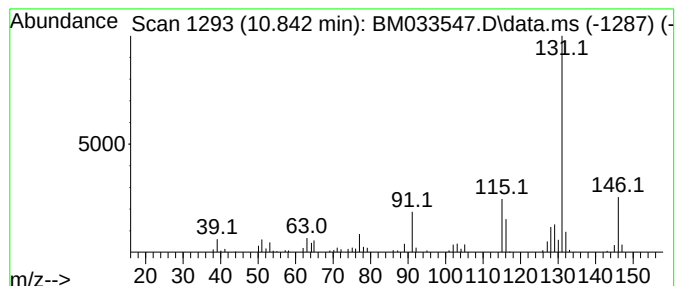
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, (2-methyl-1-butenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.842	8.08 ng	120896	Naphthalene-d8	10.730

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	96
2			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	91
4			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	91
5			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	90



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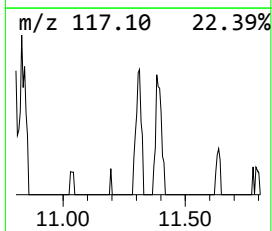
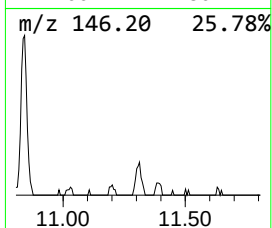
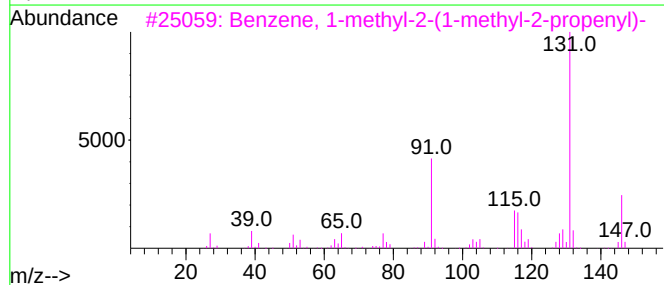
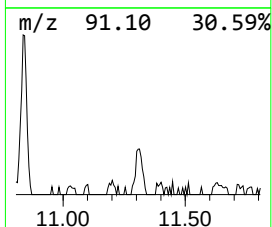
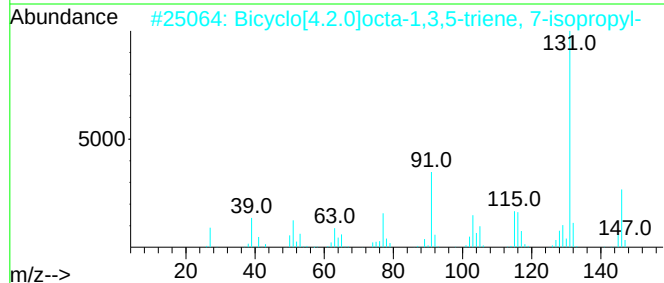
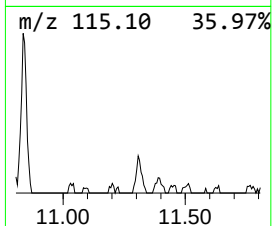
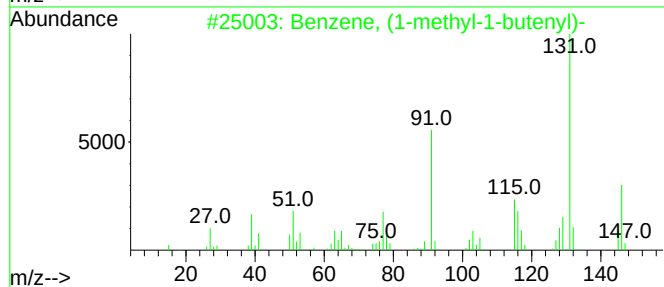
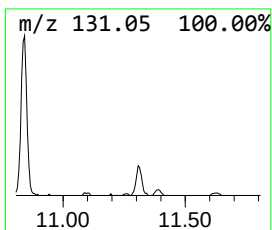
