

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140122.D
 Acq On : 29 Oct 2024 19:55
 Operator : RC/JU
 Sample : P4567-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	16	26	rVB	1062269	1699165	60.82%	8.027%
2	3.999	318	324	329	rBV	20594	33454	1.20%	0.158%
3	5.116	506	514	521	rVB2	17780	33240	1.19%	0.157%
4	5.504	574	580	586	rBV	1766182	2405305	86.10%	11.362%
5	6.463	737	743	745	rBV	19208	32977	1.18%	0.156%
6	6.510	745	751	763	rVB	1693479	2456696	87.93%	11.605%
7	6.887	810	815	821	rVB	661843	813890	29.13%	3.845%
8	7.445	900	910	915	rBV	1274208	1685924	60.35%	7.964%
9	7.698	948	953	962	rVB	68210	86721	3.10%	0.410%
10	8.169	1019	1033	1046	rBV	849266	1095321	39.21%	5.174%
11	9.245	1210	1216	1226	rBV	2109506	2793775	100.00%	13.197%
12	9.316	1226	1228	1237	rVB3	16865	29339	1.05%	0.139%
13	9.922	1326	1331	1346	rVB	871144	1123023	40.20%	5.305%
14	10.633	1447	1452	1459	rBV	304740	393354	14.08%	1.858%
15	10.710	1459	1465	1476	rBV	1105444	1445007	51.72%	6.826%
16	11.410	1579	1584	1592	rBV	718551	966588	34.60%	4.566%
17	11.933	1669	1673	1685	rBV2	317777	502366	17.98%	2.373%
18	12.622	1787	1790	1796	rBV	57320	85817	3.07%	0.405%
19	12.721	1803	1807	1819	rBV	103666	201695	7.22%	0.953%
20	12.998	1849	1854	1861	rBV	1396704	1798738	64.38%	8.497%
21	13.474	1933	1935	1941	rVB	61824	76458	2.74%	0.361%
22	14.057	2029	2034	2045	rVB	523836	742200	26.57%	3.506%
23	15.557	2284	2289	2301	rVB	397345	668205	23.92%	3.156%

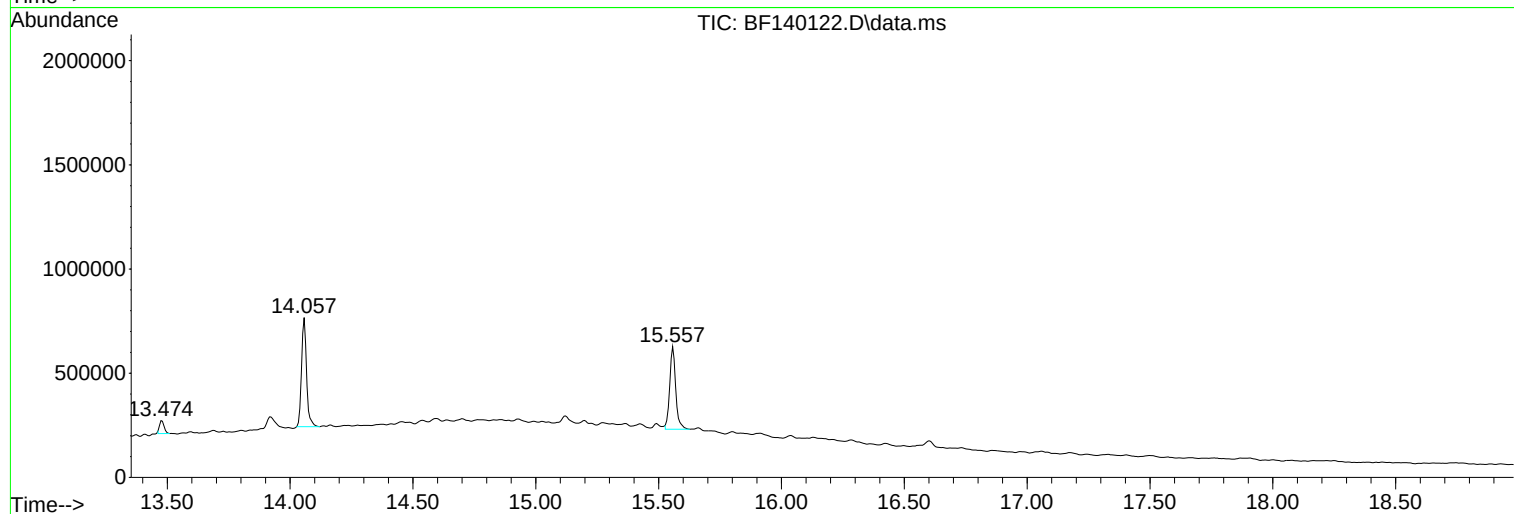
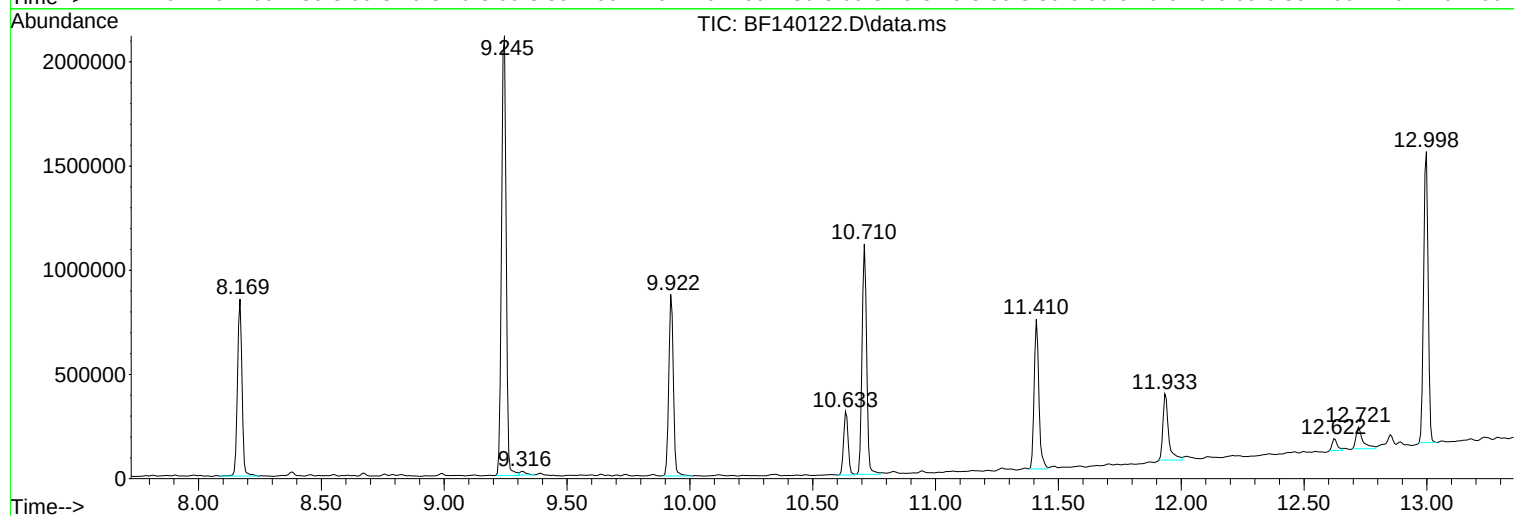
