

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
 Data File : BF132597.D
 Acq On : 01 Mar 2023 18:19
 Operator : CG\JU
 Sample : 01739-15
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-3-COMP-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_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	446	450	458	rVB	1377279	1560779	46.93%	6.002%
2	5.628	513	517	521	rBV	3616036	3313476	99.64%	12.741%
3	6.628	682	687	690	rBV	3331296	3184494	95.76%	12.245%
4	7.004	747	751	754	rBV	1227913	1012847	30.46%	3.895%
5	7.563	842	846	849	rBV	2387477	2073217	62.34%	7.972%
6	8.286	966	969	973	rBV	1554480	1194188	35.91%	4.592%
7	9.363	1148	1152	1155	rBV	4156026	3325513	100.00%	12.787%
8	10.051	1265	1269	1272	rBV	1337050	1162663	34.96%	4.471%
9	10.763	1386	1390	1395	rBV	225259	188772	5.68%	0.726%
10	10.839	1399	1403	1407	rBV	2000135	1717573	51.65%	6.604%
11	11.545	1519	1523	1526	rBV	1182721	1034345	31.10%	3.977%
12	12.057	1606	1610	1619	rBV2	278353	334949	10.07%	1.288%
13	12.763	1726	1730	1734	rBV	59981	69506	2.09%	0.267%
14	12.845	1740	1744	1749	rBV	113953	142088	4.27%	0.546%
15	12.992	1764	1769	1772	rBV2	62274	69788	2.10%	0.268%
16	13.133	1789	1793	1796	rBV	3361757	2921221	87.84%	11.233%
17	13.692	1883	1888	1891	rBV2	46442	52921	1.59%	0.203%
18	14.045	1941	1948	1962	rBV5	81514	283762	8.53%	1.091%
19	14.198	1970	1974	1978	rBV	1250735	1192246	35.85%	4.584%
20	14.339	1995	1998	2007	rBV2	37669	42319	1.27%	0.163%
