

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
 Data File : BF132352.D
 Acq On : 07 Feb 2023 19:15
 Operator : CG\JU
 Sample : 01464-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-8

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: BF132352.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	408	417	426	rBV	949741	1161850	29.94%	3.995%
2	5.672	477	482	485	rBV	2872438	2857530	73.63%	9.826%
3	6.666	645	651	654	rBV	2747075	2804289	72.26%	9.643%
4	7.048	713	716	720	rVB	1023658	816142	21.03%	2.806%
5	7.613	807	812	815	rBV	2196083	1879333	48.42%	6.462%
6	8.337	931	935	938	rBV	1432479	1111588	28.64%	3.822%
7	9.413	1114	1118	1121	rBV	4755652	3881089	100.00%	13.345%
8	10.101	1231	1235	1238	rBV	1521435	1290404	33.25%	4.437%
9	10.813	1350	1356	1359	rBV	226362	173945	4.48%	0.598%
10	10.889	1365	1369	1373	rBV	2705037	2574969	66.35%	8.854%
11	11.595	1485	1489	1492	rBV	1603993	1360538	35.06%	4.678%
12	11.619	1492	1493	1497	rVB	205134	116707	3.01%	0.401%
13	11.672	1497	1502	1504	rBV2	45553	72523	1.87%	0.249%
14	12.107	1572	1576	1579	rBV	580451	518202	13.35%	1.782%
15	12.213	1591	1594	1597	rBV2	48972	61208	1.58%	0.210%
16	12.819	1693	1697	1700	rBV	320352	273166	7.04%	0.939%
17	12.895	1706	1710	1716	rBV2	114149	132735	3.42%	0.456%
18	13.048	1729	1736	1742	rBV	329696	360314	9.28%	1.239%
19	13.189	1756	1760	1763	rBV	4163563	3677526	94.76%	12.645%
20	13.619	1828	1833	1837	rBV2	59924	80175	2.07%	0.276%
21	14.077	1908	1911	1924	rVB2	210382	386679	9.96%	1.330%
22	14.254	1937	1941	1944	rBV	985364	973528	25.08%	3.348%
23	14.277	1944	1945	1951	rVB	115503	94919	2.45%	0.326%
24	14.342	1951	1956	1963	rBV	796559	874832	22.54%	3.008%
