

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013125\
 Data File : BF141349.D
 Acq On : 31 Jan 2025 23:10
 Operator : RC/JU
 Sample : Q1194-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-110-SB01

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_F\Methods\8270-BF012925.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	5	11	17	rBV	72385	108401	3.20%	0.463%
2	2.346	31	43	57	rVB	51666	186216	5.50%	0.795%
3	5.010	491	496	502	rVB	40951	67045	1.98%	0.286%
4	5.422	560	566	584	rBV	2282457	3033055	89.59%	12.948%
5	5.981	656	661	670	rBV	59009	79311	2.34%	0.339%
6	6.440	733	739	756	rBV	2177653	3055889	90.26%	13.045%
7	6.798	795	800	805	rBV	735261	899199	26.56%	3.839%
8	7.357	889	895	900	rBV	1516199	2002245	59.14%	8.547%
9	7.616	933	939	947	rBV	81440	104051	3.07%	0.444%
10	8.081	1010	1018	1023	rBV	942087	1208483	35.69%	5.159%
11	8.298	1051	1055	1062	rVB	33531	43882	1.30%	0.187%
12	8.669	1113	1118	1122	rBV	44461	58728	1.73%	0.251%
13	9.157	1195	1201	1206	rBV	2631881	3385629	100.00%	14.453%
14	9.234	1210	1214	1219	rVB	41207	56425	1.67%	0.241%
15	9.834	1310	1316	1328	rBV	1032656	1291141	38.14%	5.512%
16	10.545	1432	1437	1445	rBV	169420	221757	6.55%	0.947%
17	10.622	1445	1450	1468	rBV	1387377	1843411	54.45%	7.869%
18	11.322	1564	1569	1576	rVB	873519	1099316	32.47%	4.693%
19	11.857	1654	1660	1674	rBV2	122009	244818	7.23%	1.045%
20	12.104	1698	1702	1710	rVB	42057	54385	1.61%	0.232%
21	12.645	1787	1794	1805	rBV6	23026	65109	1.92%	0.278%
