

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
 Data File : BF132349.D
 Acq On : 07 Feb 2023 17:38
 Operator : CG\JU
 Sample : 01466-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.290	405	417	426	rBV	995168	1356442	27.65%	4.091%
2	5.678	477	483	486	rBV	3224960	3315852	67.60%	10.001%
3	6.666	646	651	654	rBV	2957206	3310710	67.49%	9.986%
4	7.048	713	716	720	rVB	1100027	870970	17.76%	2.627%
5	7.613	807	812	815	rBV	2504983	2227166	45.40%	6.718%
6	8.336	931	935	938	rBV	1535029	1182899	24.11%	3.568%
7	9.413	1114	1118	1121	rBV	5269774	4515830	92.06%	13.621%
8	10.101	1231	1235	1238	rBV	1682676	1397474	28.49%	4.215%
9	10.813	1350	1356	1360	rVB	220969	167076	3.41%	0.504%
10	10.895	1365	1370	1373	rBV	3711680	3284886	66.97%	9.908%
11	11.595	1485	1489	1492	rBV	1812273	1510044	30.78%	4.555%
12	12.107	1571	1576	1591	rBV	708042	693215	14.13%	2.091%
13	12.818	1691	1697	1703	rBV	112115	118528	2.42%	0.358%
14	12.895	1705	1710	1720	rBV	158577	170543	3.48%	0.514%
15	13.048	1730	1736	1742	rVB	135986	156148	3.18%	0.471%
16	13.189	1756	1760	1764	rBV	4793249	4905304	100.00%	14.795%
17	14.077	1907	1911	1929	rBV	376458	635929	12.96%	1.918%
18	14.254	1937	1941	1944	rBV	1245830	1102207	22.47%	3.324%
19	14.342	1951	1956	1963	rBV	826533	891812	18.18%	2.690%
20	14.601	1990	2000	2011	rBV10	47866	170975	3.49%	0.516%
21	15.130	2086	2090	2095	rVB	76755	80829	1.65%	0.244%
22	15.830	2203	2209	2221	rBV2	746542	1004896	20.49%	3.031%
23	16.418	2302	2309	2322	rBV2	18851	84610	1.72%	0.255%

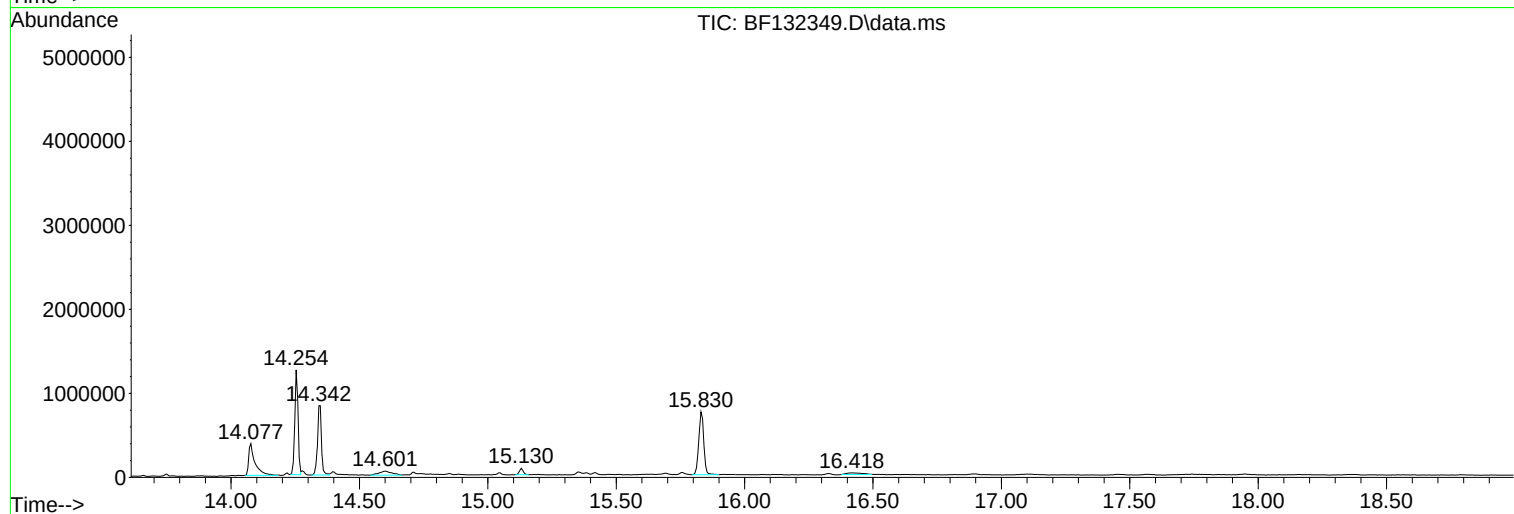
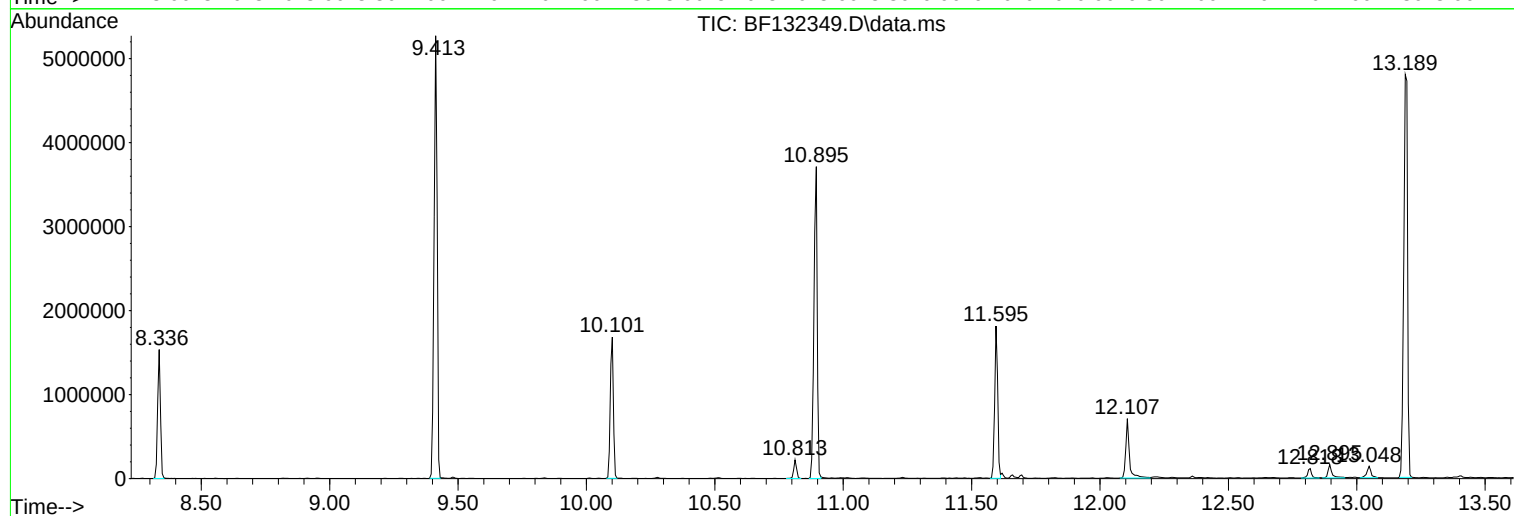
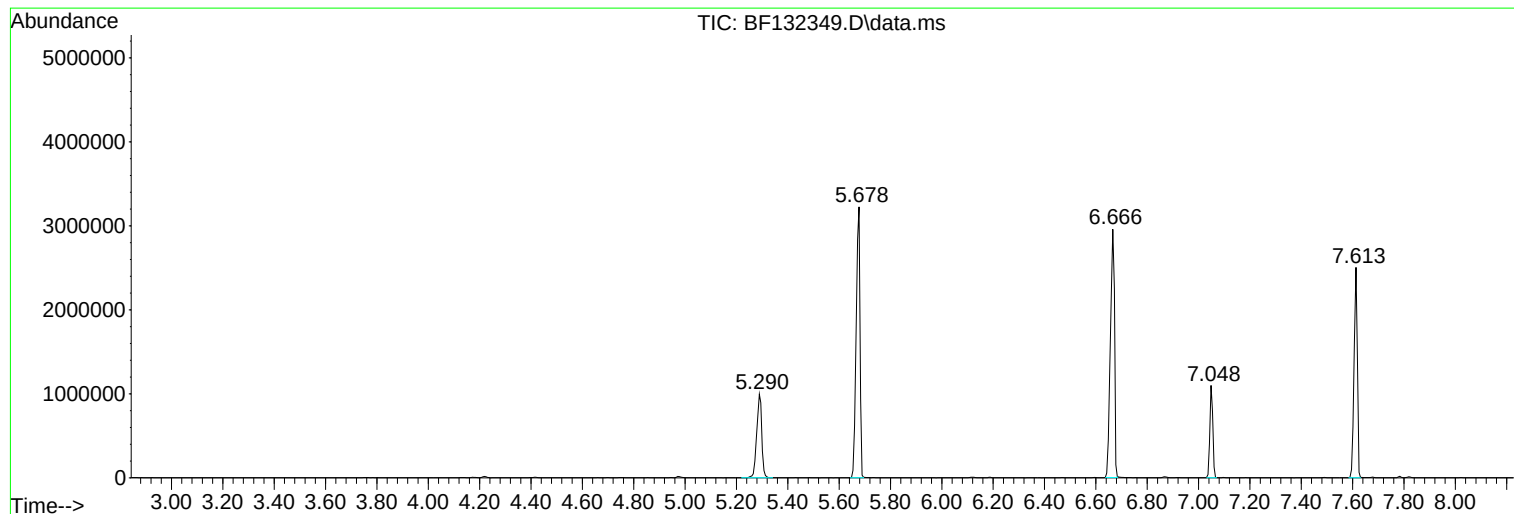
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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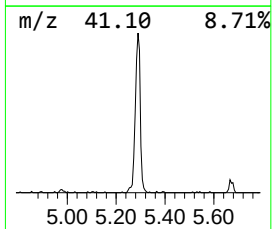