25	15.130	2087	2090	2095	rVB	105164	102466	2.64%	0.352%
26	15.354	2124	2128	2131	rBV	102142	150663	3.88%	0.518%
27	15.689	2182	2185	2192	rVB	62637	83865	2.16%	0.288%
28	15.760	2193	2197	2203	rVB	87774	121297	3.13%	0.417%
29	15.830	2204	2209	2214	rBV2	704818	953264	24.56%	3.278%
30	17.454	2480	2485	2495	rVB2	35163	80053	2.06%	0.275%
31	17.948	2565	2569	2575	rVB3	29020	56069	1.44%	0.193%

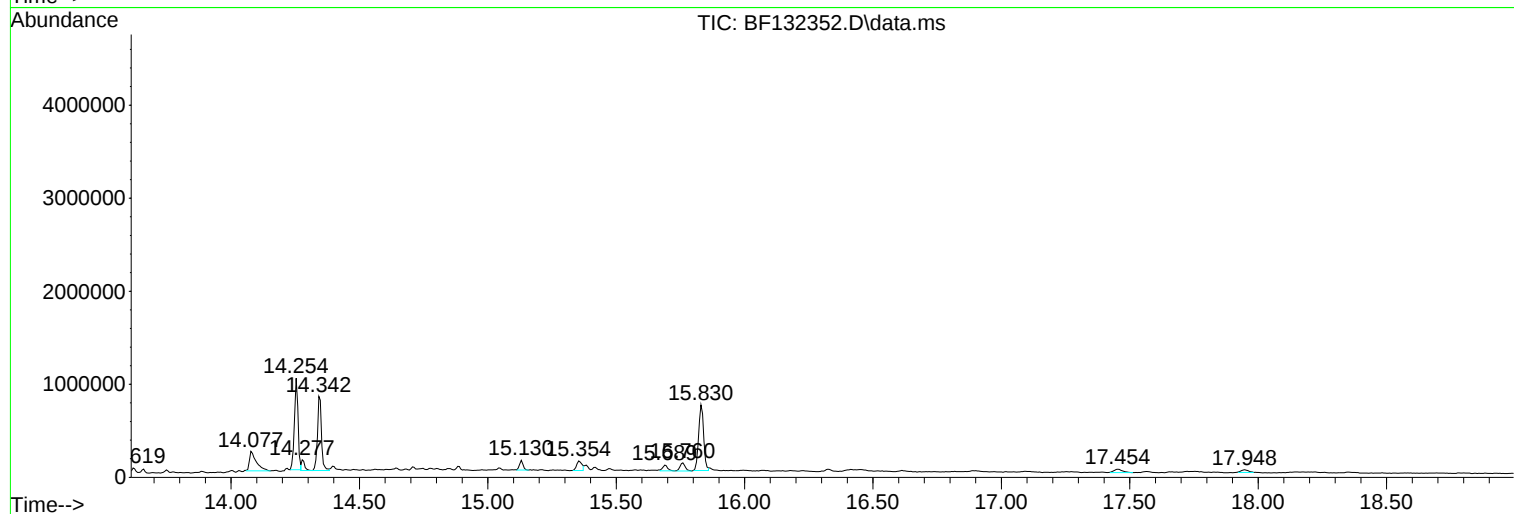
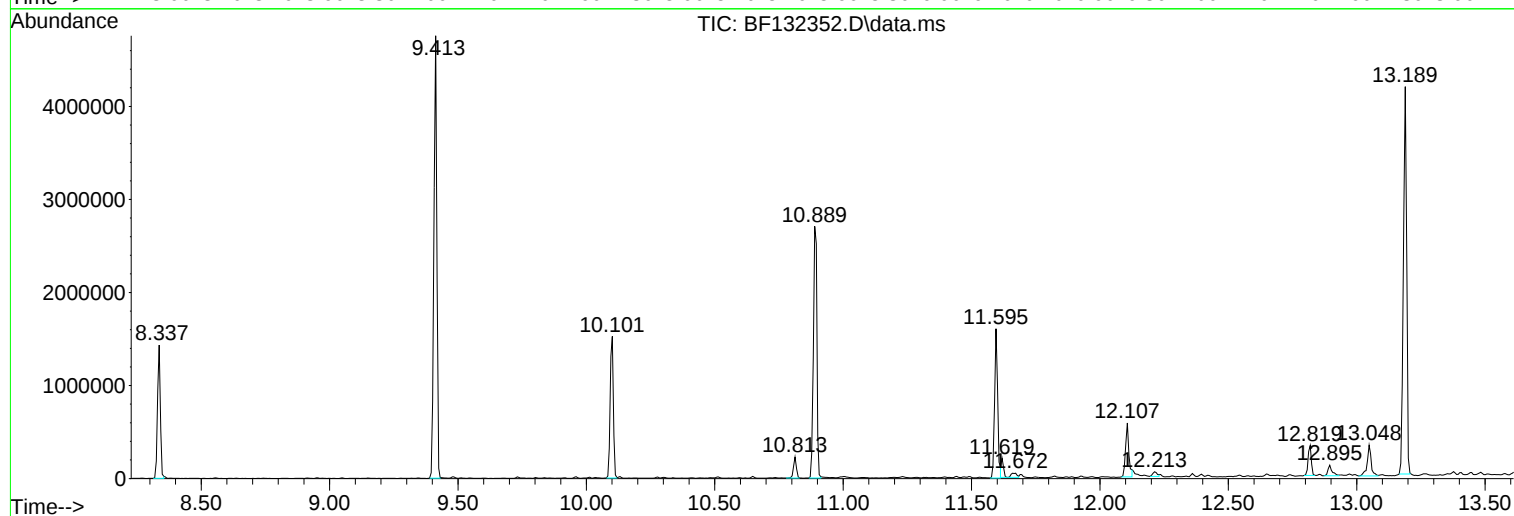
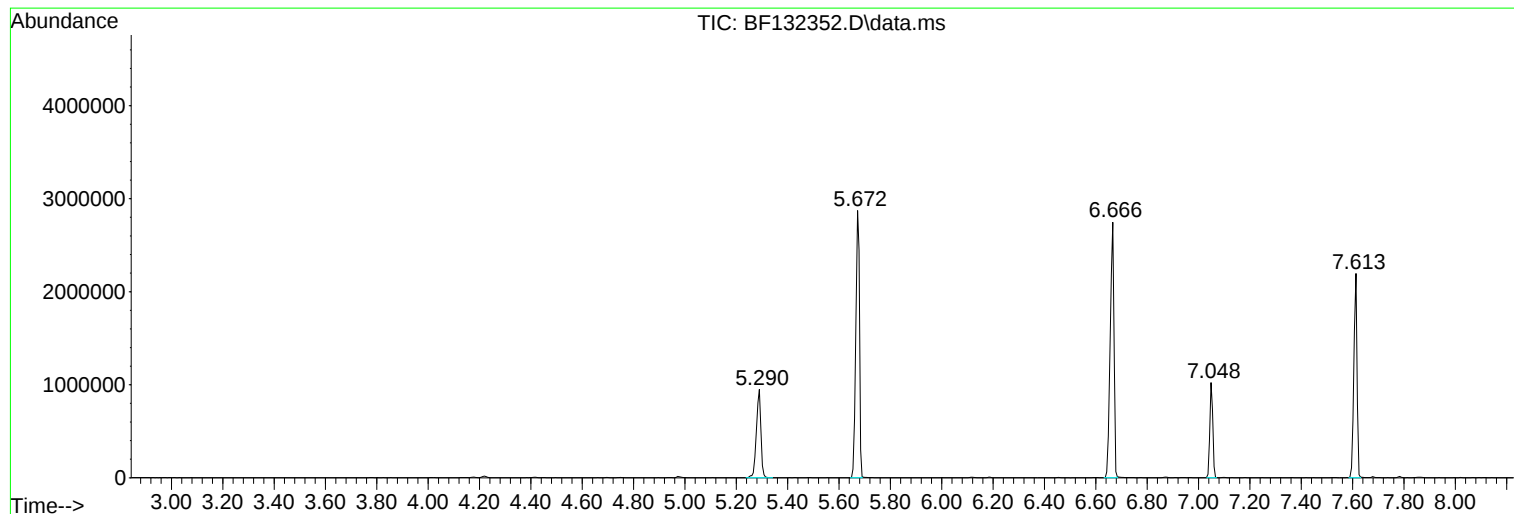
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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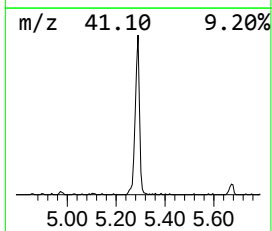
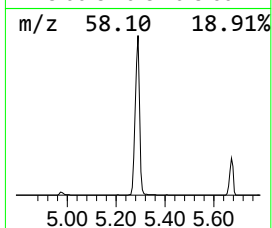
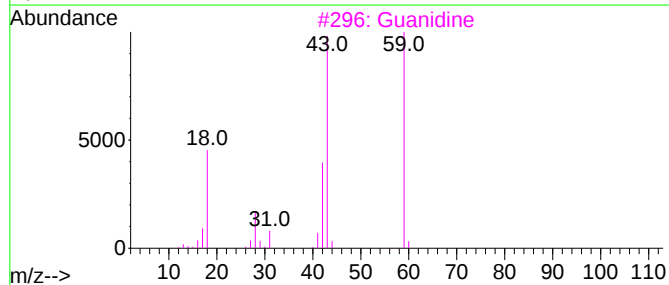
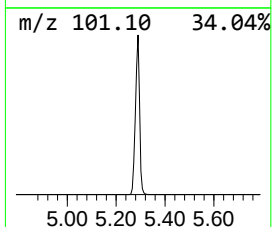
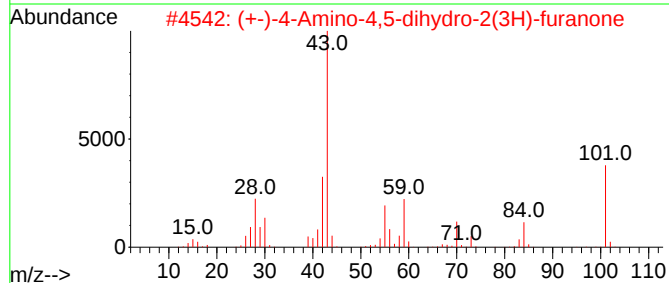