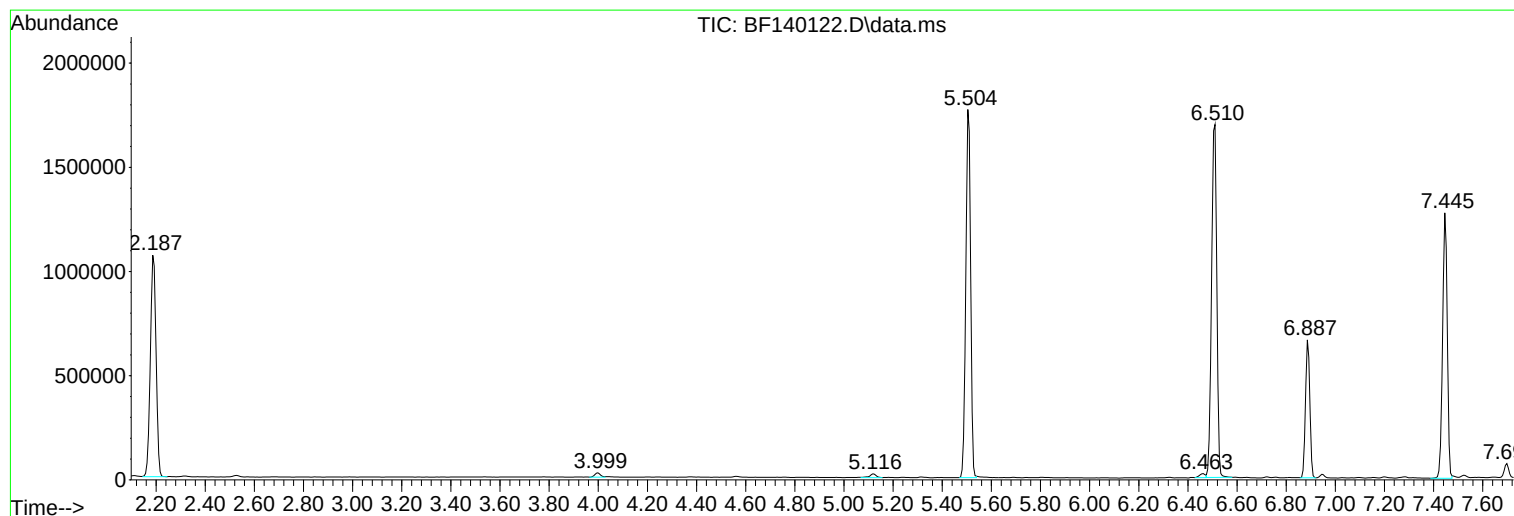
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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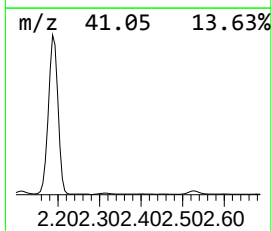
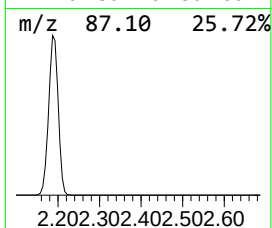
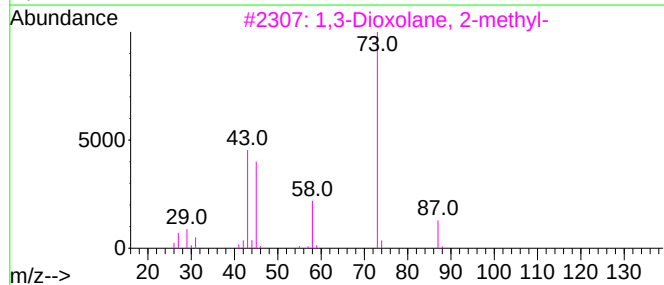
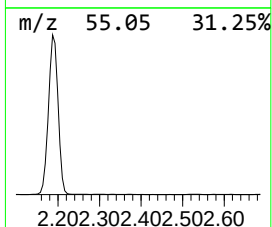
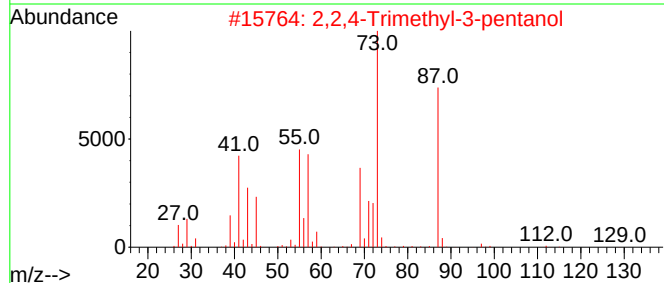
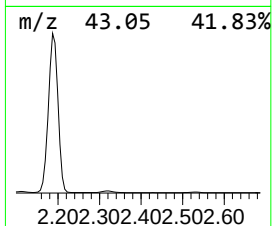
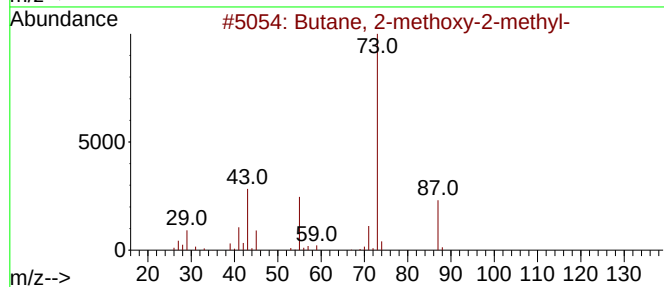
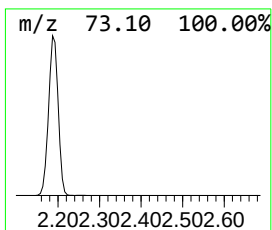
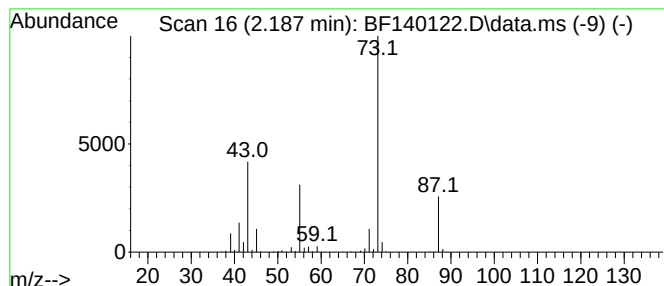
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.187	41.75 ng	1699170	1,4-Dichlorobenzene-d4	6.887

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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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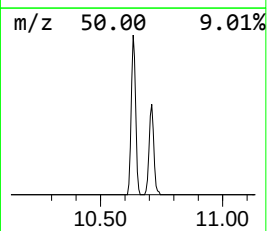