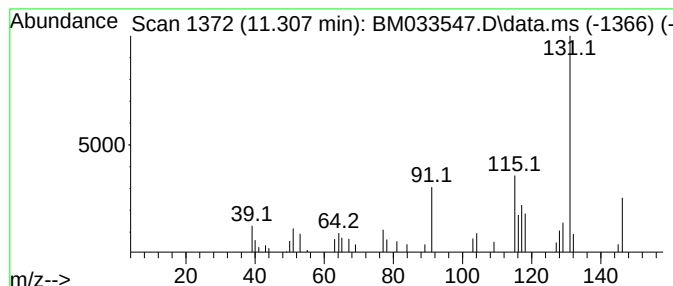
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Peak Number 4 Benzene, (1-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.307	2.00 ng	29983	Naphthalene-d8	10.730

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	81
2			Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	72
3			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	64
4			1,2,3,4-Tetrahydro-1-naphthalene...	236	C13H20Si	1000470-19-9	58
5			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	58



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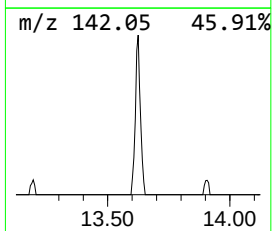
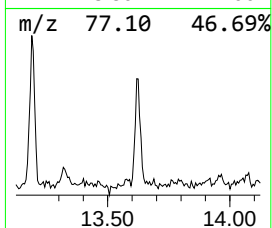
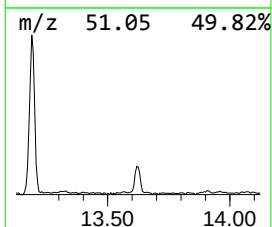
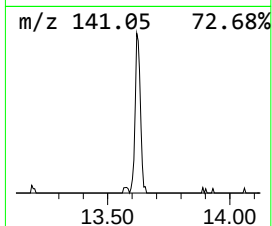
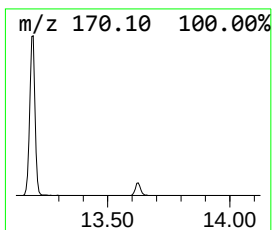
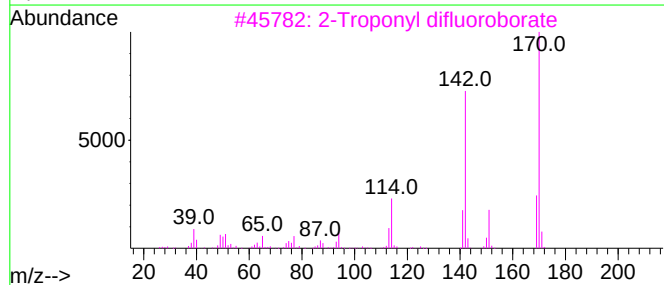
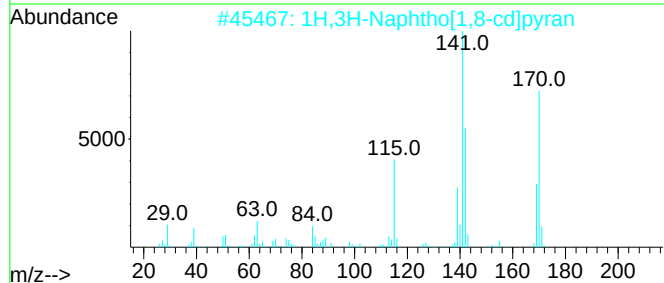