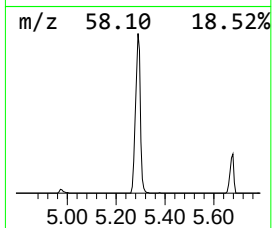
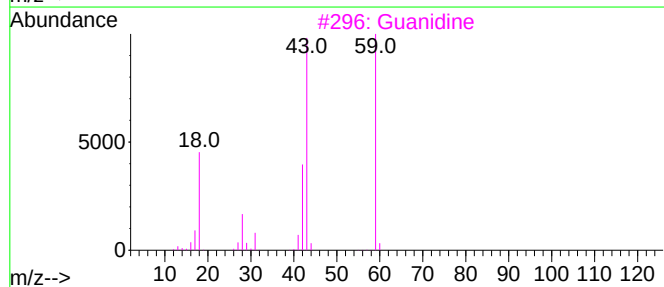
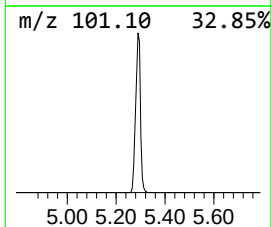
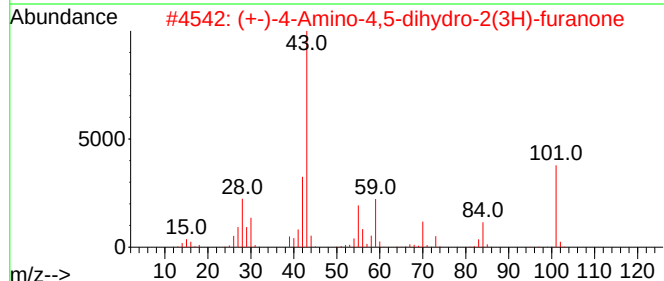
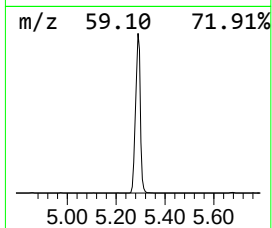
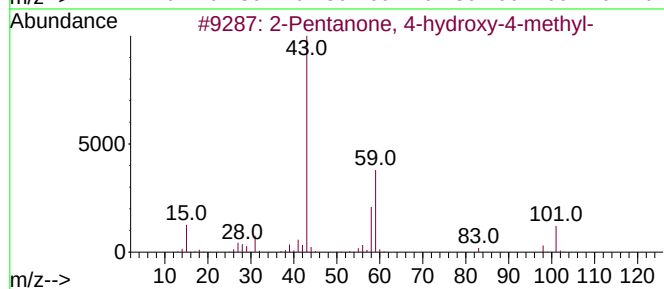
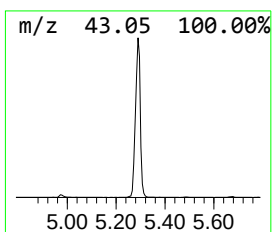
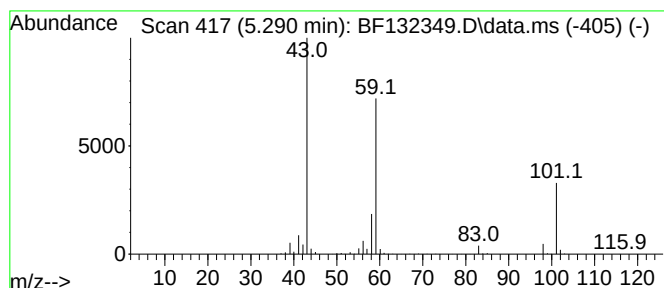
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.290	31.15 ng	1356440	1,4-Dichlorobenzene-d4	7.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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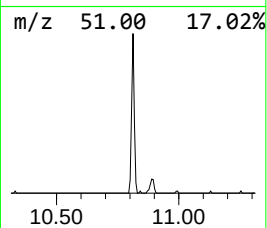
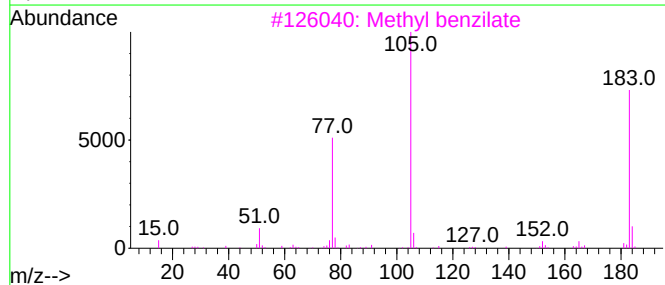
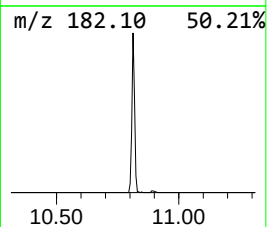
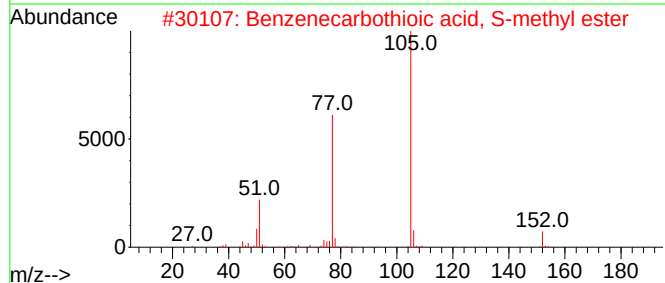
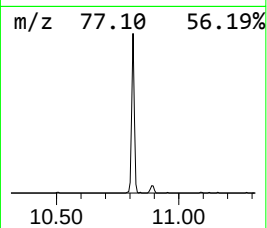
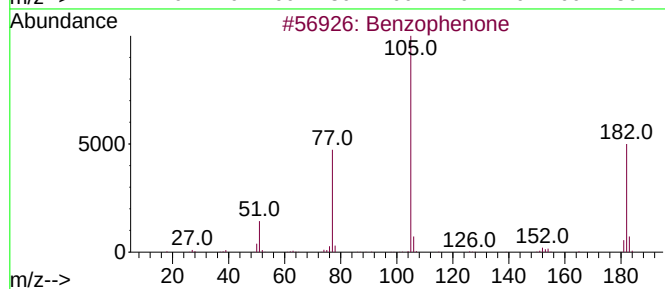
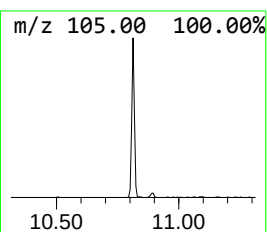
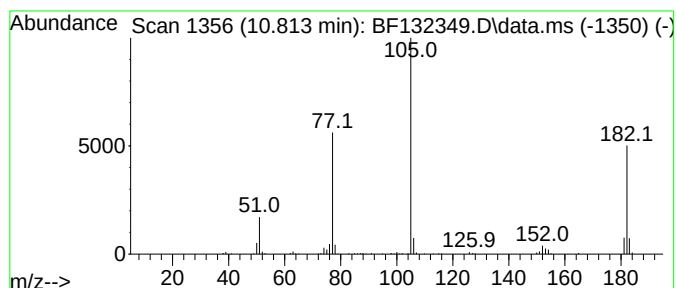