21	15.062	2118	2121	2124	rVB	57756	56723	1.71%	0.218%
22	15.751	2233	2238	2247	rBV	765229	1072943	32.26%	4.126%

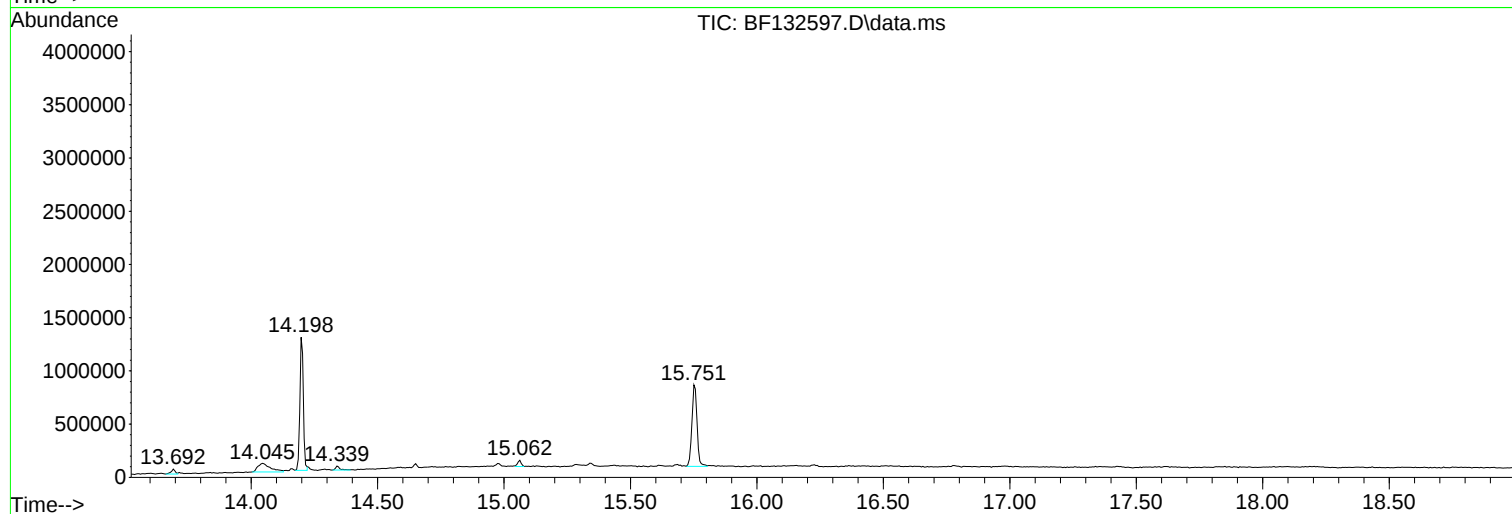
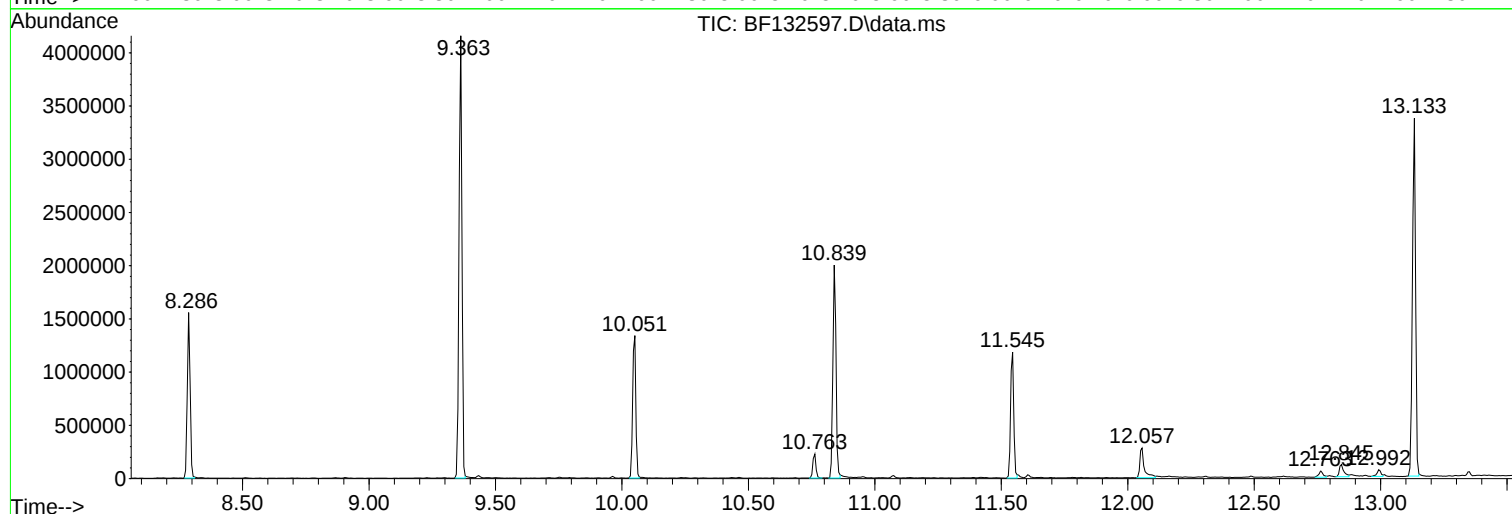
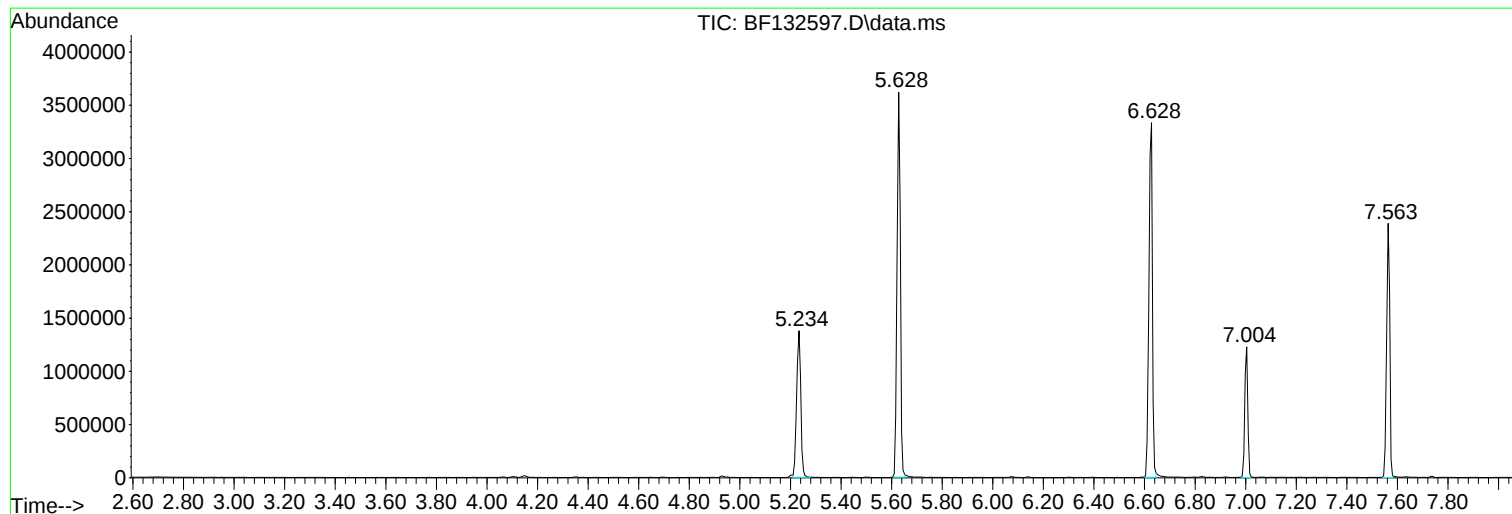
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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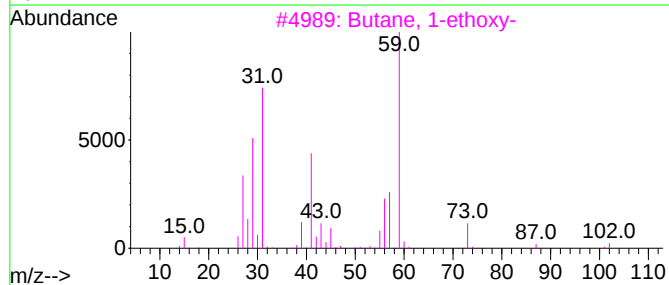
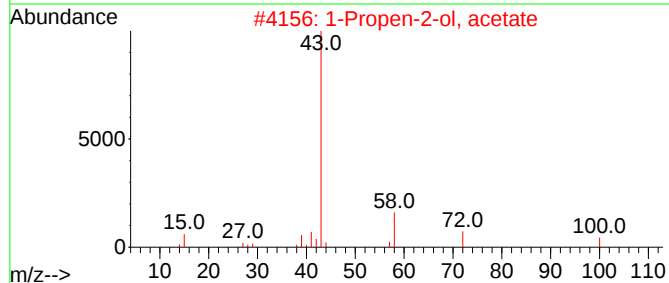
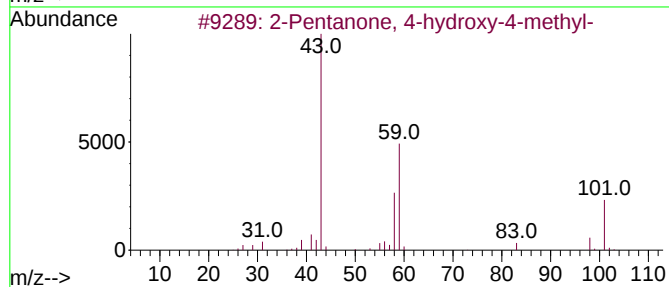
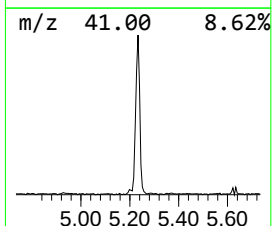
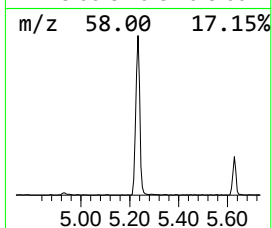
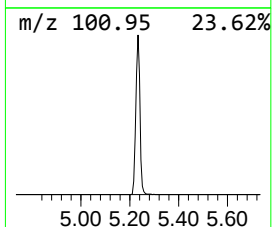
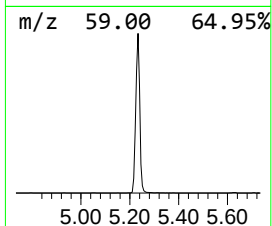
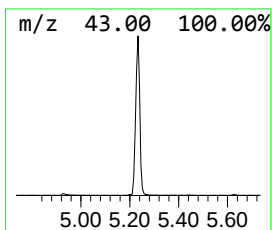
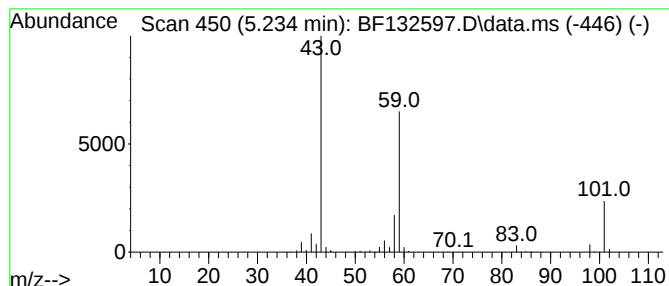