22	12.910	1833	1839	1844	rBV	1885314	2389896	70.59%	10.202%
23	13.451	1926	1931	1939	rBV	169032	231058	6.82%	0.986%
24	13.880	1996	2004	2010	rBV6	14878	43408	1.28%	0.185%
25	13.963	2012	2018	2025	rVB	641075	867094	25.61%	3.701%
26	15.416	2259	2265	2281	rVB	463911	734594	21.70%	3.136%
27	18.210	2736	2740	2750	rVB3	19926	51064	1.51%	0.218%

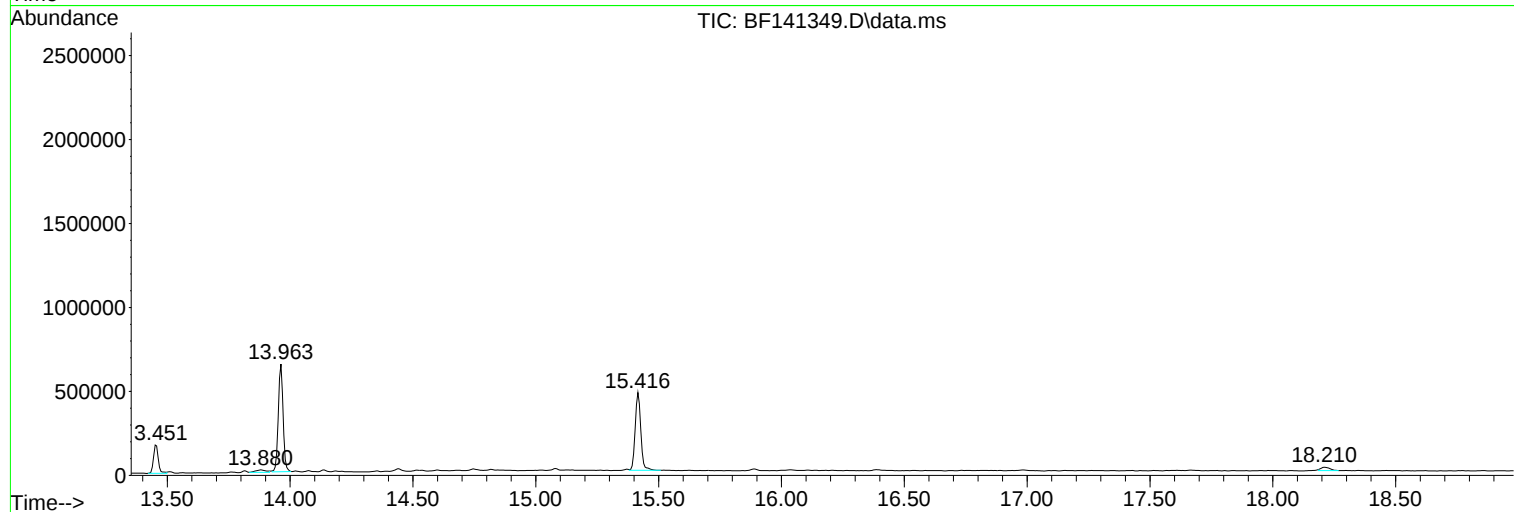
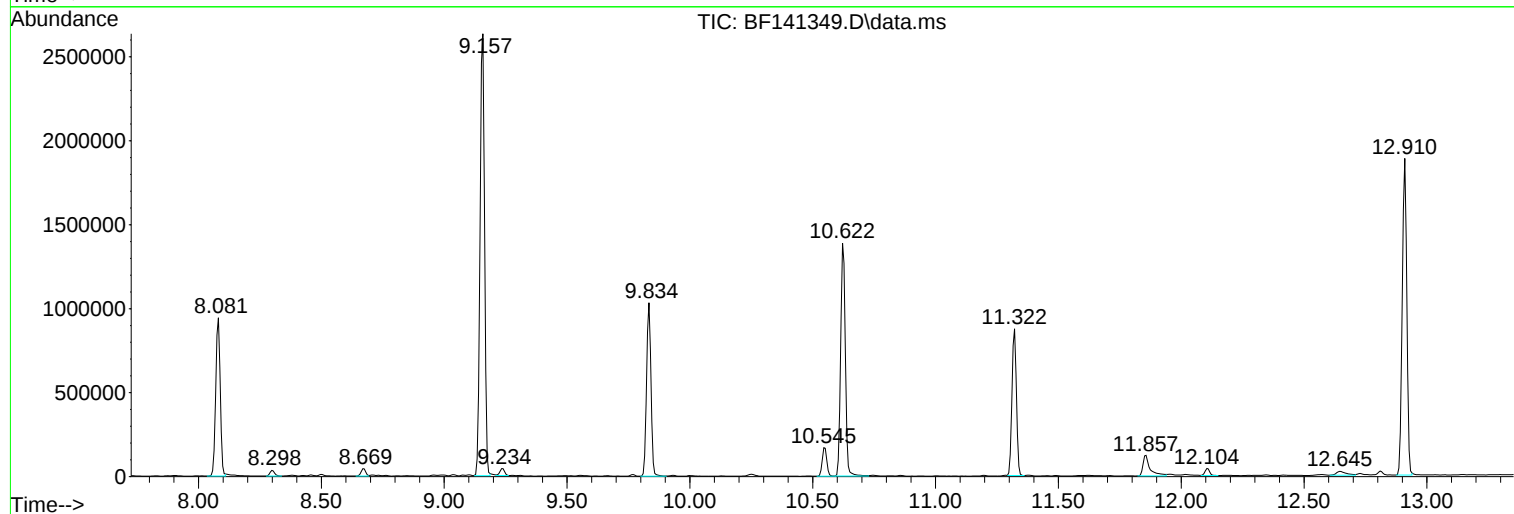
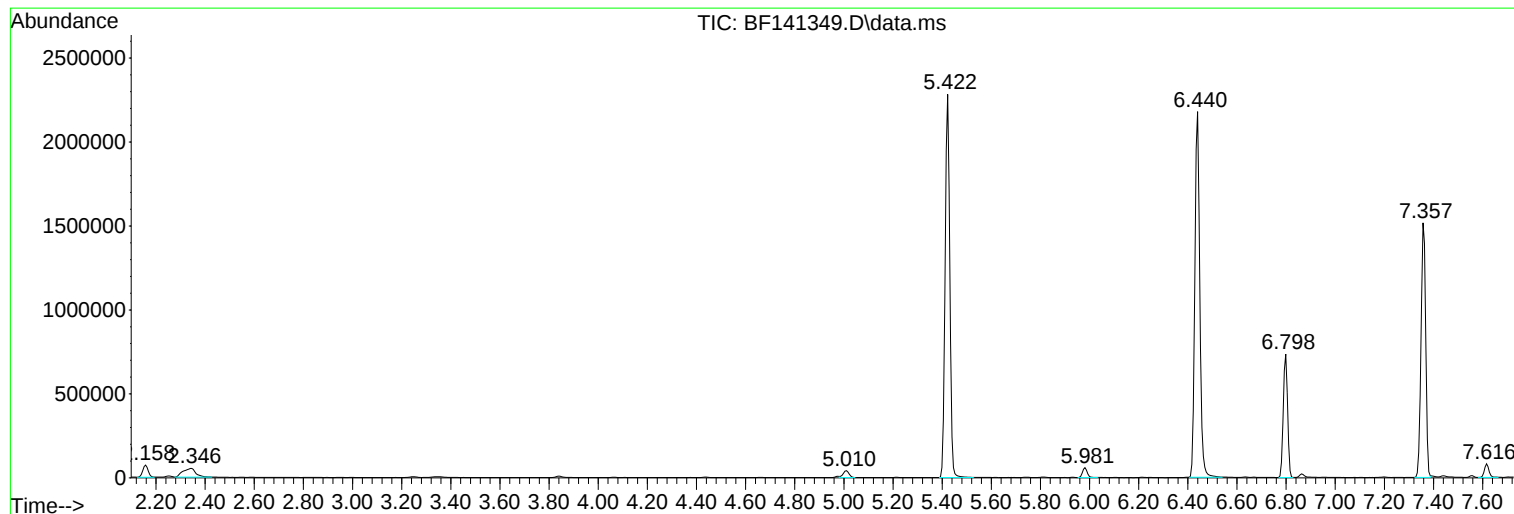
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-110-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.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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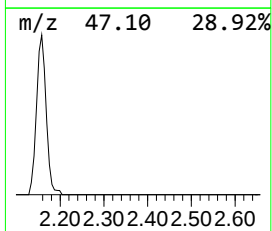