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Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.813	2.39 ng	167076	Acenaphthene-d10	10.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Methyl benzilate	242	C15H14O3	000076-89-1	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43



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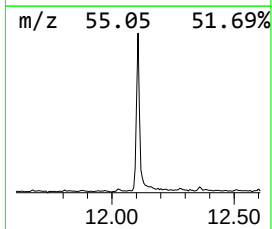
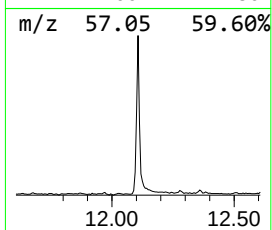
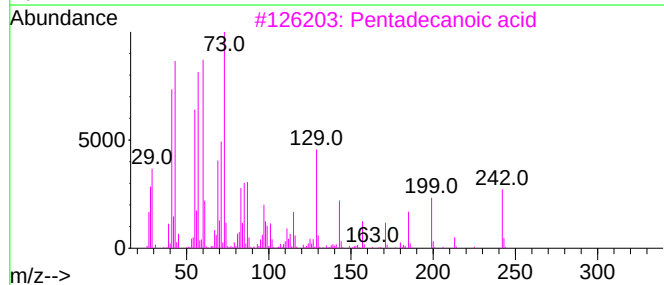
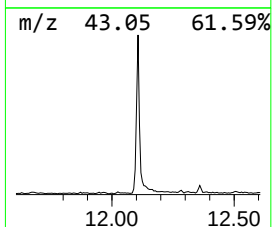
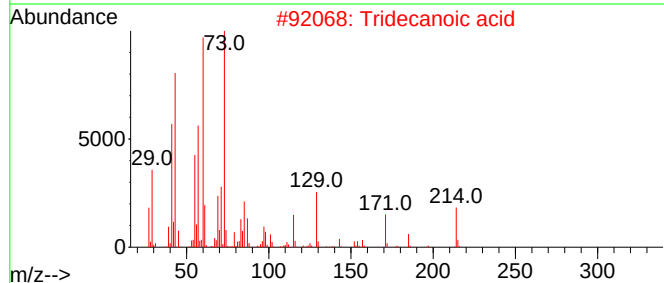
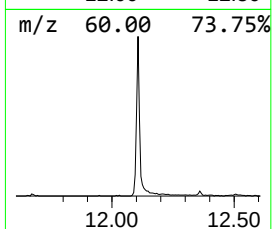
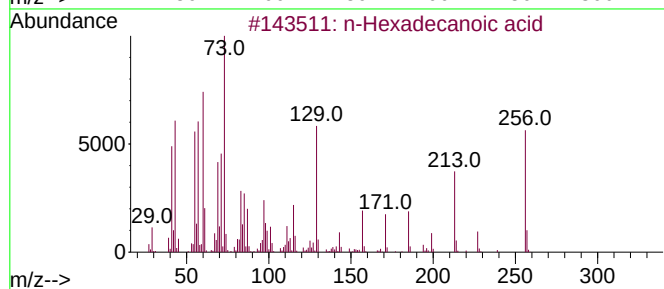
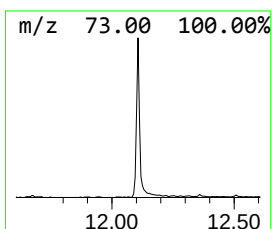
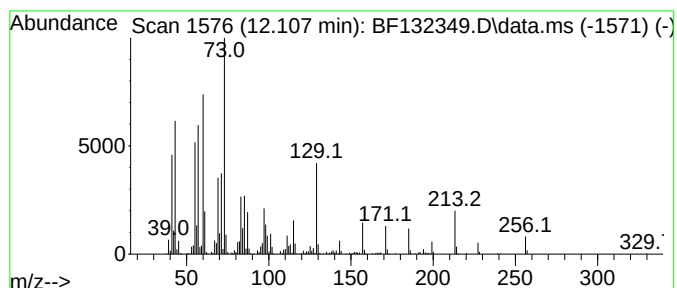
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.107	9.18 ng	693215	Phenanthrene-d10	11.595	
