

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100724\
 Data File : BF139691.D
 Acq On : 07 Oct 2024 17:31
 Operator : RC/JU
 Sample : P4290-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IB-4

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-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	3	12	25	rVB	1799290	2896796	100.00%	14.891%
2	5.081	503	508	524	rVB	97911	151806	5.24%	0.780%
3	5.487	568	577	582	rBV	1493165	1945069	67.15%	9.999%
4	6.498	738	749	767	rBV	1469019	2043494	70.54%	10.505%
5	6.863	806	811	816	rBV	419112	500867	17.29%	2.575%
6	7.428	898	907	912	rBV	998941	1327244	45.82%	6.823%
7	7.681	944	950	958	rVB	39337	51311	1.77%	0.264%
8	8.145	1022	1029	1042	rBV	524942	656470	22.66%	3.375%
9	9.222	1206	1212	1217	rBV	1865110	2375159	81.99%	12.209%
10	9.898	1322	1327	1332	rVB	595918	734926	25.37%	3.778%
11	10.616	1443	1449	1454	rBV	363689	470965	16.26%	2.421%
12	10.692	1456	1462	1477	rVV	1115231	1515623	52.32%	7.791%
13	11.386	1575	1580	1588	rBV	655868	810534	27.98%	4.167%
14	11.910	1664	1669	1683	rBV	149210	259561	8.96%	1.334%
15	12.698	1798	1803	1815	rBV3	15078	32899	1.14%	0.169%
16	12.974	1844	1850	1855	rBV	1978308	2568203	88.66%	13.202%
17	13.874	1998	2003	2017	rBV5	11430	38423	1.33%	0.198%
18	14.027	2023	2029	2037	rBV	449408	574794	19.84%	2.955%
19	14.780	2153	2157	2164	rBV2	24742	46749	1.61%	0.240%
20	15.498	2273	2279	2289	rVB	292091	452539	15.62%	2.326%