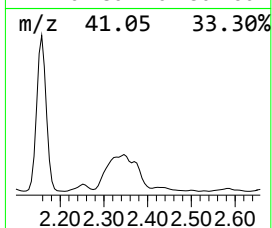
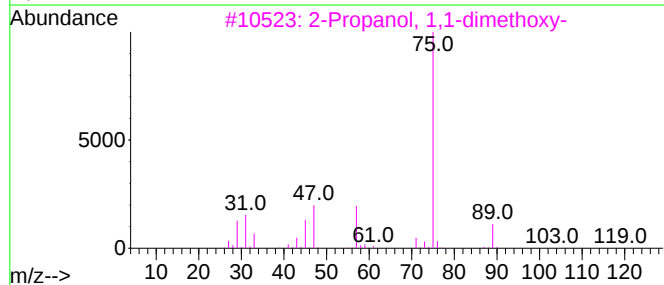
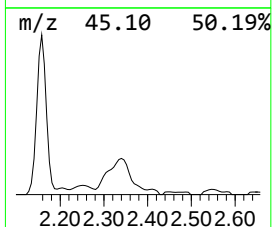
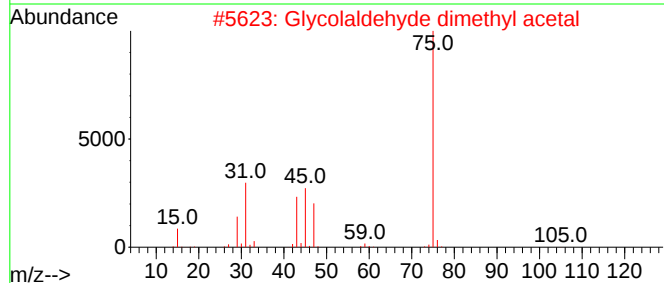
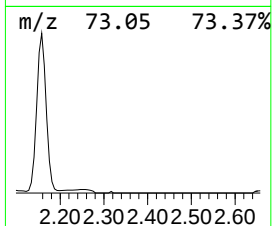
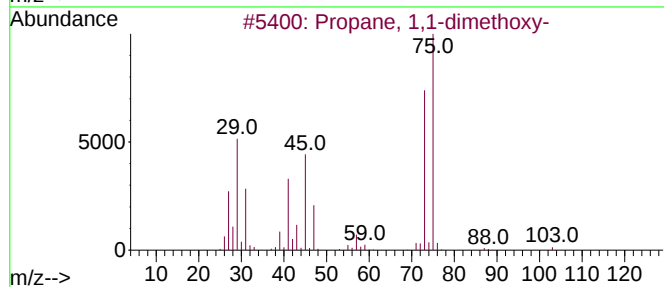
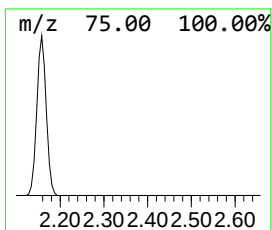
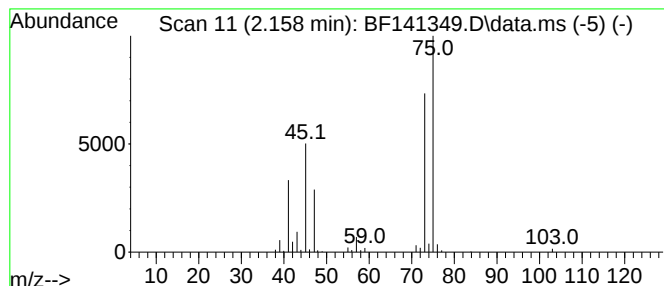
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	2.41 ng	108401	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	42
3			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
4			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	38
5			Methane, trimethoxy-	106	C4H10O3	000149-73-5	38



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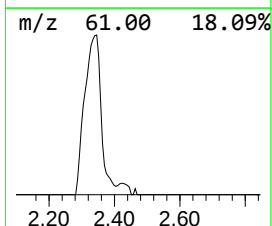
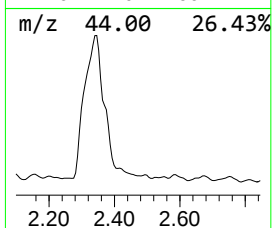