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	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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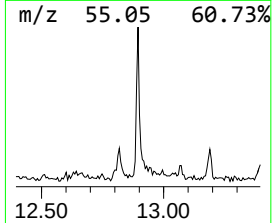
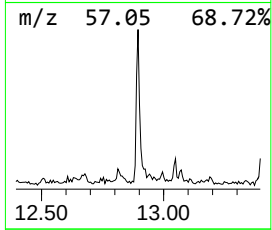
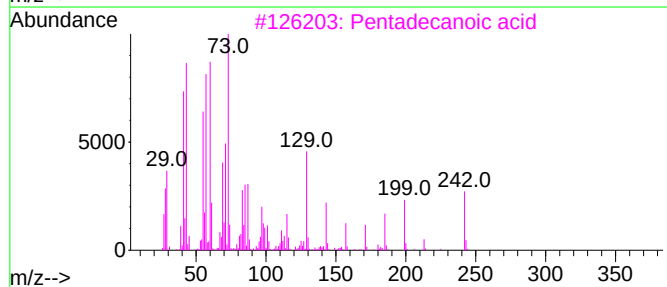
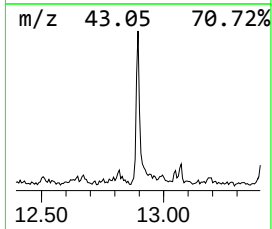
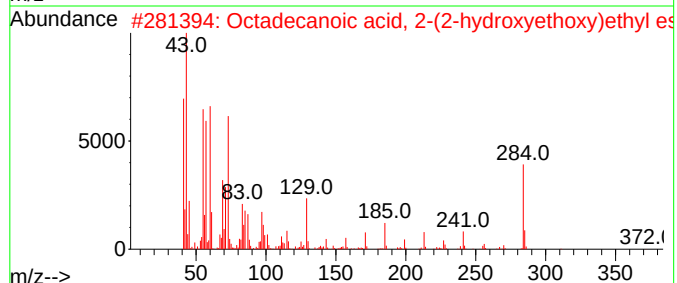
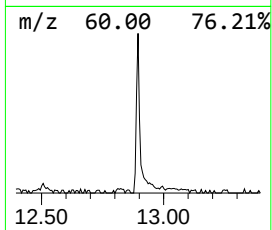
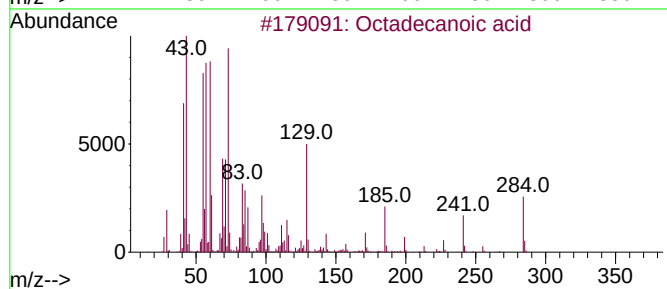
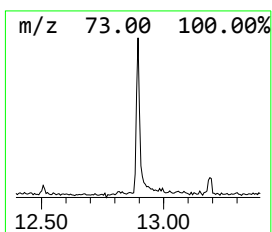
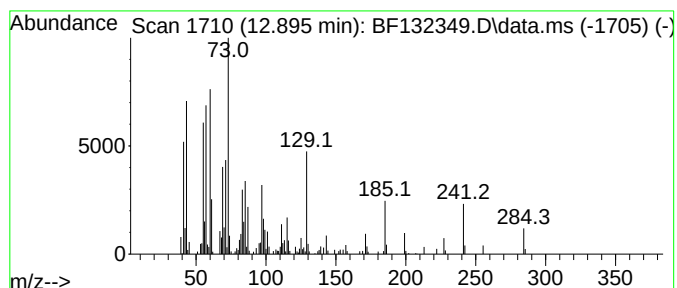
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Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.895	2.26 ng	170543	Phenanthrene-d10	11.595	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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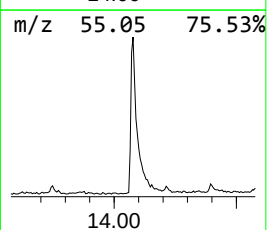
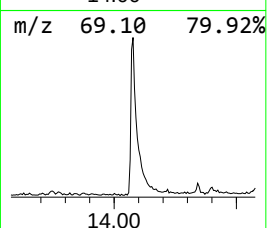
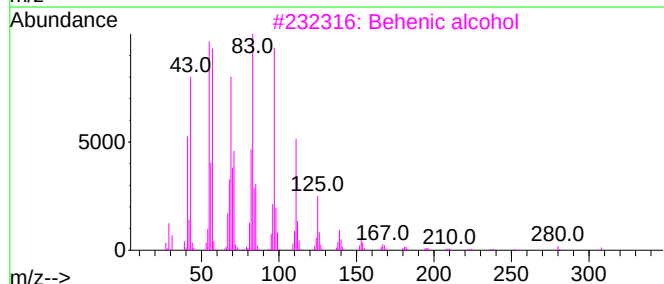