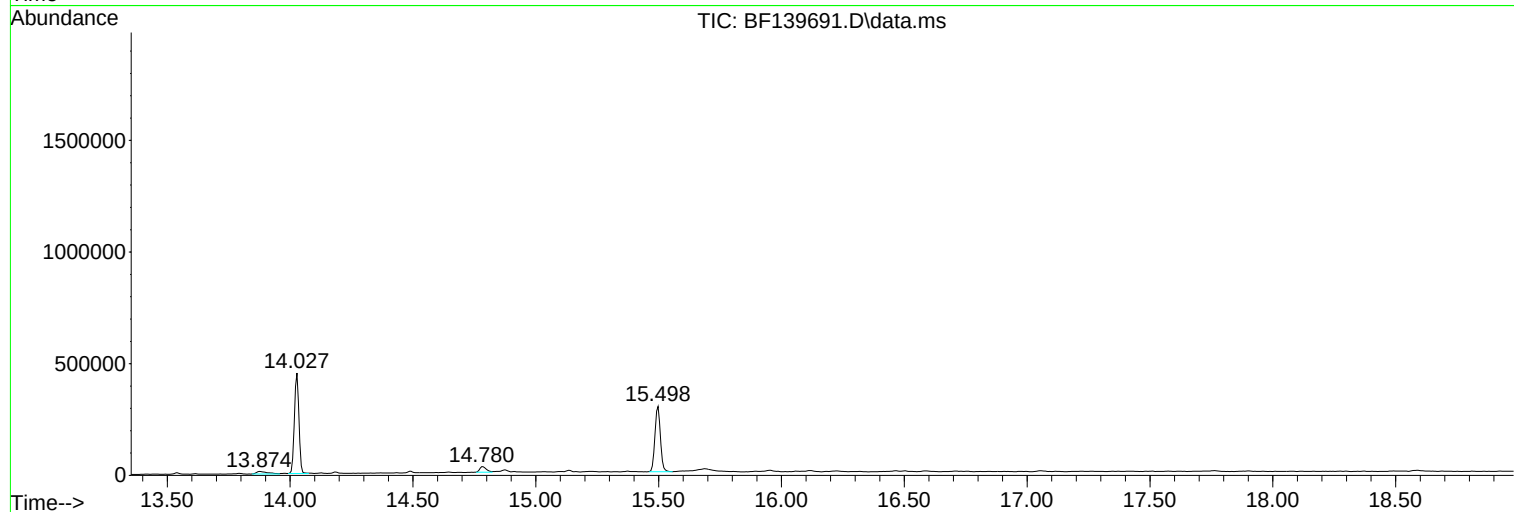
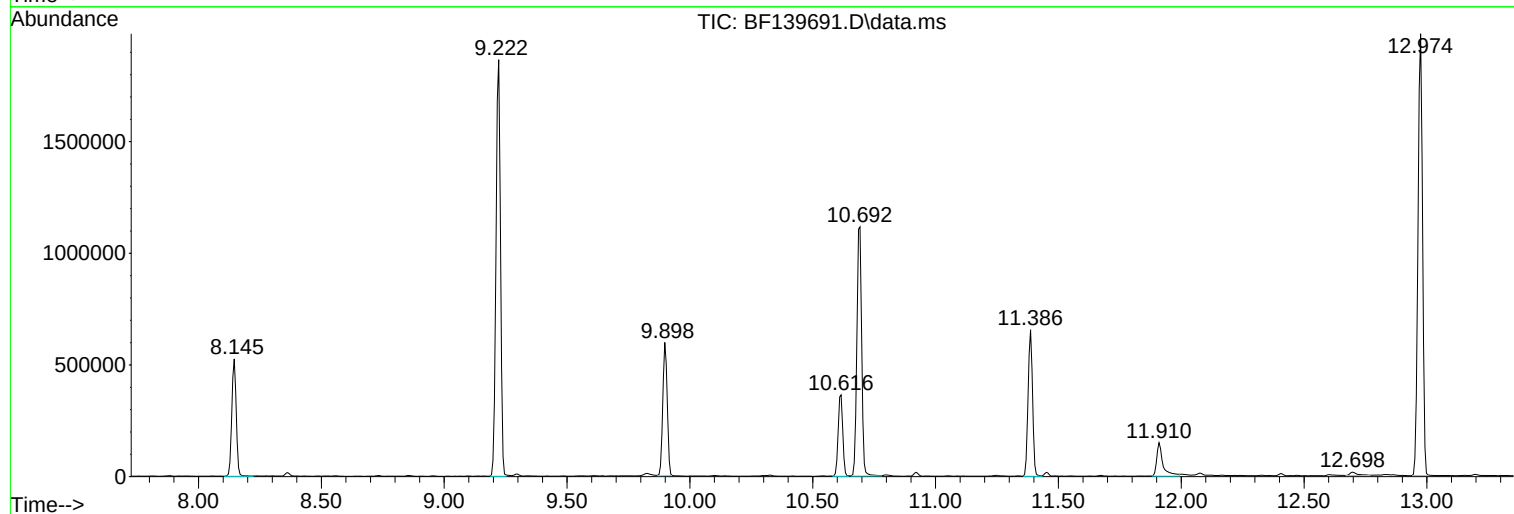
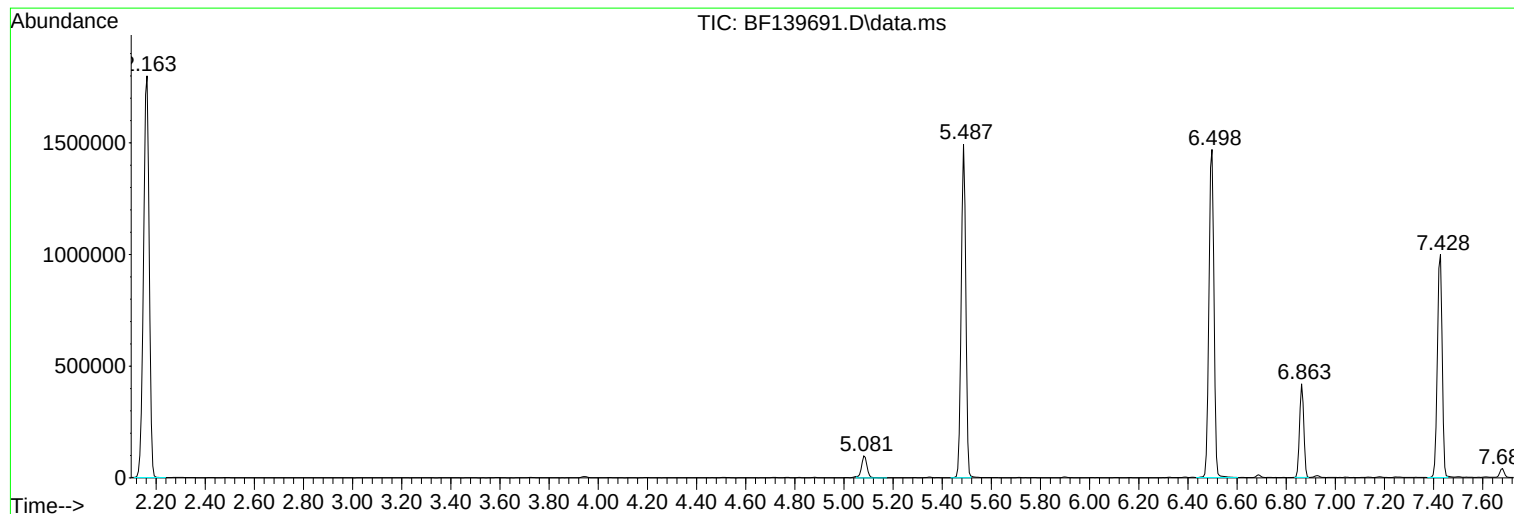
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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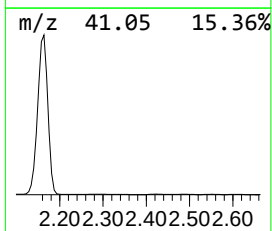
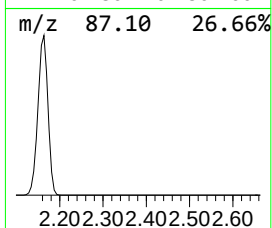
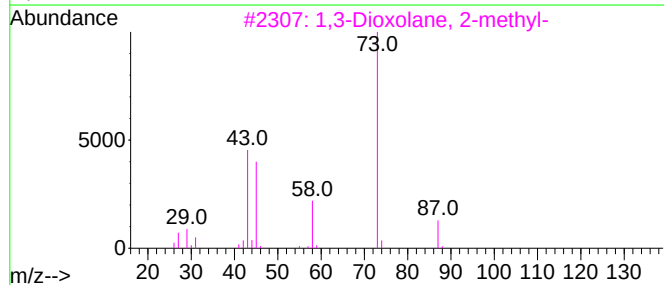
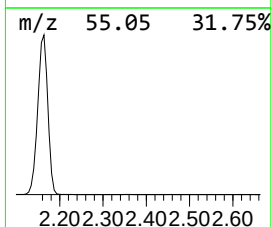
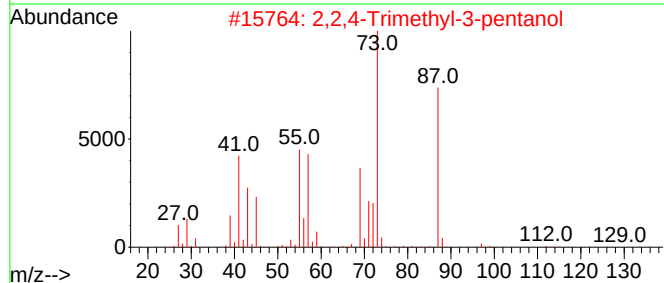
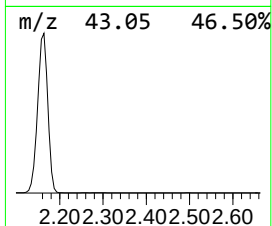
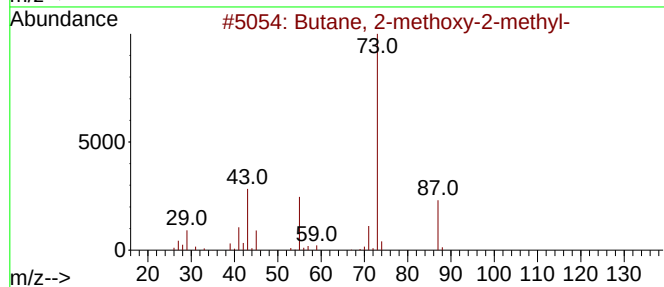
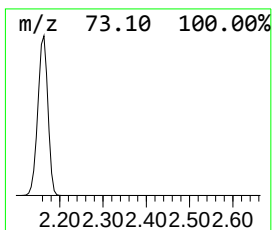
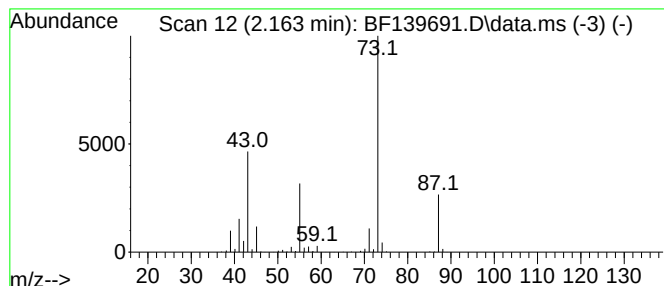
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	115.67 ng	2896800	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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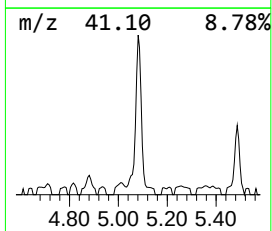