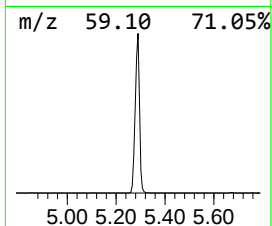
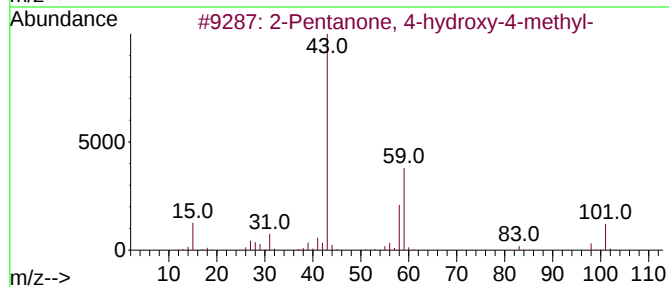
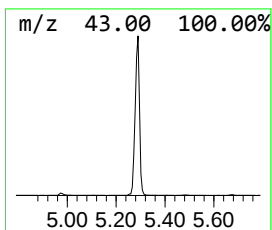
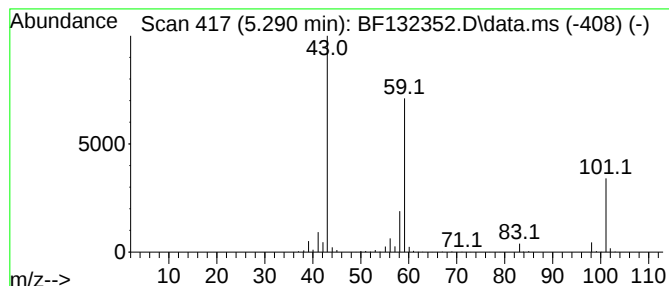
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.290	28.47 ng	1161850	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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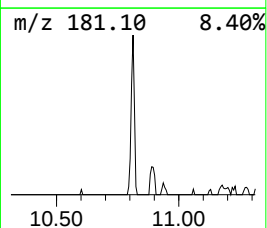
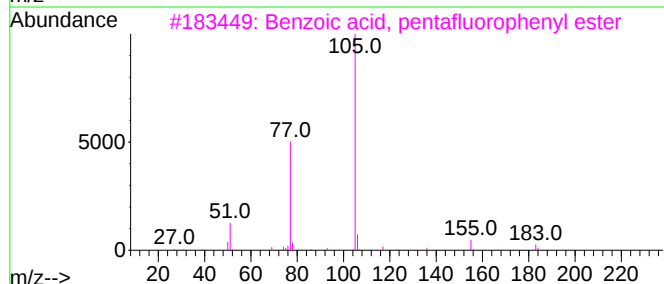
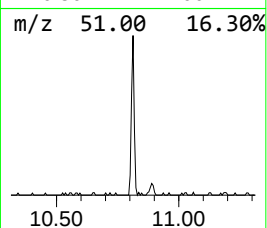
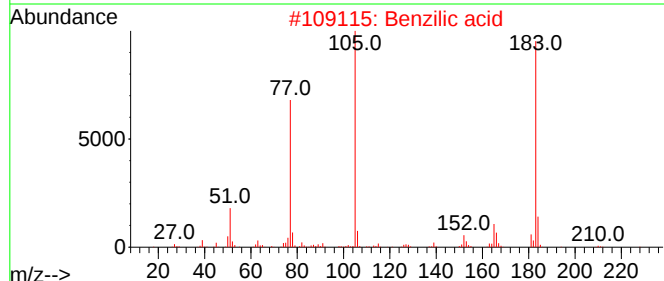
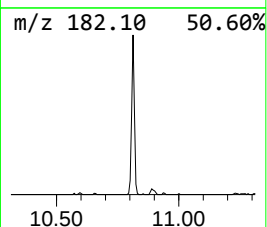
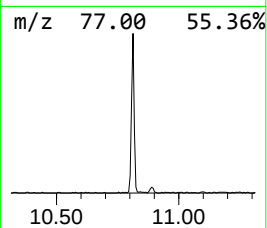
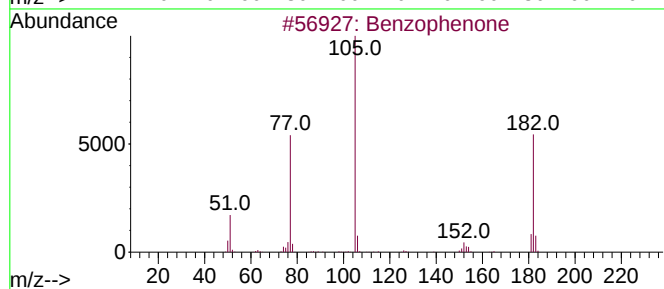
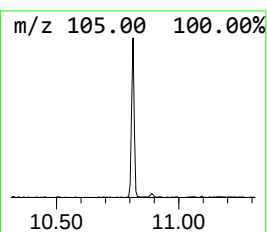
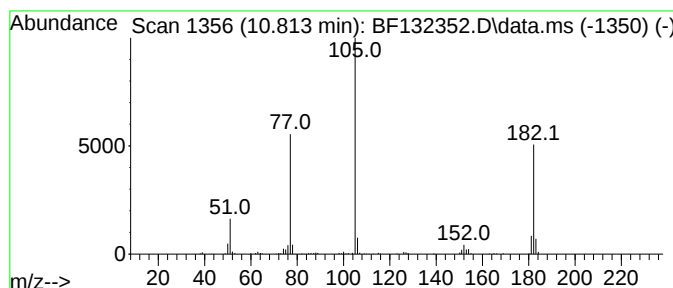
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.813	2.70 ng	173945	Acenaphthene-d10	10.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzilic acid	228	C14H12O3	000076-93-7	50