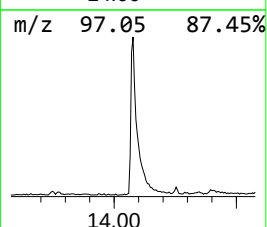
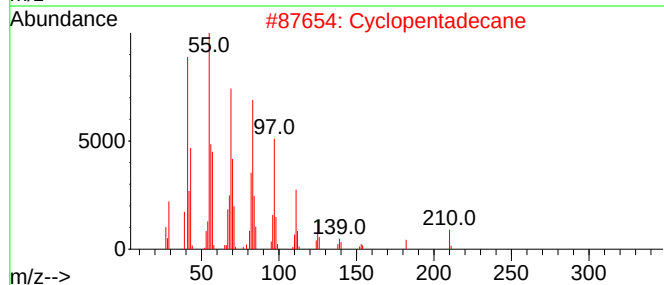
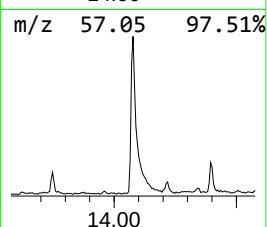
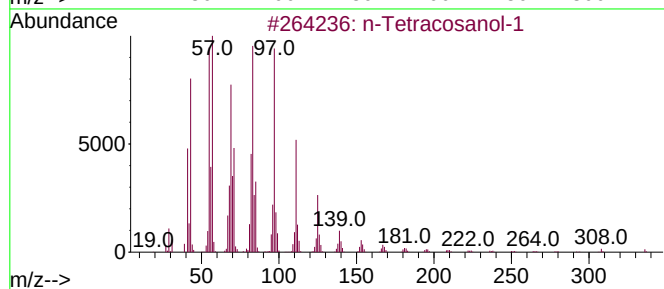
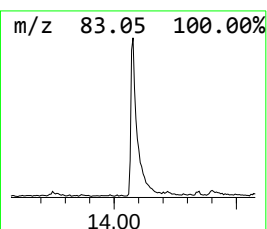
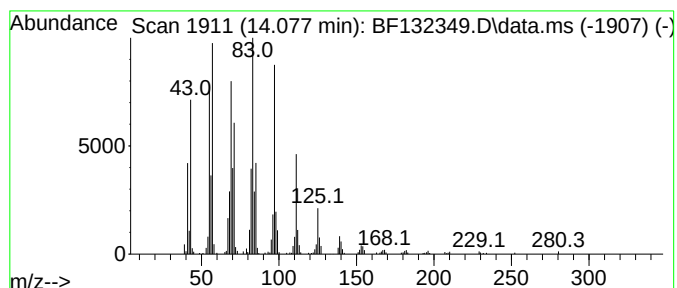
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.077	11.54 ng	635929	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2			Cyclopentadecane	210	C15H30	000295-48-7	94
3			Behenic alcohol	326	C22H46O	000661-19-8	93
4			1-Hexacosene	364	C26H52	018835-33-1	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



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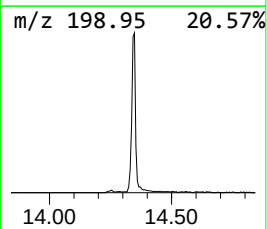
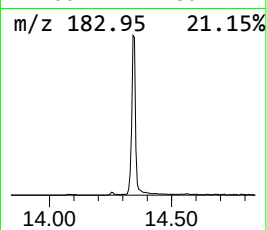
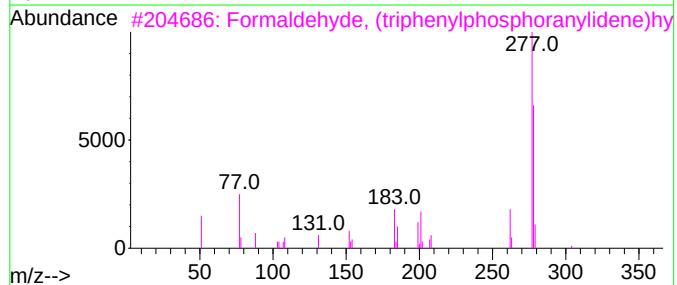
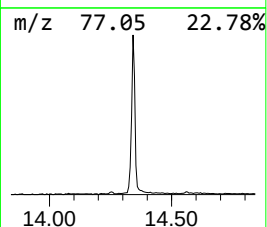
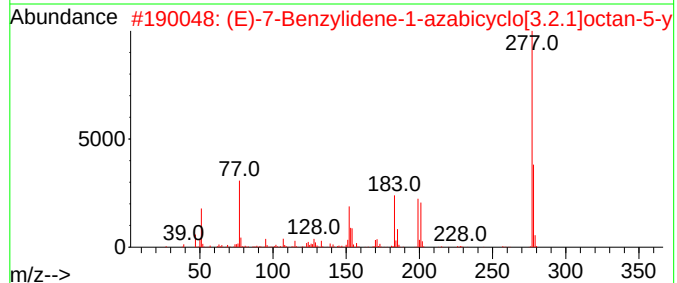
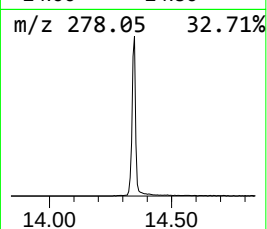
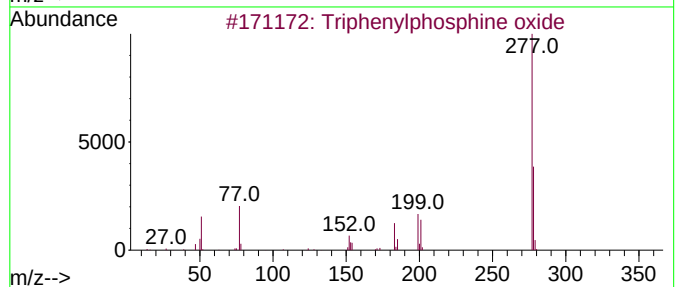