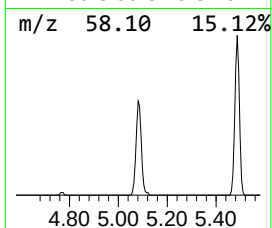
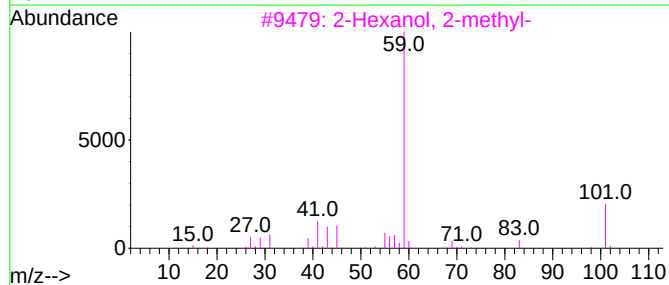
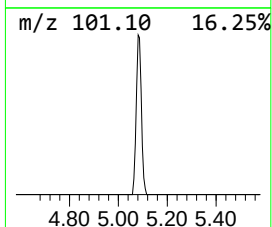
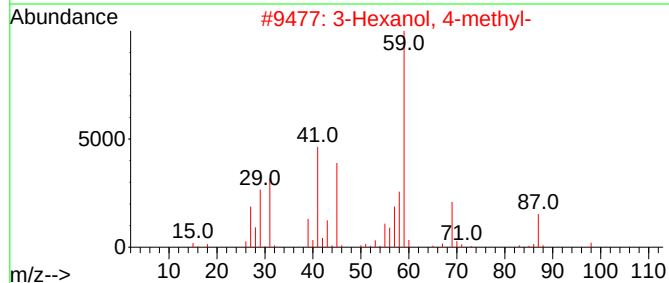
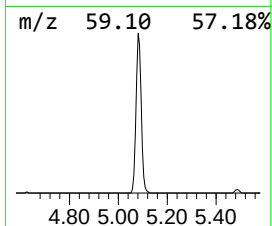
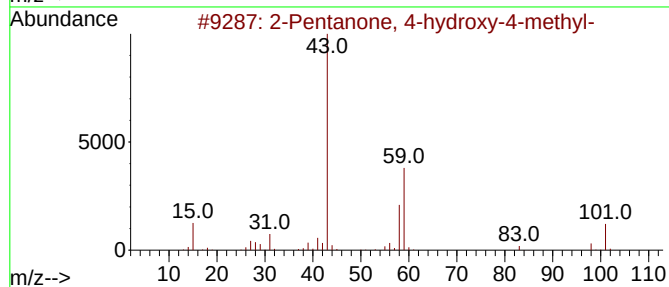
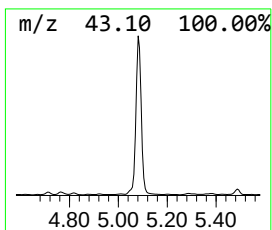
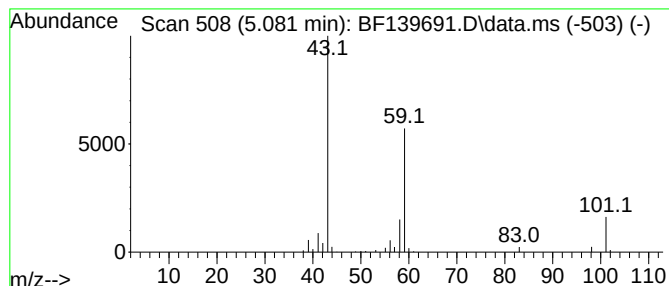
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	6.06 ng	151806	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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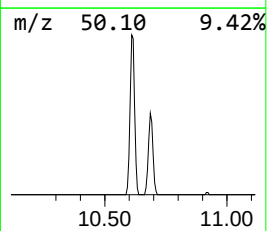
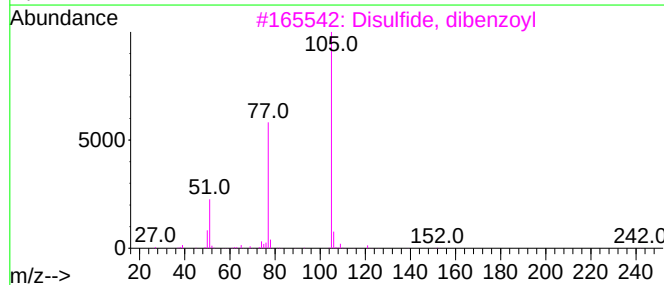
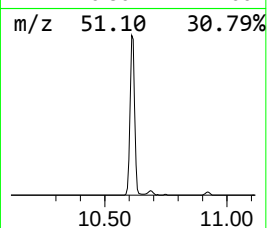