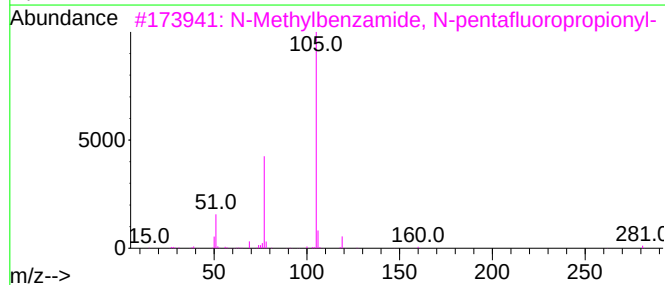
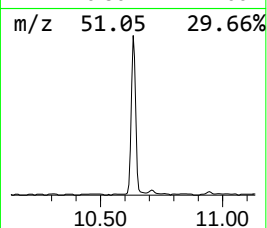
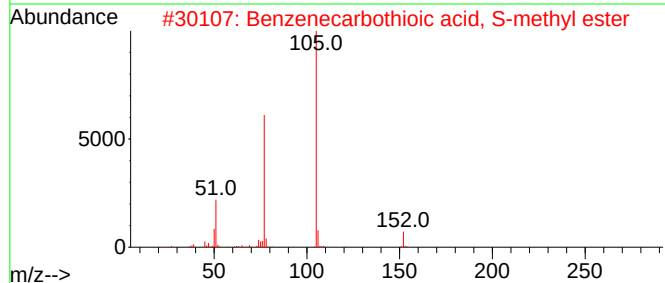
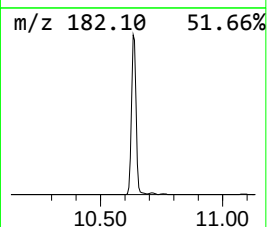
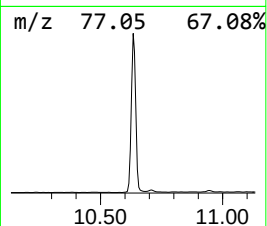
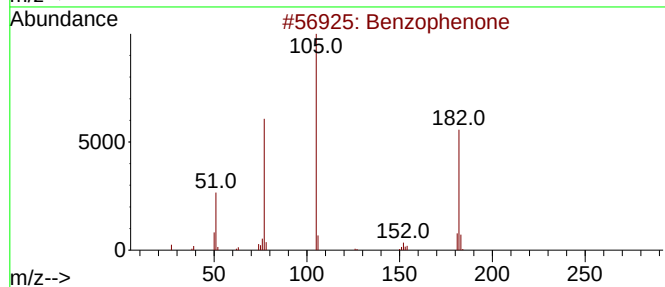
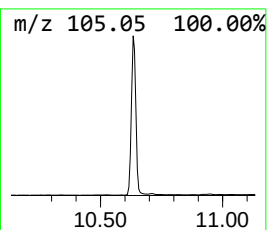
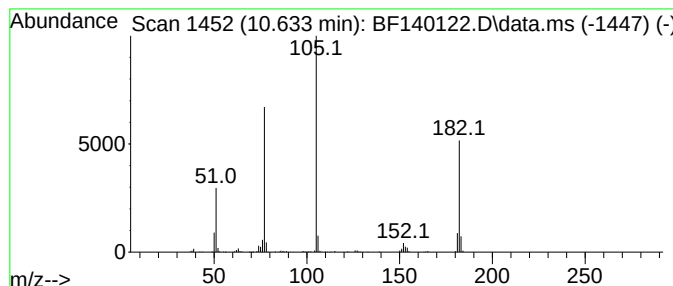
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	7.01 ng	393354	Acenaphthene-d10	9.922

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			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	50



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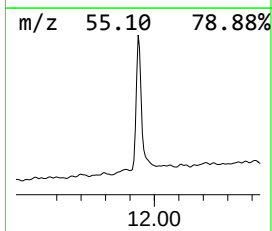
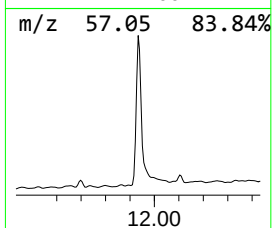