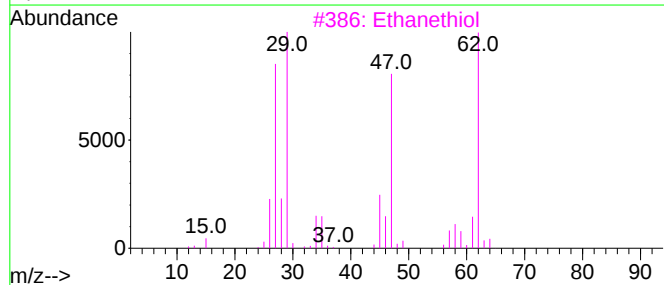
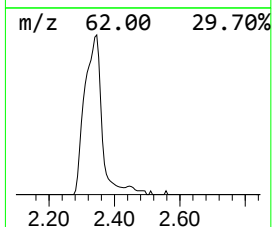
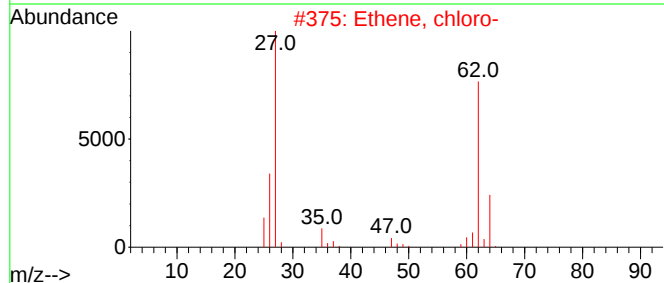
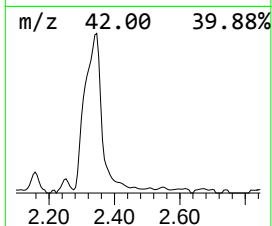
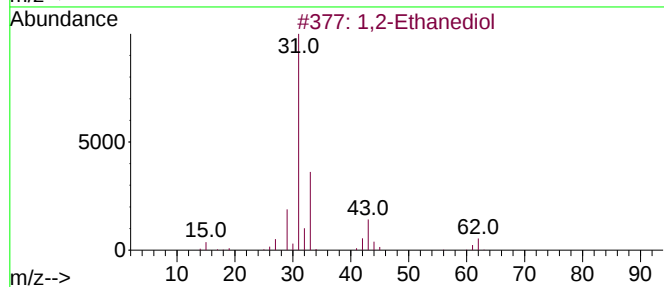
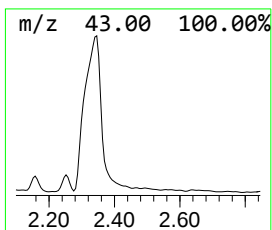
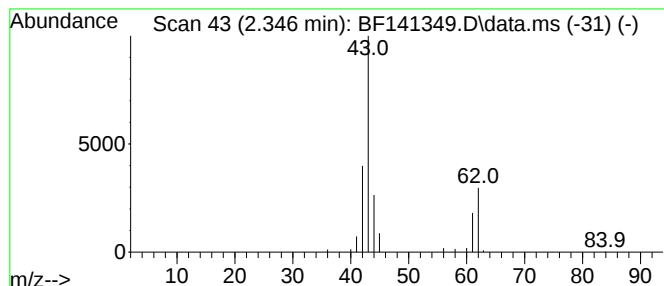
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.346 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.346	4.14 ng	186216	1,4-Dichlorobenzene-d4	6.798

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Ethanediol	62	C2H6O2	000107-21-1	9
2		Ethene, chloro-	62	C2H3Cl	000075-01-4	5
3		Ethanethiol	62	C2H6S	000075-08-1	4
4		Peroxide, dimethyl	62	C2H6O2	000690-02-8	4
5		Diazirine	42	CH2N2	1000305-84-1	3