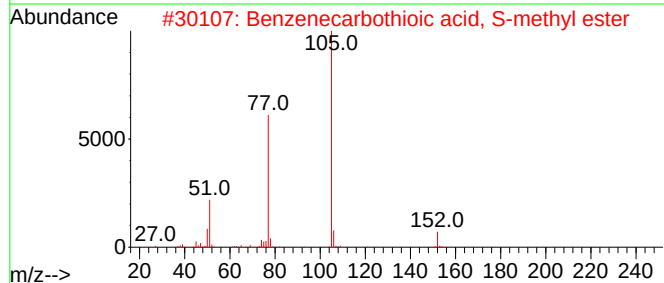
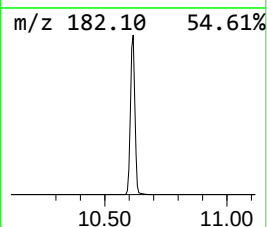
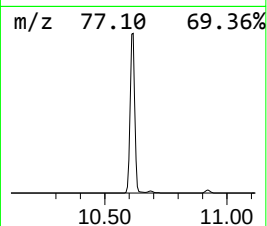
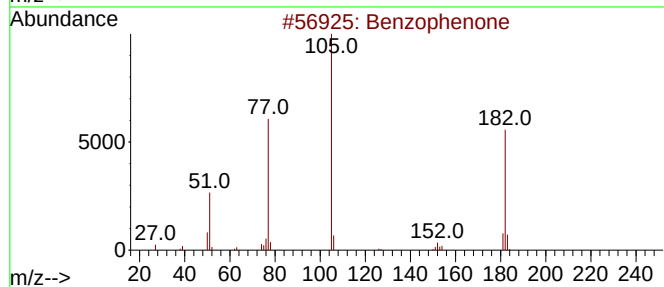
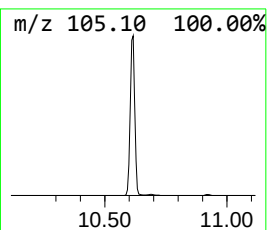
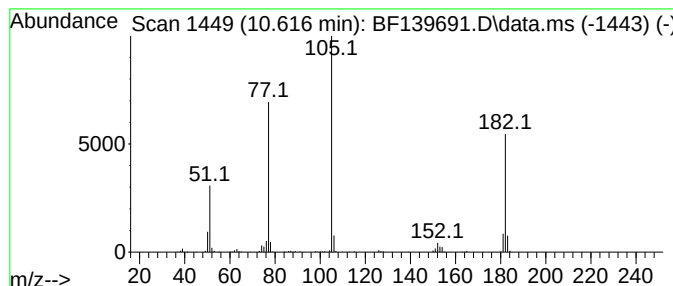
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	12.82 ng	470965	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	52
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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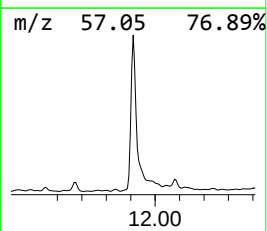
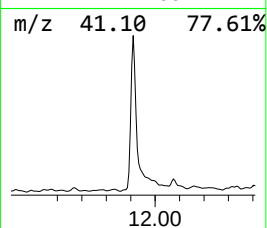
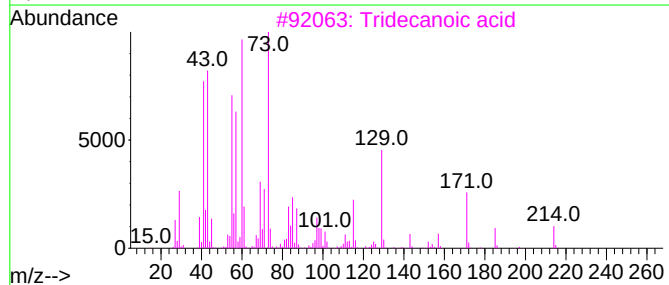
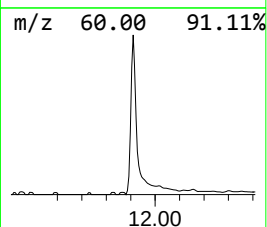
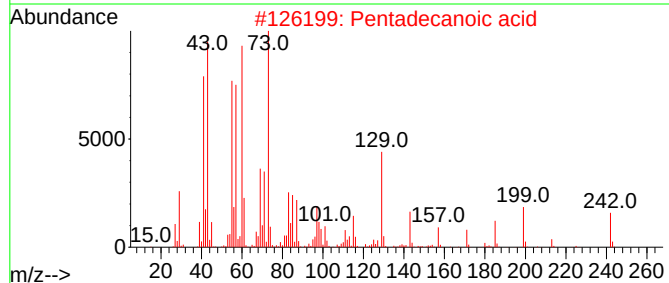
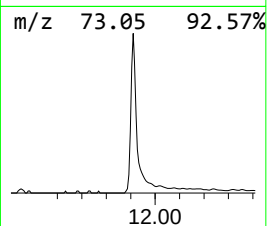