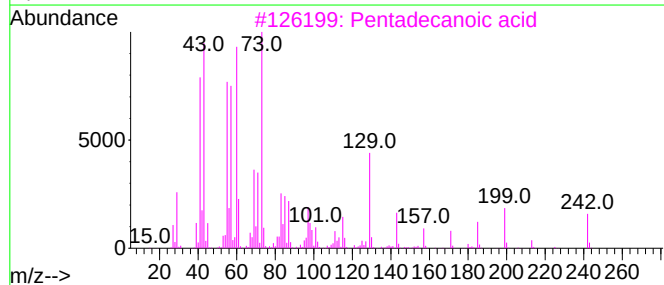
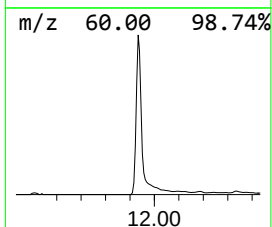
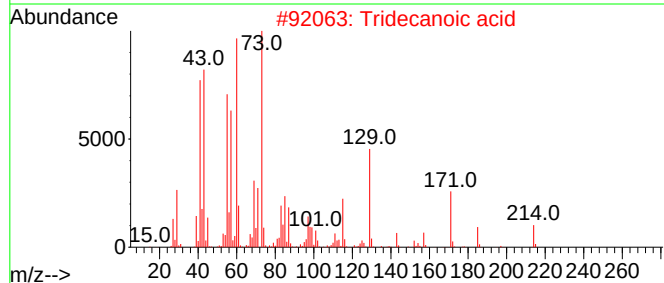
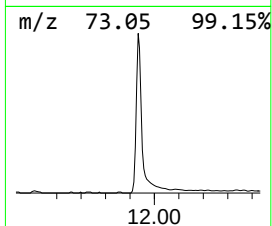
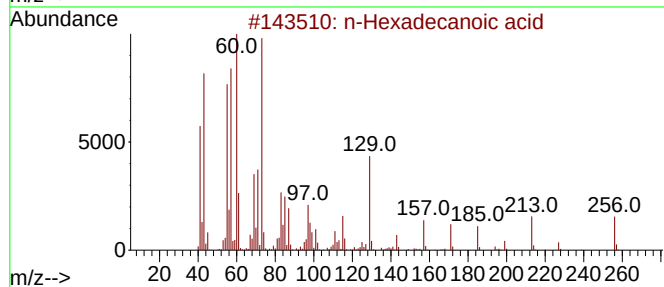
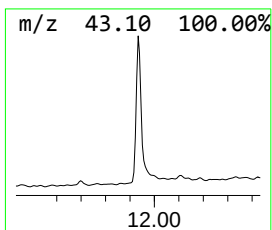
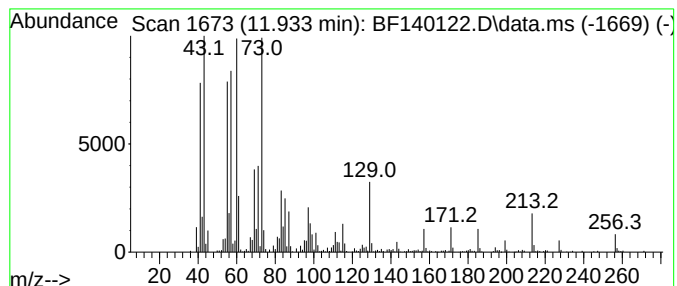
Instrument :
BNA_F
ClientSampleId :
WC-2

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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 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	10.39 ng	502366	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	78



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Instrument :
BNA_F
ClientSampleId :
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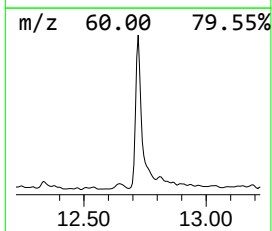