3			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	43



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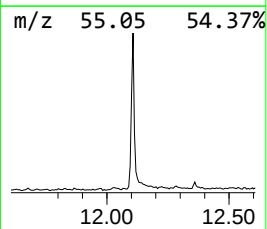
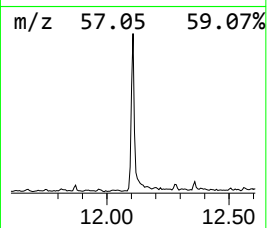
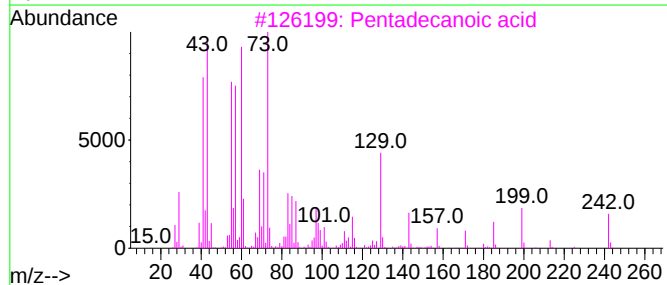
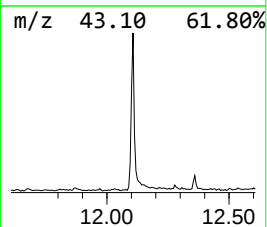
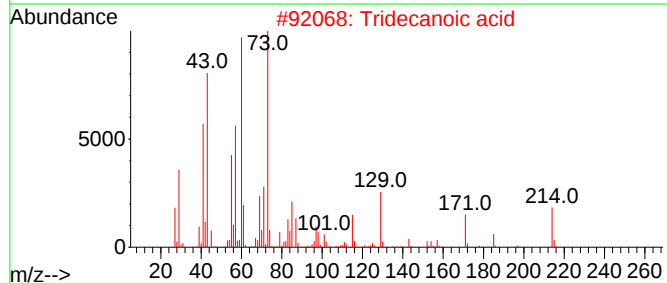
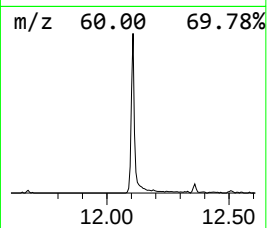
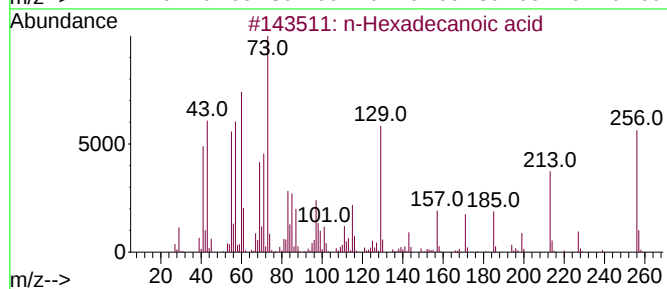
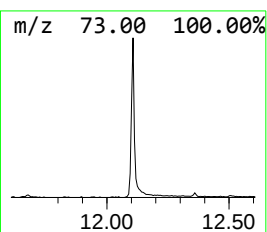
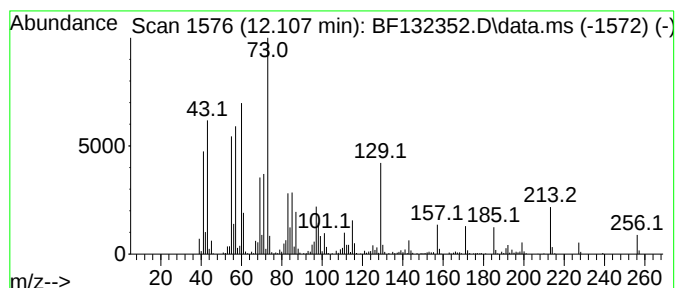
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.107	7.62 ng	518202	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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



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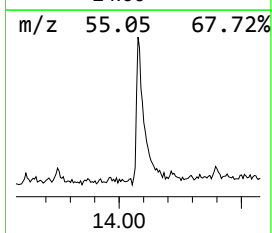