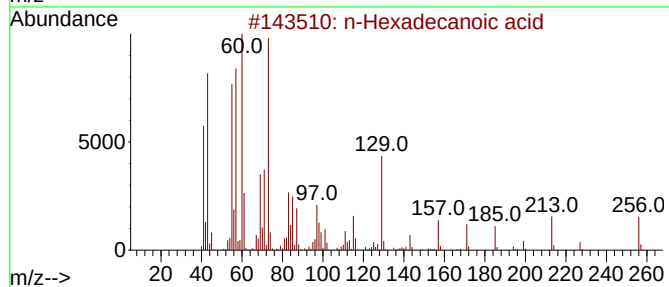
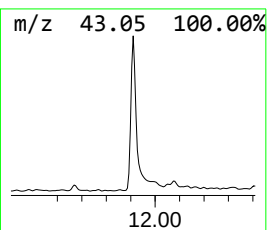
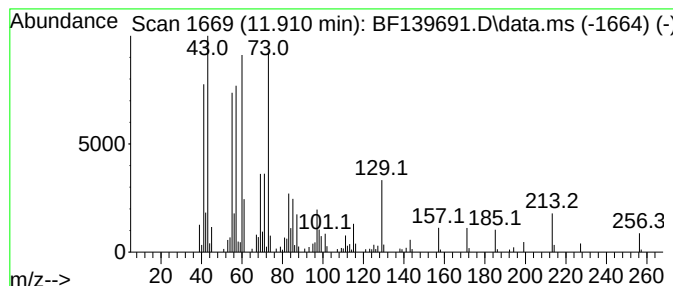
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	6.40 ng	259561	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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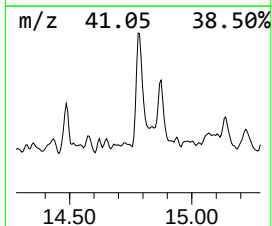
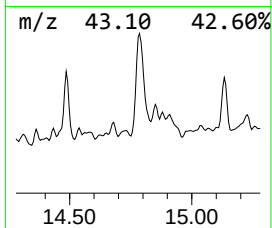
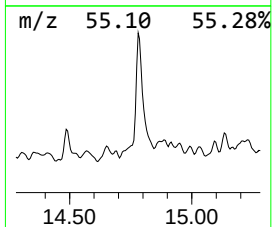
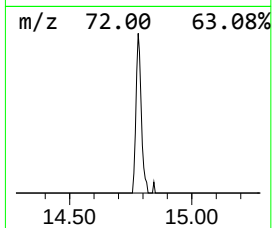
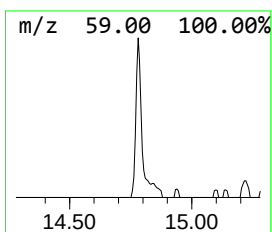
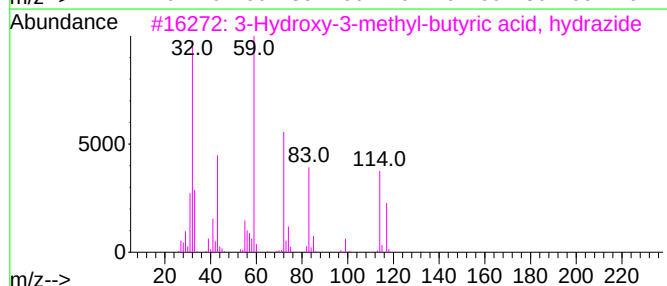
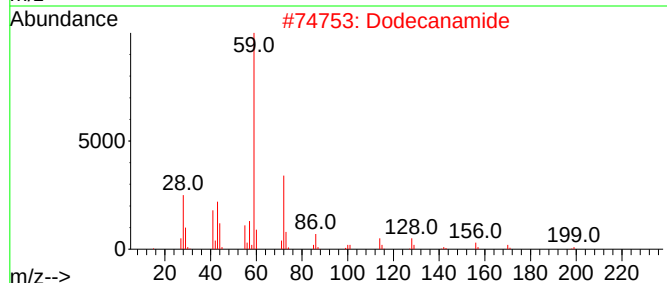
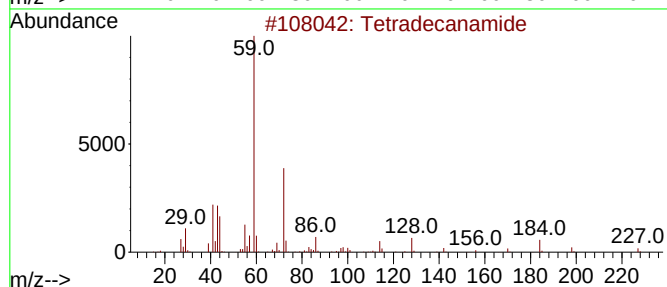
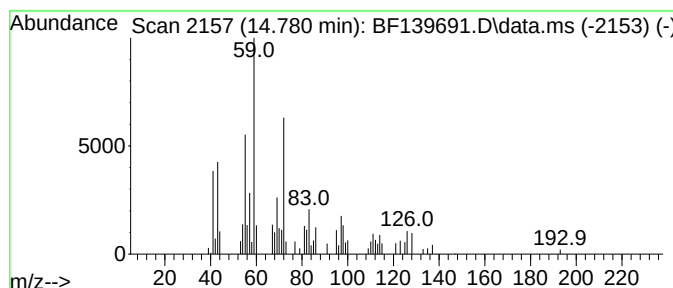
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 5 Tetradecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	2.07 ng	46749	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanamide	227	C14H29NO	000638-58-4	59
2			Dodecanamide	199	C12H25NO	001120-16-7	59
3			3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	50
4			3-Butenoic acid, 2-methyl-, meth...	114	C6H10O2	051747-33-2	38
5			Silane, hexyl-	116	C6H16Si	001072-14-6	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	115.7	ng	2896800	1	6.863	500867	20.0
2-Pentanone, 4-...	5.081	6.1	ng	151806	1	6.863	500867	20.0
Benzophenone	10.616	12.8	ng	470965	3	9.898	734926	20.0
n-Hexadecanoic ...	11.910	6.4	ng	259561	4	11.386	810534	20.0
Tetradecanamide	14.780	2.1	ng	46749	6	15.498	452539	20.0