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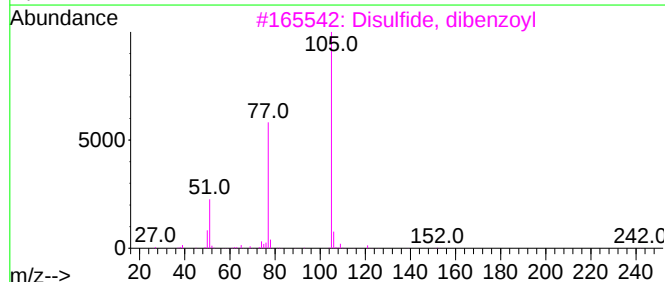
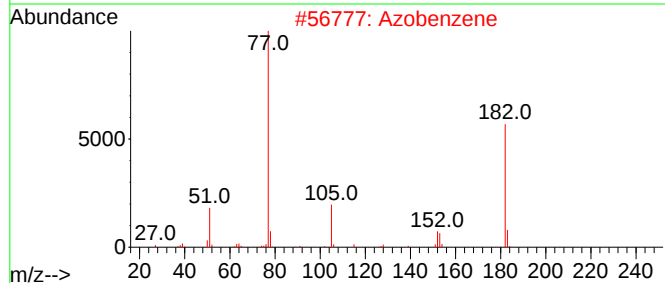
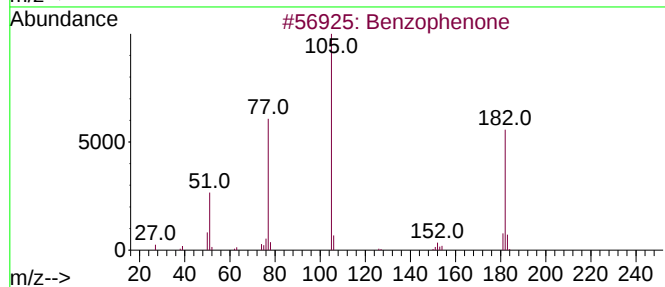
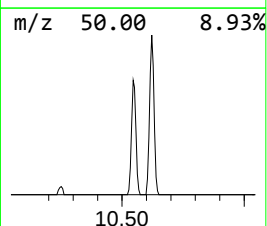
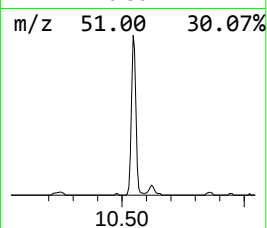
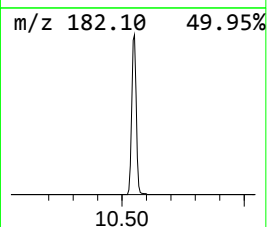
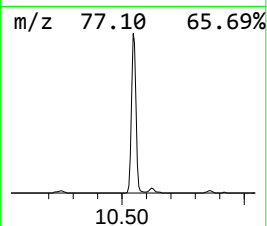
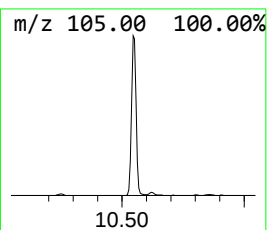
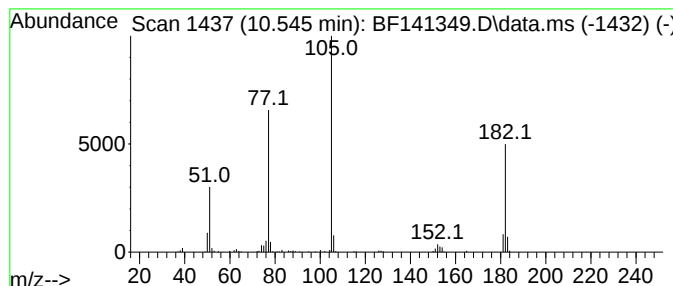
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	3.44 ng	221757	Acenaphthene-d10	9.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			Methyl benzilate	242	C15H14O3	000076-89-1	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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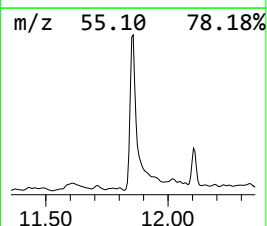