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.234	30.82 ng	1560780	1,4-Dichlorobenzene-d4	7.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Acetone	58	C3H6O	000067-64-1	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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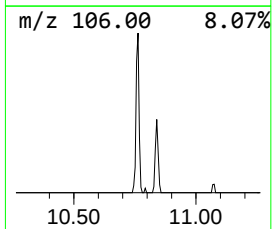
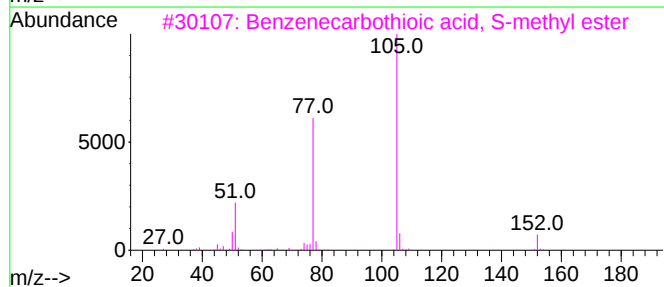
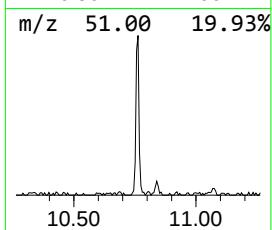
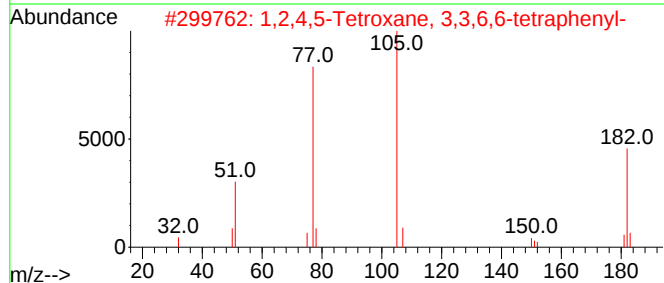
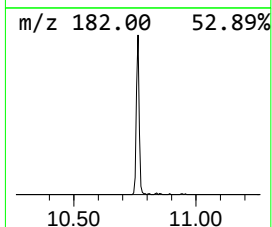
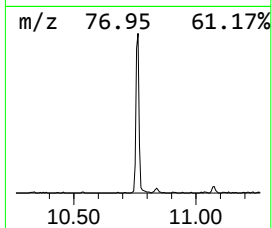
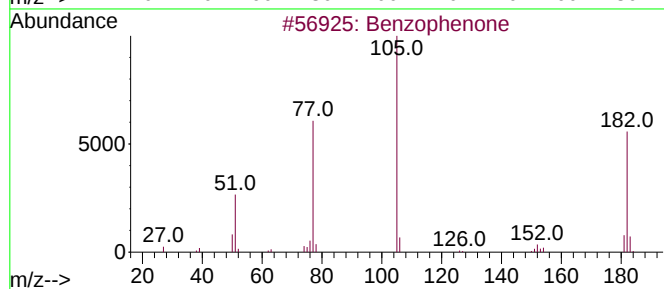
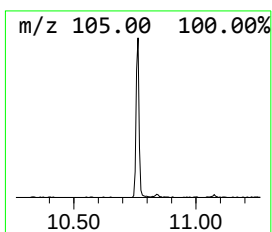
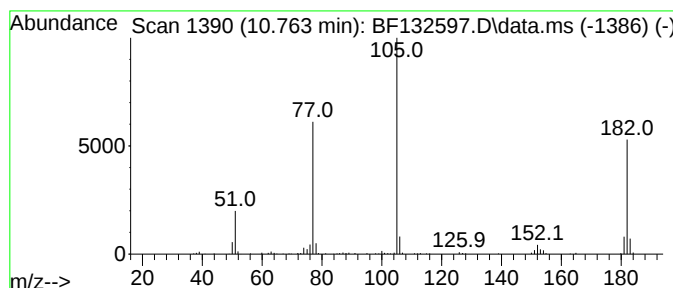
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	3.25 ng	188772	Acenaphthene-d10	10.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47