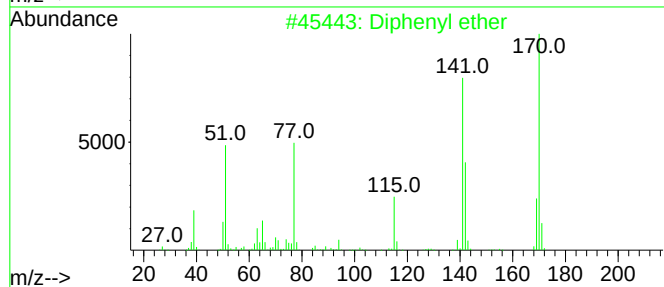
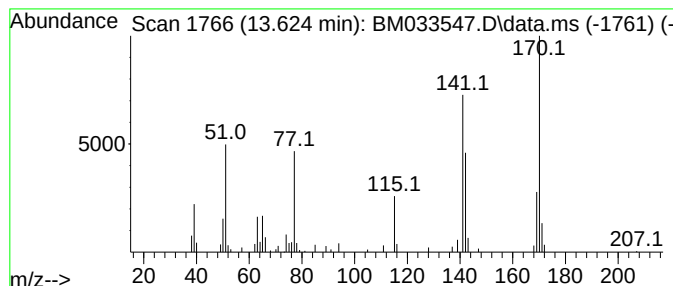
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Peak Number 5 Diphenyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.624	3.28 ng	61613	Acenaphthene-d10	14.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diphenyl ether	170	C12H10O	000101-84-8	98
2			1H,3H-Naphtho[1,8-cd]pyran	170	C12H10O	000203-84-9	47
3			2-Troponyl difluoroborate	170	C7H5BF2O2	022502-10-9	46
4			2-(3-Hydroxybenzylidene)malononi...	170	C10H6N2O	007255-96-1	43
5			3-Hydroxybiphenyl	170	C12H10O	000580-51-8	38



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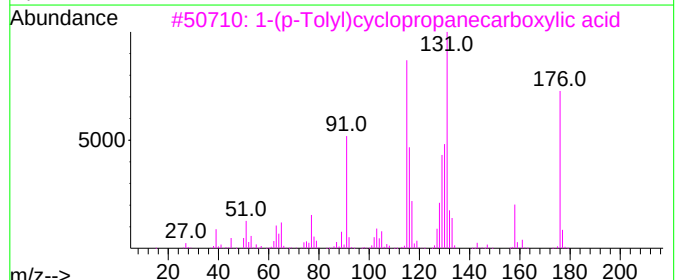
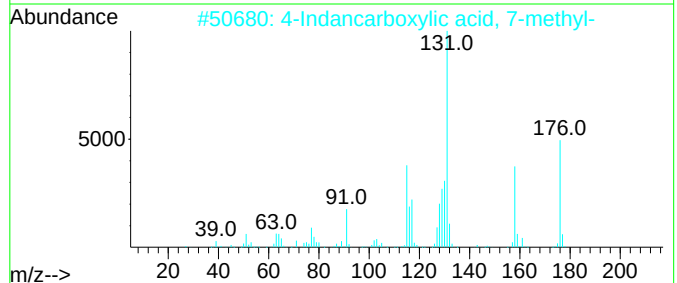
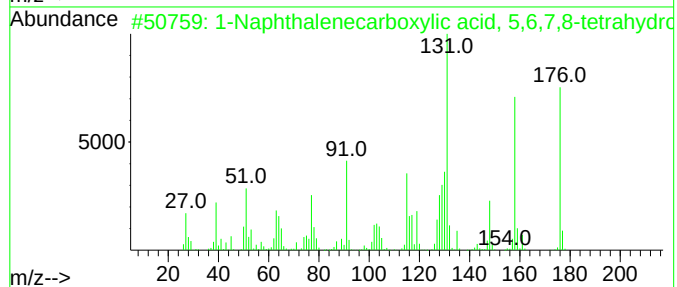
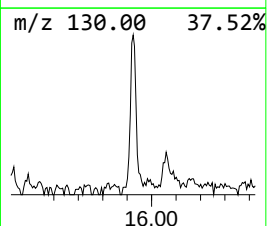
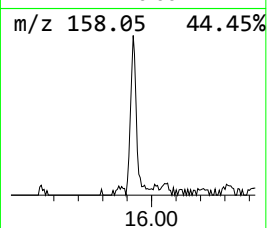