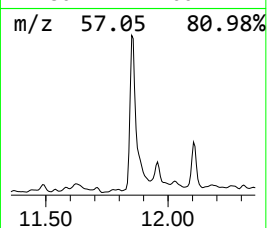
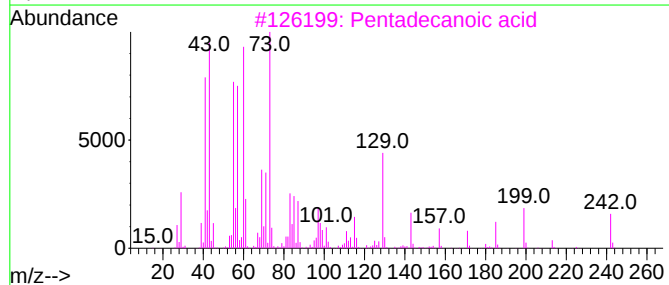
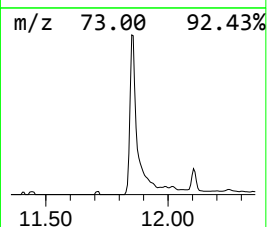
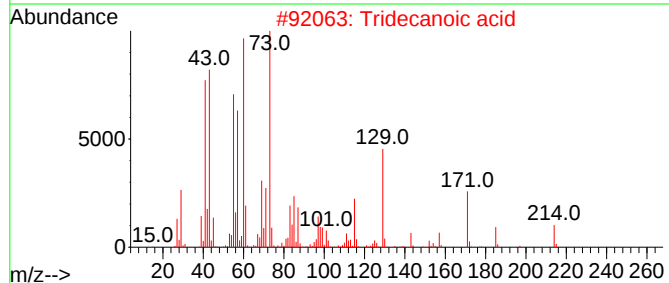
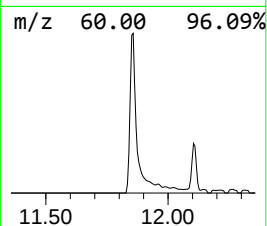
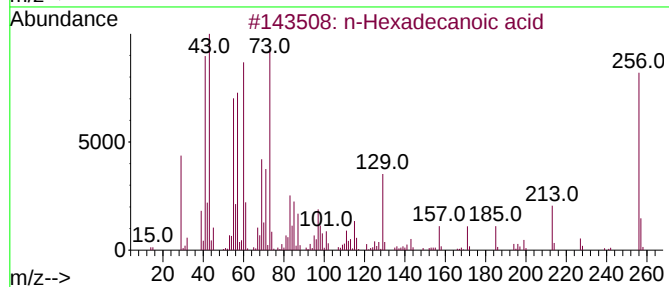
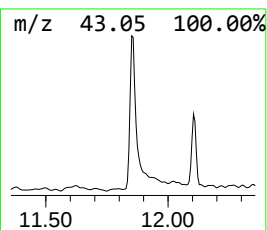
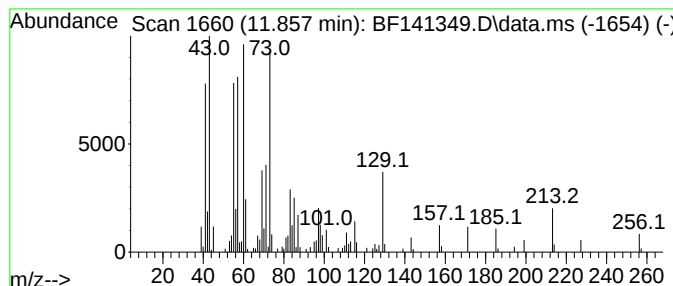
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.45 ng	244818	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Octanoic acid	144	C8H16O2	000124-07-2	43



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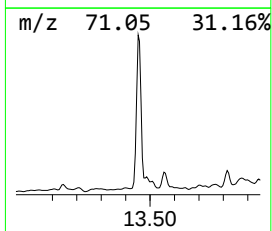
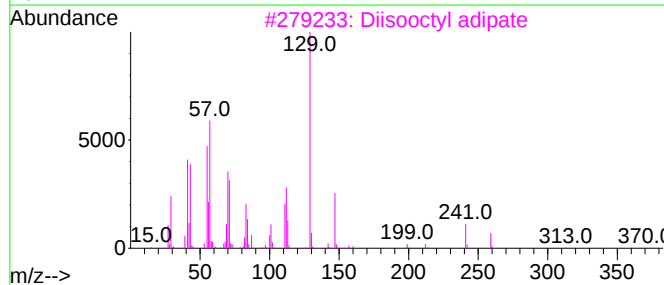
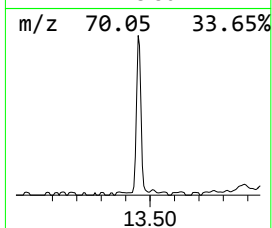
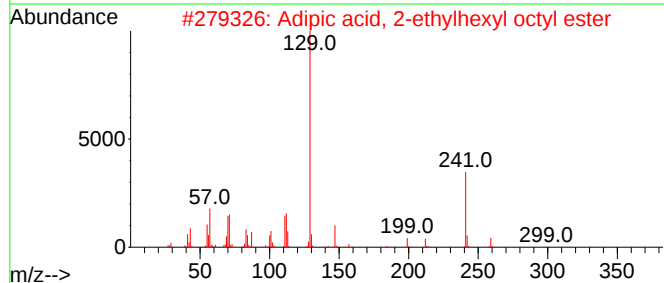
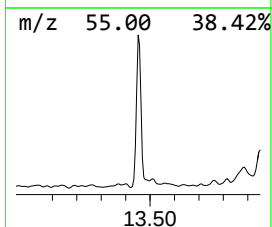