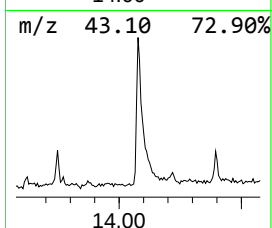
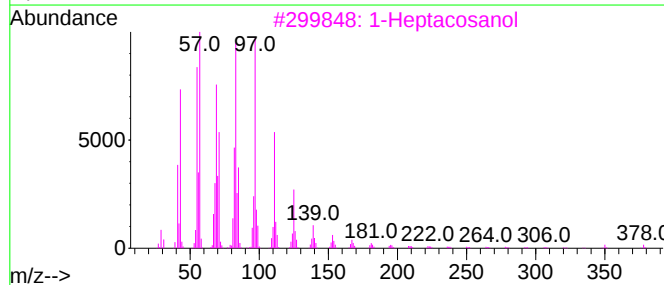
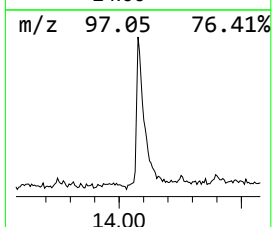
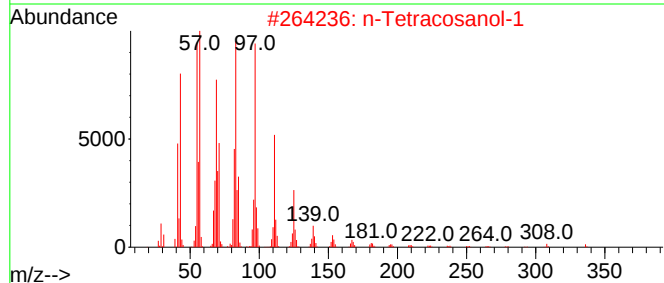
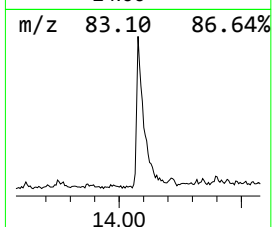
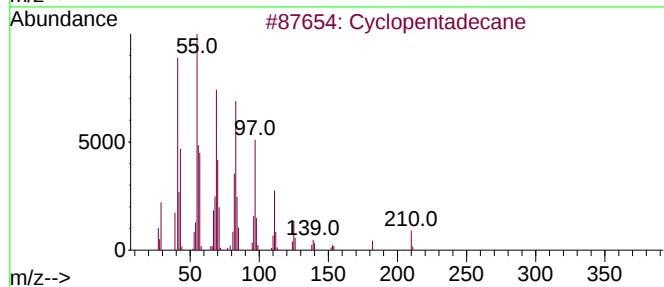
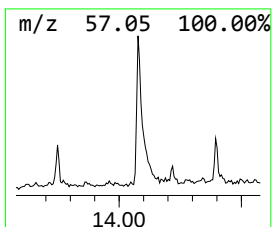
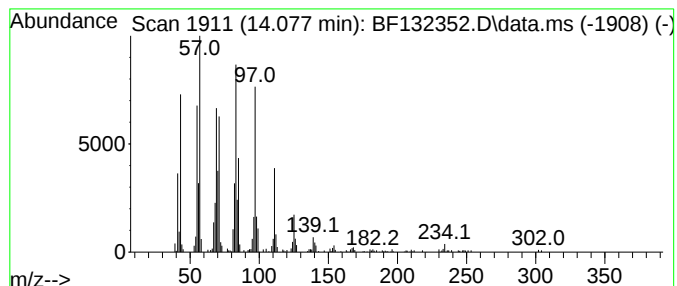
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Peak Number 4 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.077	7.94 ng	386679	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3			1-Heptacosanol	396	C27H56O	002004-39-9	90
4			1-Docosene	308	C22H44	001599-67-3	90
5			1-Heneicosanol	312	C21H44O	015594-90-8	81



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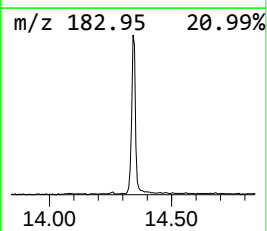
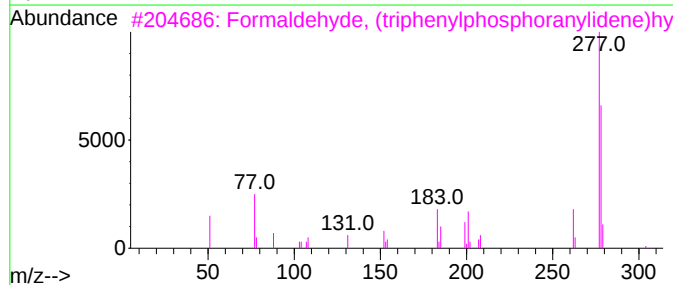