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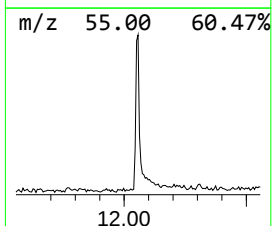
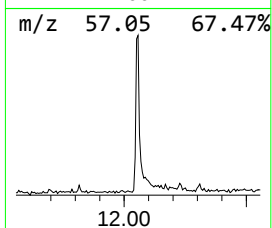
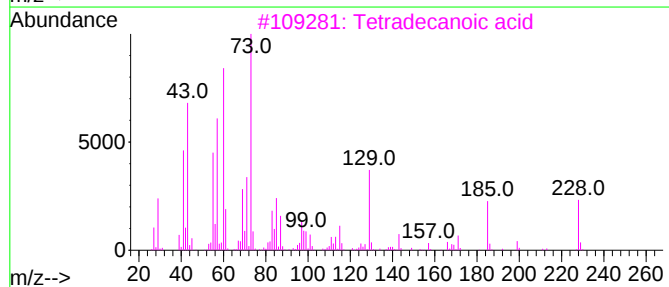
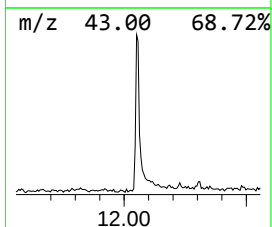
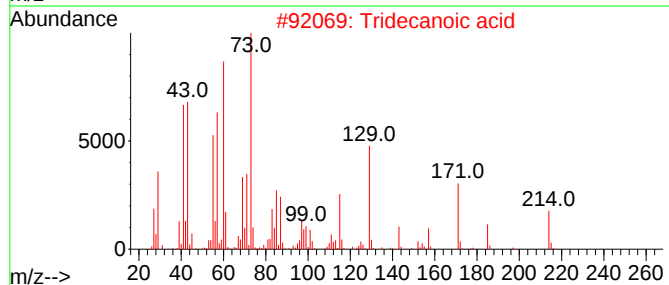
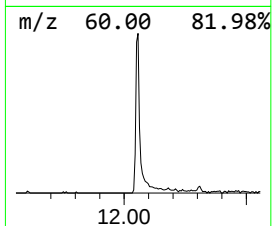
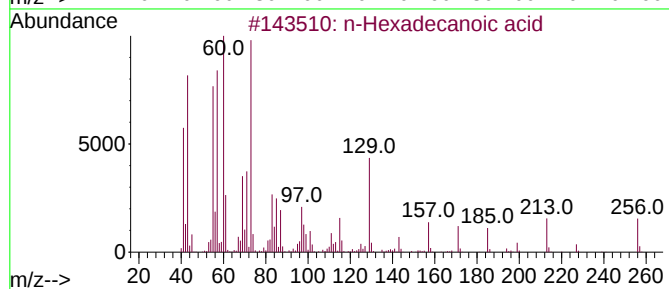
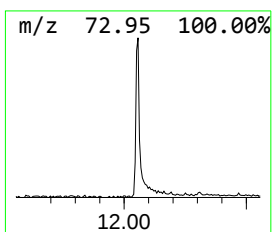
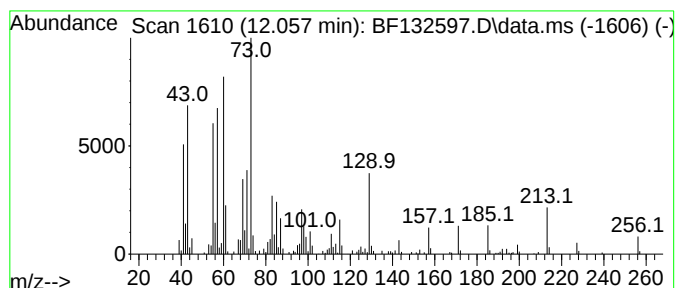
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.057	6.48 ng	334949	Phenanthrene-d10	11.545	
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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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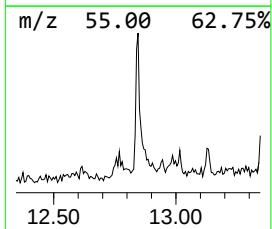