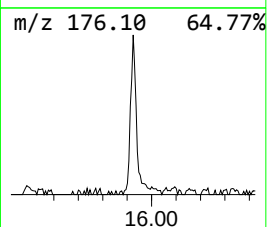
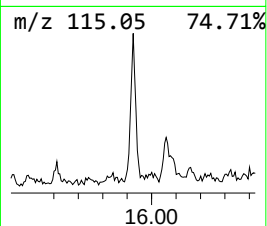
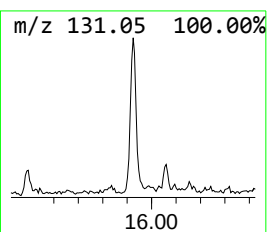
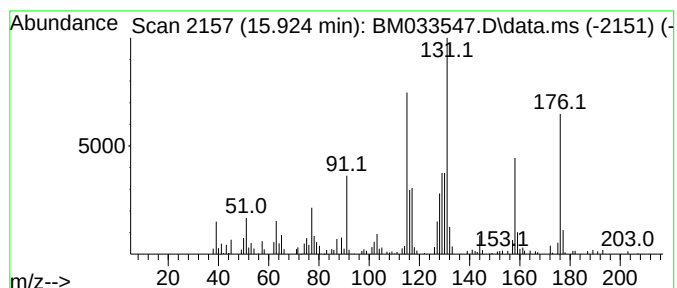
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Naphthalenecarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.924	8.48 ng	159492	Acenaphthene-d10	14.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	97
2			4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	91
3			1-(p-Tolyl)cyclopropanecarboxyli...	176	C11H12O2	083846-66-6	74
4			1,2-Disilacyclopentane, 1,1,2,2-...	158	C7H18Si2	015003-82-4	46
5			Benzene, 1-hexynyl-	158	C12H14	001129-65-3	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033547.D
Acq On : 20 Dec 2021 19:20
Operator : CG/JU
Sample : M5115-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-3

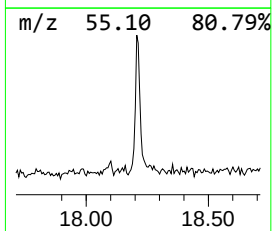