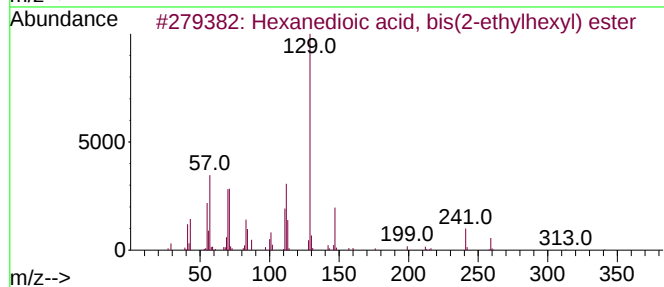
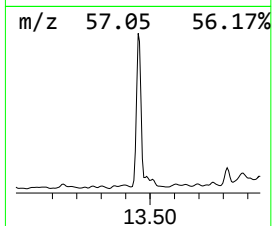
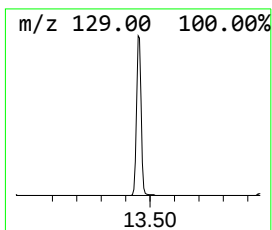
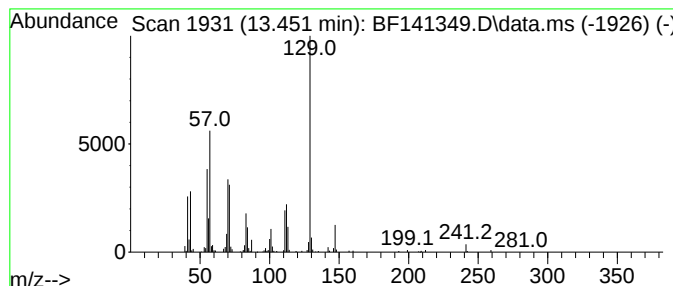
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.451	5.33 ng	231058	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3	Diisooctyl adipate	370	C22H42O4	001330-86-5	86
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	70
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.158	2.4	ng	108401	1	6.798	899199	20.0
unknown2.346	2.346	4.1	ng	186216	1	6.798	899199	20.0
Benzophenone	10.545	3.4	ng	221757	3	9.834	1291140	20.0
n-Hexadecanoic ...	11.857	4.5	ng	244818	4	11.322	1099320	20.0
Hexanedioic aci...	13.451	5.3	ng	231058	5	13.963	867094	20.0