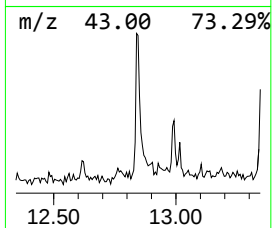
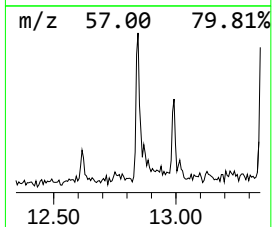
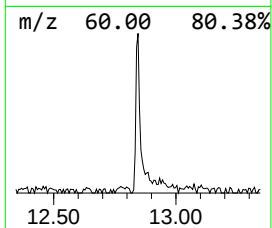
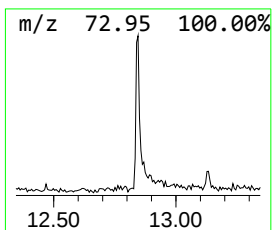
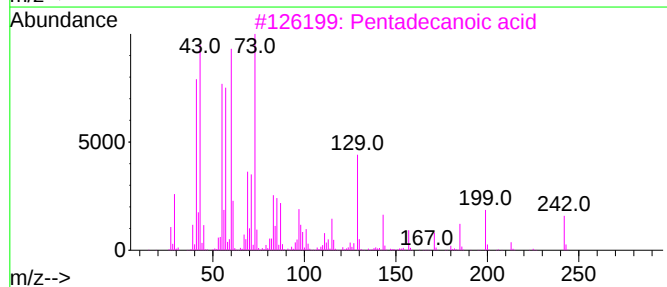
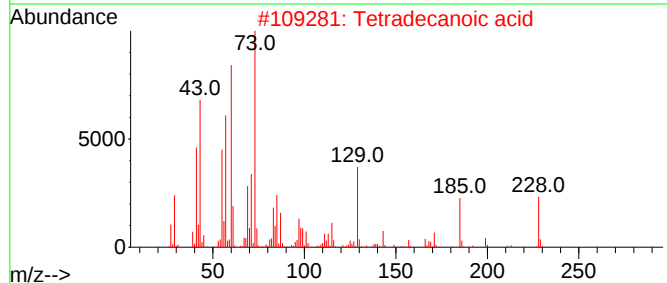
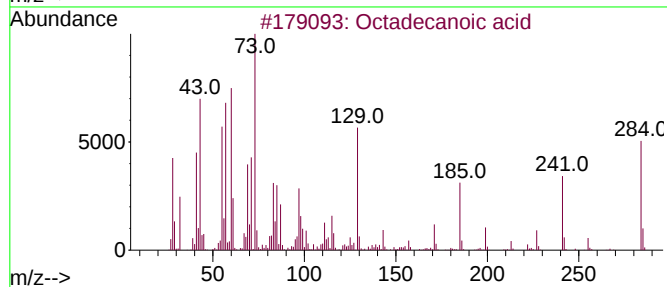
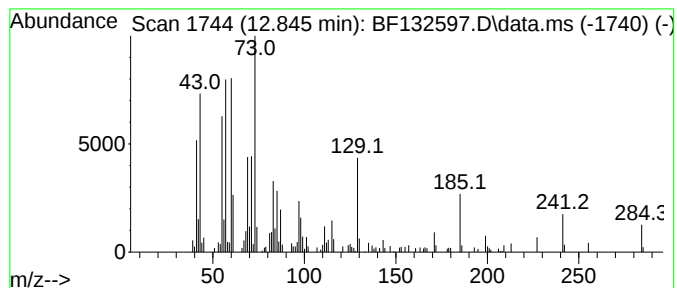
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.845	2.75 ng	142088	Phenanthrene-d10	11.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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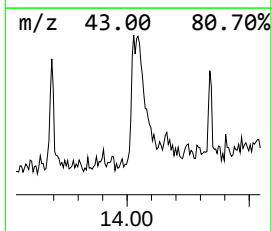
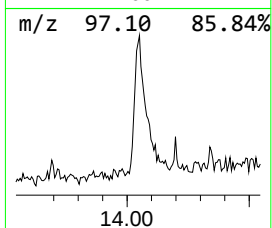
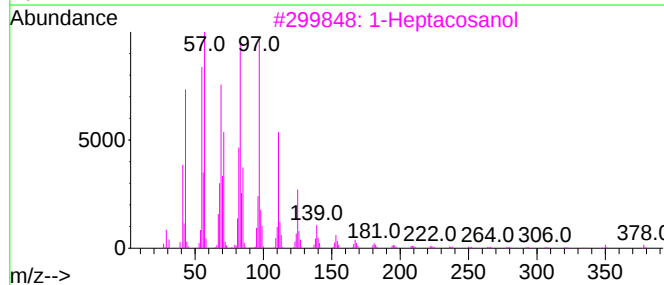