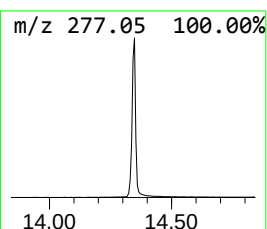
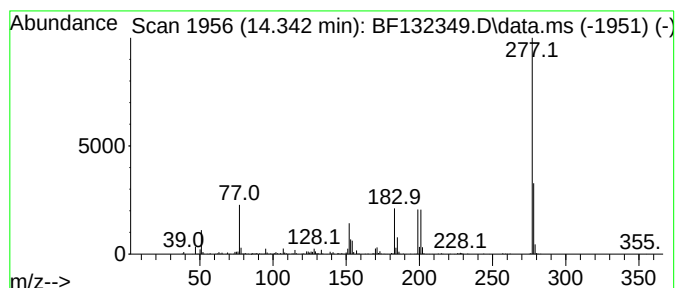
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.342	16.18 ng	891812	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	37
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132349.D
Acq On : 07 Feb 2023 17:38
Operator : CG\JU
Sample : 01466-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-3

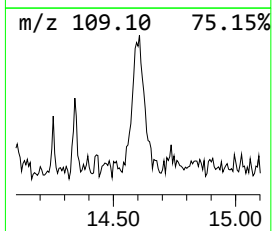
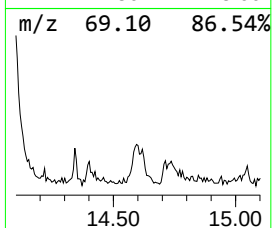
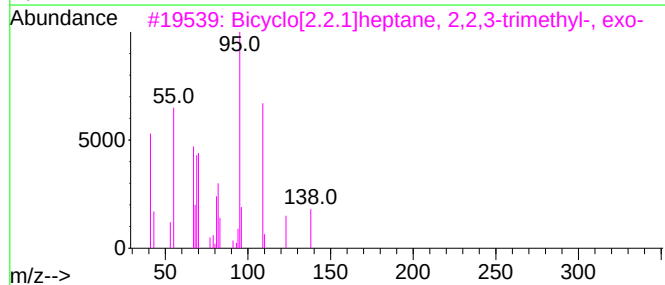
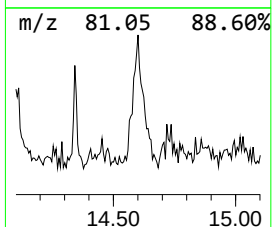
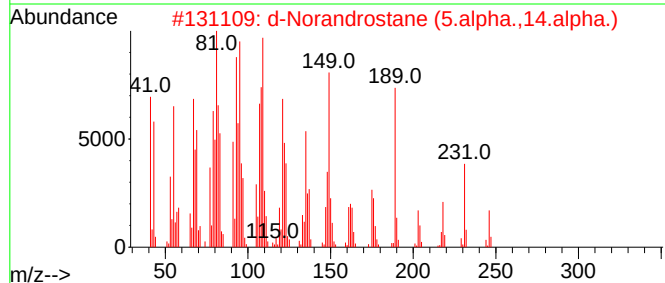
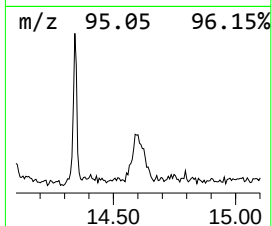
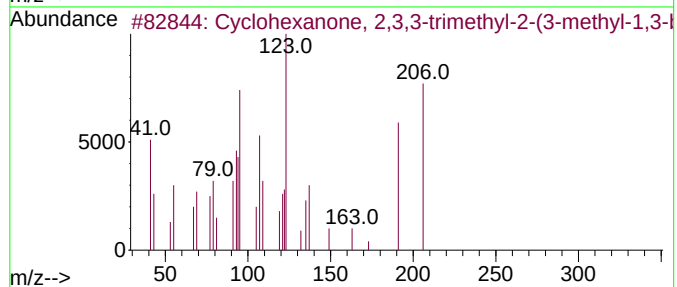
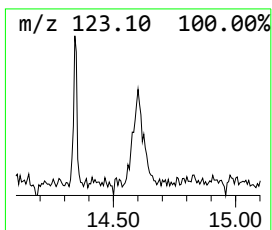
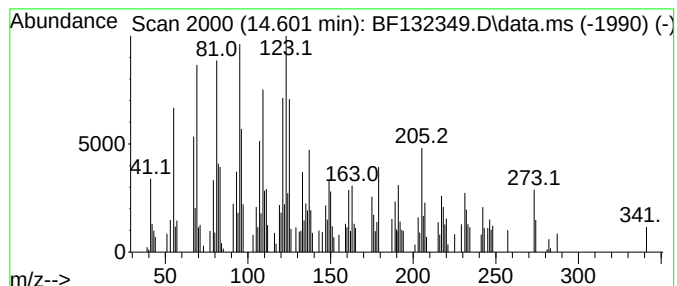
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.601 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.601	3.10 ng	170975	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	45
2			d-Norandrostane (5.alpha.,14.alp...	246	C18H30	1000281-13-8	41
3			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	38
4			4-Fluoro-benzoic acid (2-ethyl-c...	248	C14H17FN2O	1000296-19-8	38
5			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132349.D
Acq On : 07 Feb 2023 17:38
Operator : CG\JU
Sample : 01466-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.290	31.1	ng	1356440	1	7.048	870970	20.0
Benzophenone	10.813	2.4	ng	167076	3	10.101	1397470	20.0
n-Hexadecanoic ...	12.107	9.2	ng	693215	4	11.595	1510040	20.0
Octadecanoic acid	12.895	2.3	ng	170543	4	11.595	1510040	20.0
n-Tetracosanol-1	14.077	11.5	ng	635929	5	14.254	1102210	20.0
Triphenylphosph...	14.342	16.2	ng	891812	5	14.254	1102210	20.0
unknown14.601	14.601	3.1	ng	170975	5	14.254	1102210	20.0