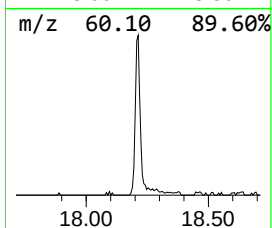
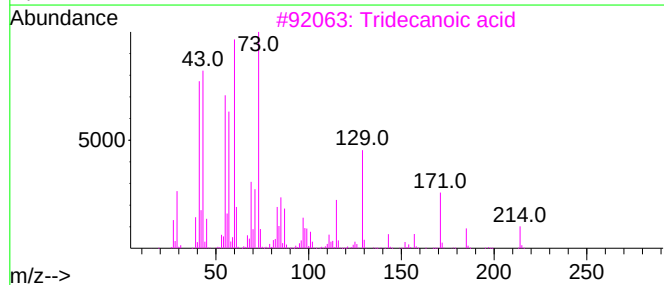
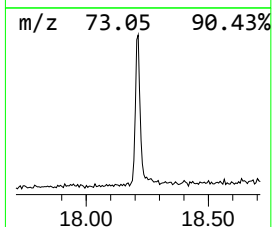
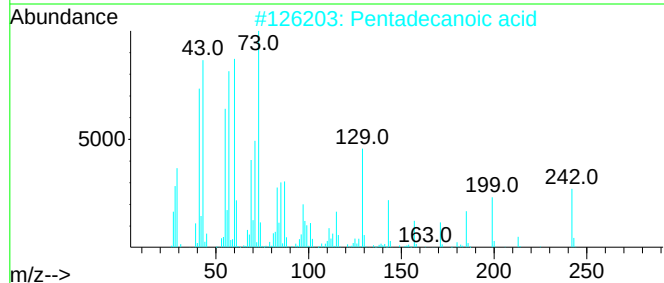
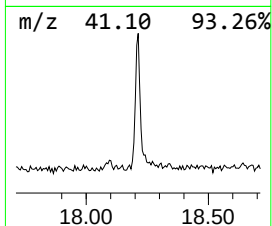
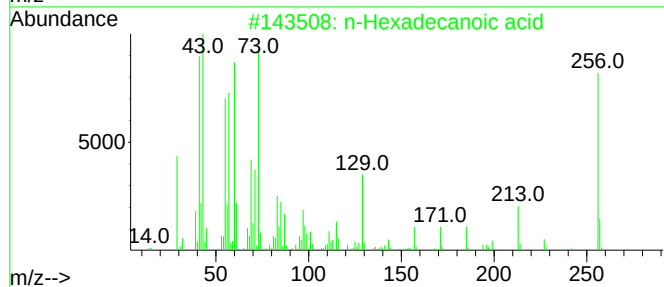
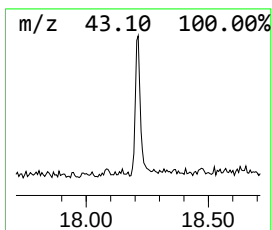
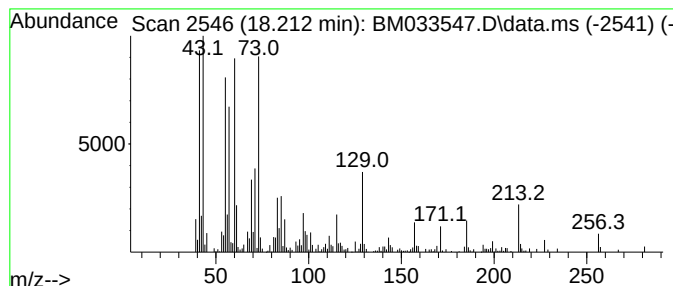
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	12.28 ng	232189	Phenanthrene-d10	17.313

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033547.D
Acq On : 20 Dec 2021 19:20
Operator : CG/JU
Sample : M5115-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-3

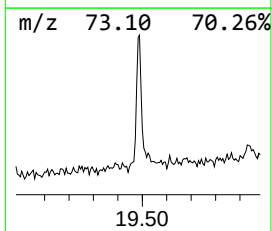
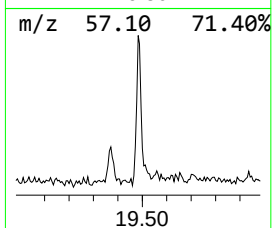
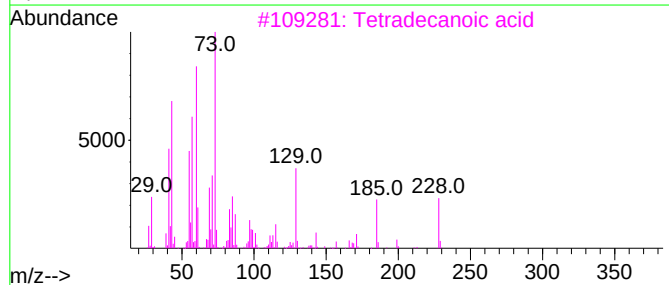
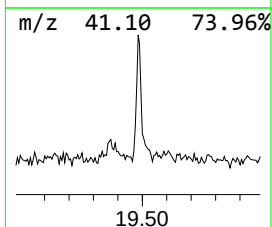
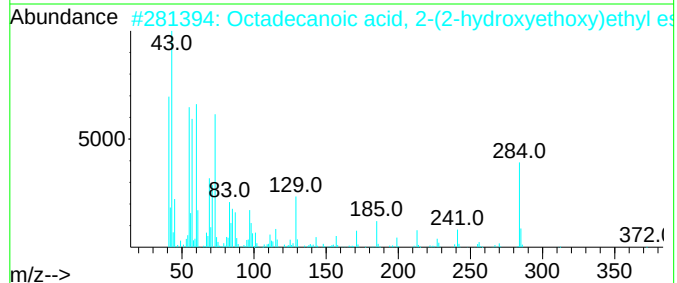
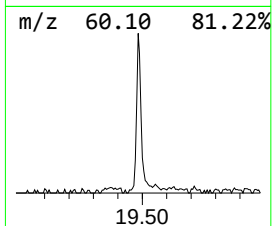