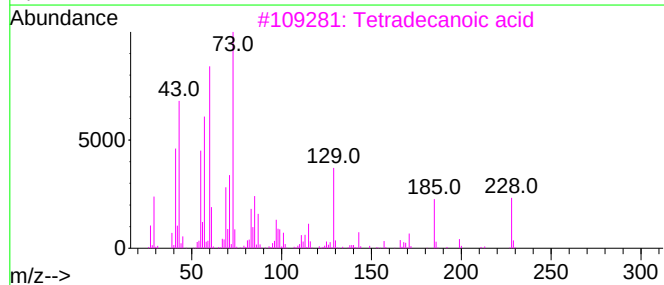
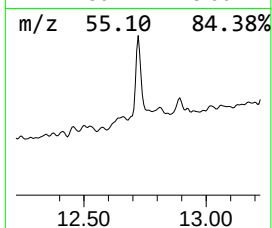
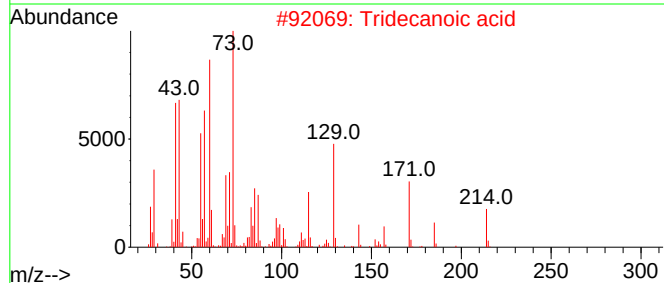
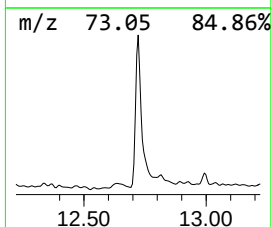
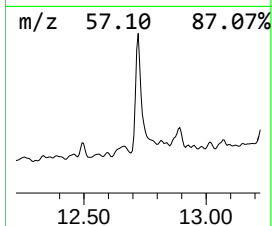
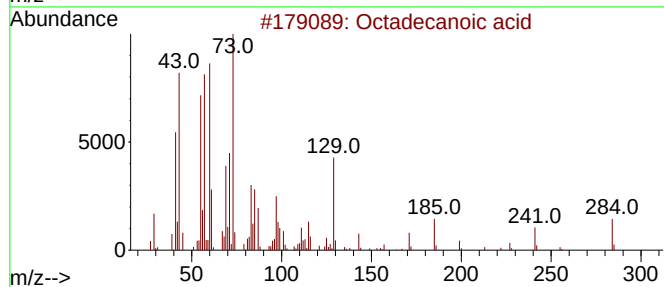
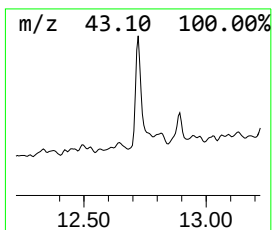
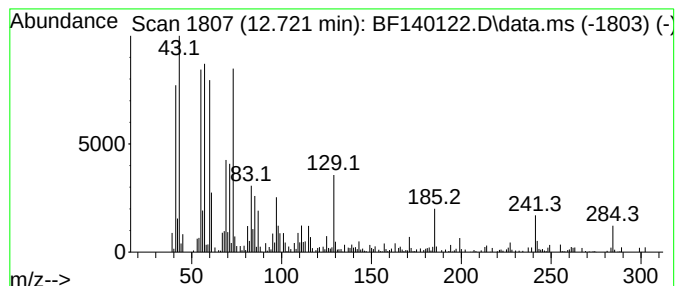
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	4.17 ng	201695	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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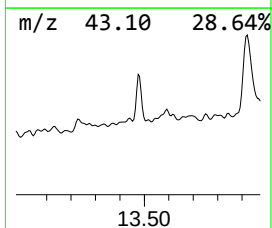
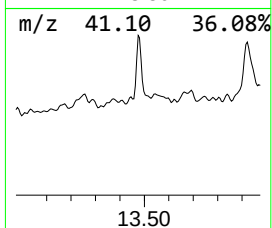
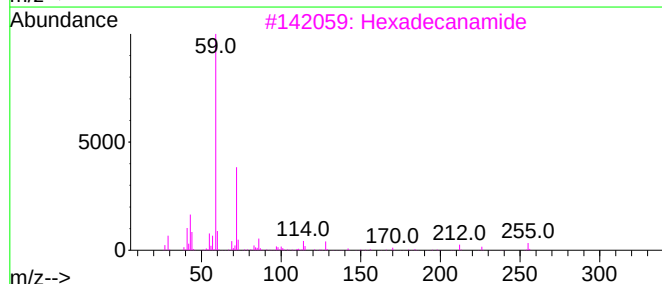
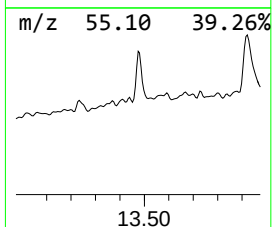
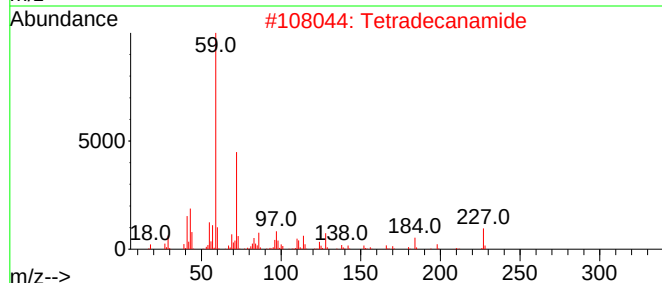
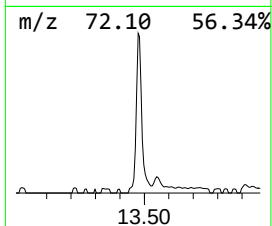