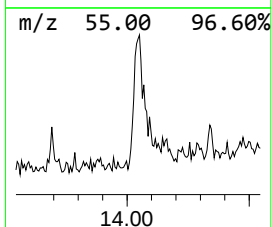
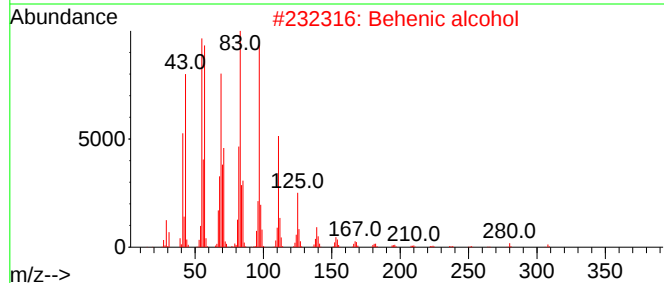
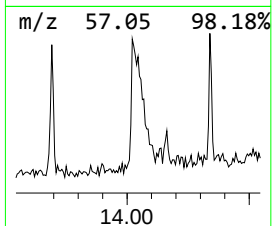
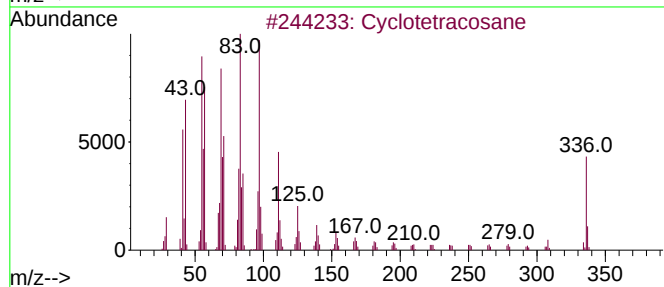
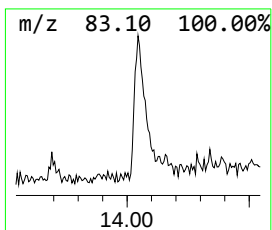
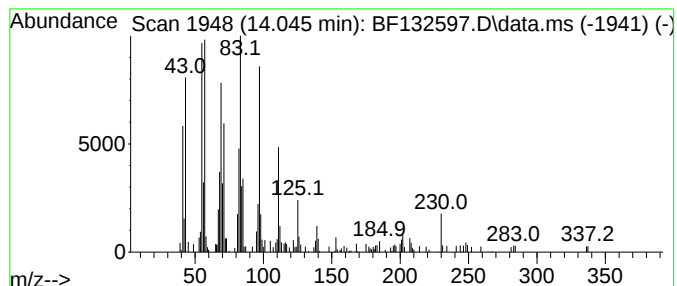
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	4.76 ng	283762	Chrysene-d12	14.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	98
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.234	30.8	ng	1560780	1	7.004	1012850	20.0
Benzophenone	10.763	3.3	ng	188772	3	10.051	1162660	20.0
n-Hexadecanoic ...	12.057	6.5	ng	334949	4	11.545	1034350	20.0
Octadecanoic acid	12.845	2.8	ng	142088	4	11.545	1034350	20.0
Cyclotetracosane	14.045	4.8	ng	283762	5	14.198	1192250	20.0