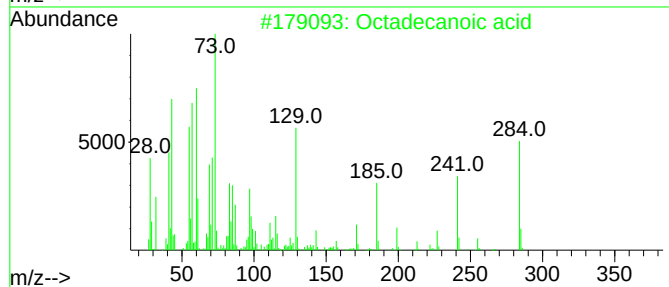
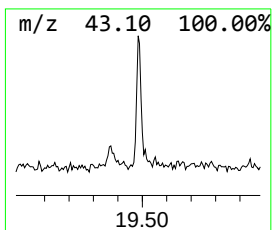
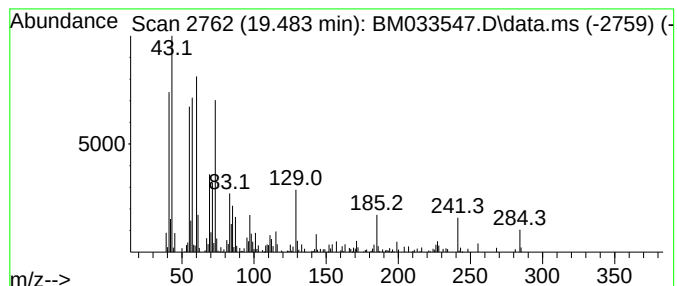
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.483	8.35 ng	150840	Chrysene-d12	21.494

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033547.D
Acq On : 20 Dec 2021 19:20
Operator : CG/JU
Sample : M5115-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

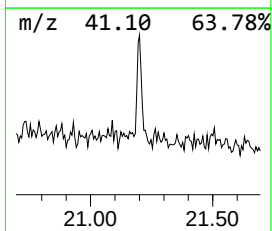
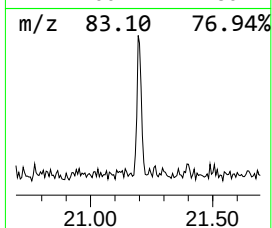
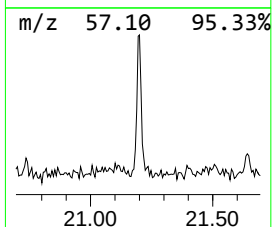
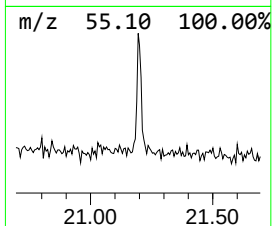
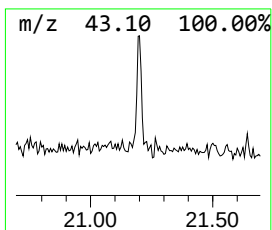
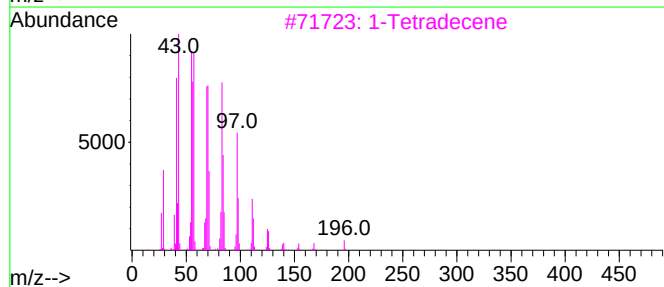
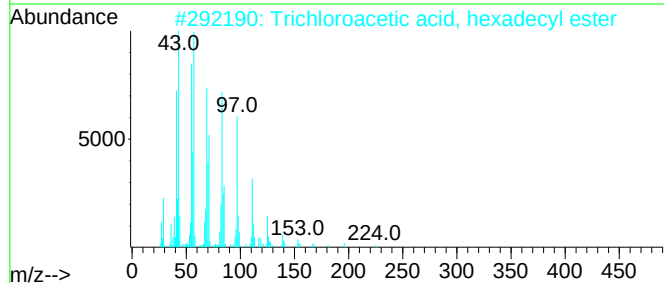
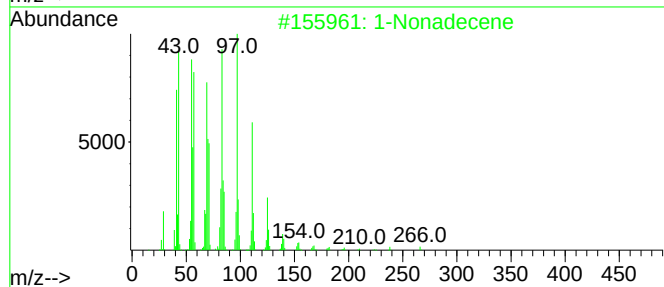
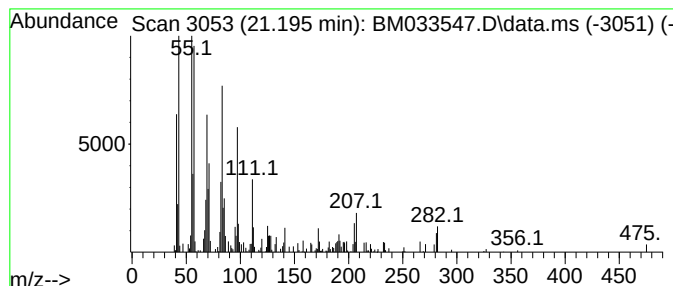
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.195	4.25 ng	76752	Chrysene-d12	21.494	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	1-Tetradecene	196	C14H28	001120-36-1	90
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033547.D
Acq On : 20 Dec 2021 19:20
Operator : CG/JU
Sample : M5115-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.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
2-Pentanone, 4-...	5.025	11.7	ng	136865	1	7.919	233783	20.0
2-Pentanone, 4-...	6.107	3.8	ng	44251	1	7.919	233783	20.0
Benzene, (2-met...	10.842	8.1	ng	120896	2	10.730	299094	20.0
Benzene, (1-met...	11.307	2.0	ng	29983	2	10.730	299094	20.0
Diphenyl ether	13.624	3.3	ng	61613	3	14.566	375987	20.0
1-Naphthaleneca...	15.924	8.5	ng	159492	3	14.566	375987	20.0
n-Hexadecanoic ...	18.212	12.3	ng	232189	4	17.313	378136	20.0
Octadecanoic acid	19.483	8.3	ng	150840	5	21.494	361201	20.0
1-Nonadecene	21.195	4.3	ng	76752	5	21.494	361201	20.0