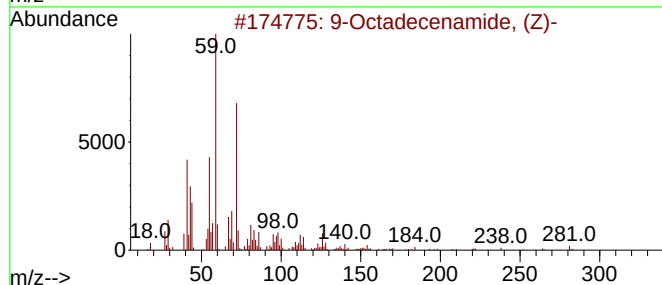
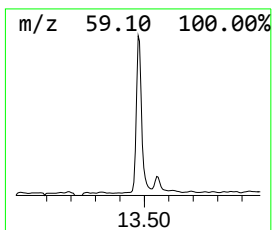
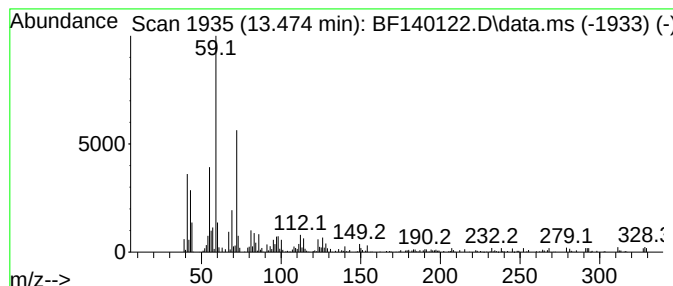
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	2.06 ng	76458	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2			Tetradecanamide	227	C14H29NO	000638-58-4	78
3			Hexadecanamide	255	C16H33NO	000629-54-9	59
4			Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
5			Dodecanamide	199	C12H25NO	001120-16-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	41.8	ng	1699170	1	6.887	813890	20.0
Benzophenone	10.633	7.0	ng	393354	3	9.922	1123020	20.0
n-Hexadecanoic ...	11.933	10.4	ng	502366	4	11.410	966588	20.0
Octadecanoic acid	12.722	4.2	ng	201695	4	11.410	966588	20.0
9-Octadecenamid...	13.474	2.1	ng	76458	5	14.057	742200	20.0