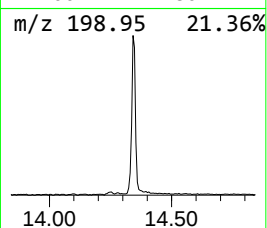
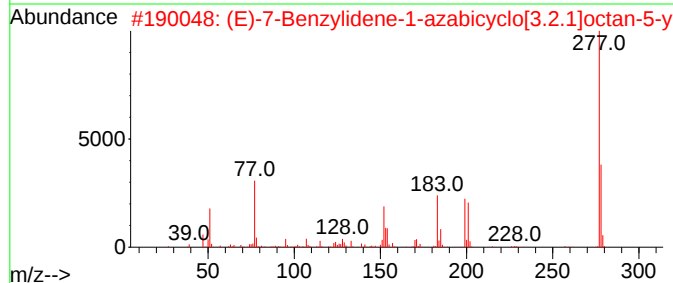
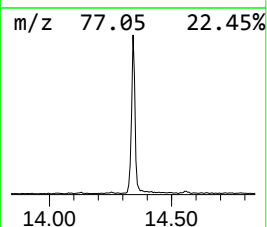
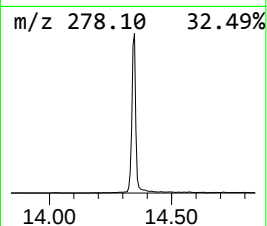
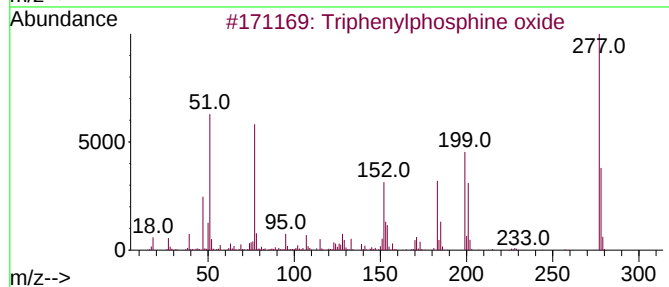
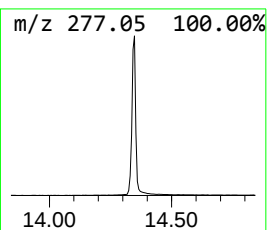
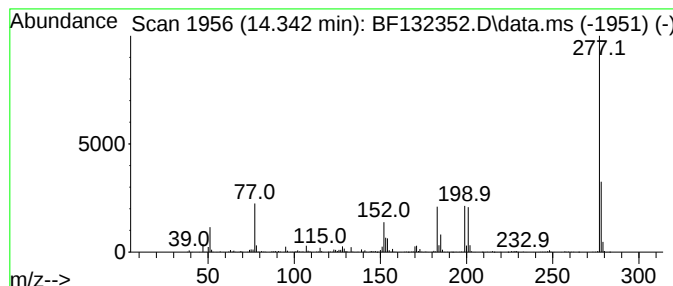
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.342	17.97 ng	874832	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32



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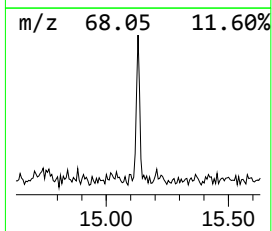
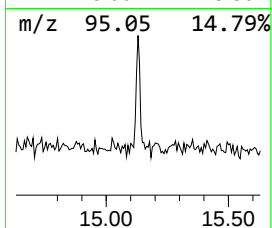
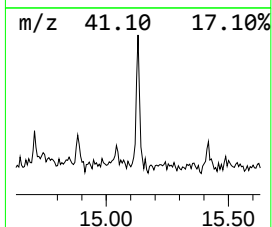
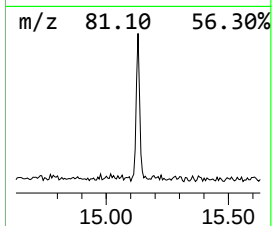
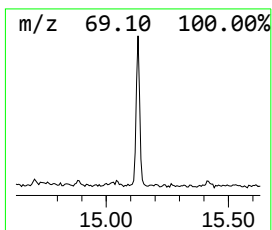
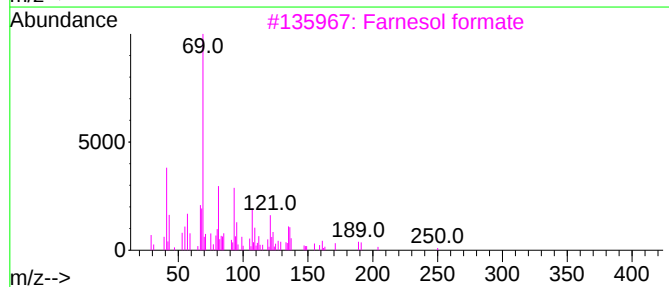
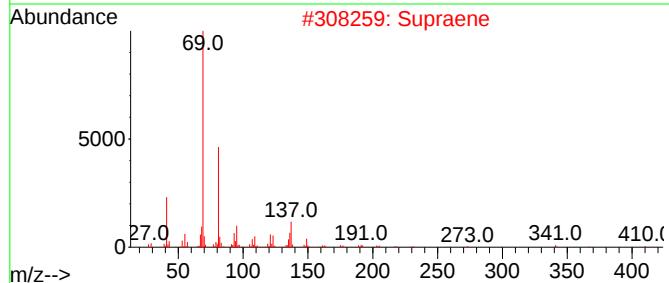
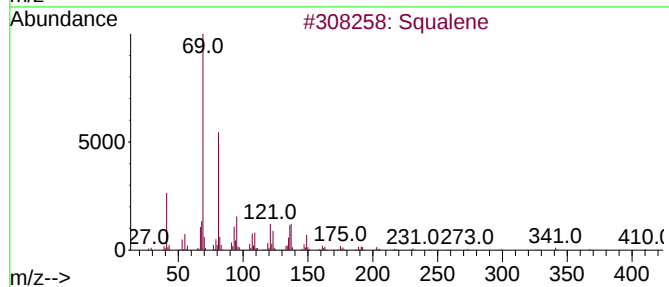
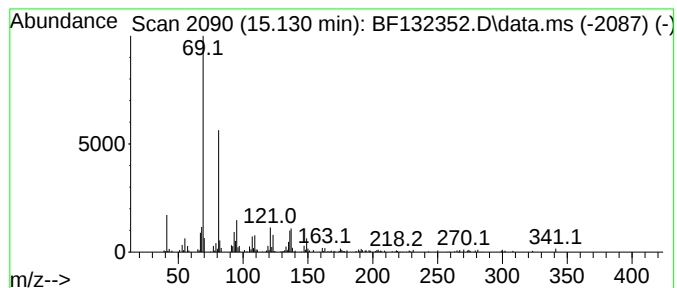
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.130	2.15 ng	102466	Perylene-d12	15.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	87
3			Farnesol formate	250	C16H26O2	917105-98-7	80
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
5			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132352.D
Acq On : 07 Feb 2023 19:15
Operator : CG\JU
Sample : 01464-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-8

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.290	28.5	ng	1161850	1	7.048	816142	20.0
Benzophenone	10.813	2.7	ng	173945	3	10.101	1290400	20.0
n-Hexadecanoic ...	12.107	7.6	ng	518202	4	11.595	1360540	20.0
Cyclopentadecane	14.077	7.9	ng	386679	5	14.254	973528	20.0
Triphenylphosph...	14.342	18.0	ng	874832	5	14.254	973528	20.0
Squalene	15.130	2.1	ng	102466	6	15.830	953264	20.0