

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021323\
 Data File : BF132422.D
 Acq On : 13 Feb 2023 21:51
 Operator : CG\JU
 Sample : 01329-16
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-9-BORING-2-28-35

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-BF021323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.278	409	415	424	rVB	1014967	1347559	35.95%	4.609%
2	5.660	475	480	483	rBV	3175237	3140886	83.79%	10.743%
3	6.649	643	648	651	rBV	2410752	2788822	74.40%	9.539%
4	7.031	709	713	716	rBV	1176053	902331	24.07%	3.086%
5	7.596	804	809	812	rBV	2073674	1878280	50.11%	6.424%
6	8.319	928	932	935	rBV	1485297	1231819	32.86%	4.213%
7	9.395	1110	1115	1118	rBV	4462059	3748575	100.00%	12.822%
8	10.084	1228	1232	1235	rVB	1610623	1454018	38.79%	4.973%
9	10.795	1349	1353	1357	rBV	256666	196129	5.23%	0.671%
10	10.878	1362	1367	1370	rBV	3120215	2818052	75.18%	9.639%
11	11.578	1482	1486	1489	rBV	1843841	1539025	41.06%	5.264%
12	12.089	1569	1573	1578	rBV	197437	217041	5.79%	0.742%
13	12.819	1688	1697	1700	rBV6	35553	62220	1.66%	0.213%
14	12.972	1719	1723	1727	rVB2	71705	68474	1.83%	0.234%
15	13.172	1752	1757	1760	rBV	4232477	3713999	99.08%	12.703%
16	13.730	1847	1852	1854	rBV2	54380	45260	1.21%	0.155%
17	14.060	1905	1908	1911	rBV	56054	44141	1.18%	0.151%
18	14.236	1934	1938	1942	rBV	1497184	1285681	34.30%	4.398%
19	14.324	1947	1953	1959	rVV	1002166	1037593	27.68%	3.549%
20	14.377	1959	1962	1970	rVB	61982	65550	1.75%	0.224%
21	14.689	2011	2015	2022	rVB	51066	52958	1.41%	0.181%
22	14.866	2041	2045	2049	rBV	184778	182741	4.87%	0.625%
23	15.107	2082	2086	2090	rVB	122146	124692	3.33%	0.426%
24	15.801	2198	2204	2214	rBV	968096	1243936	33.18%	4.255%
25	16.289	2282	2287	2292	rBV4	22911	46840	1.25%	0.160%

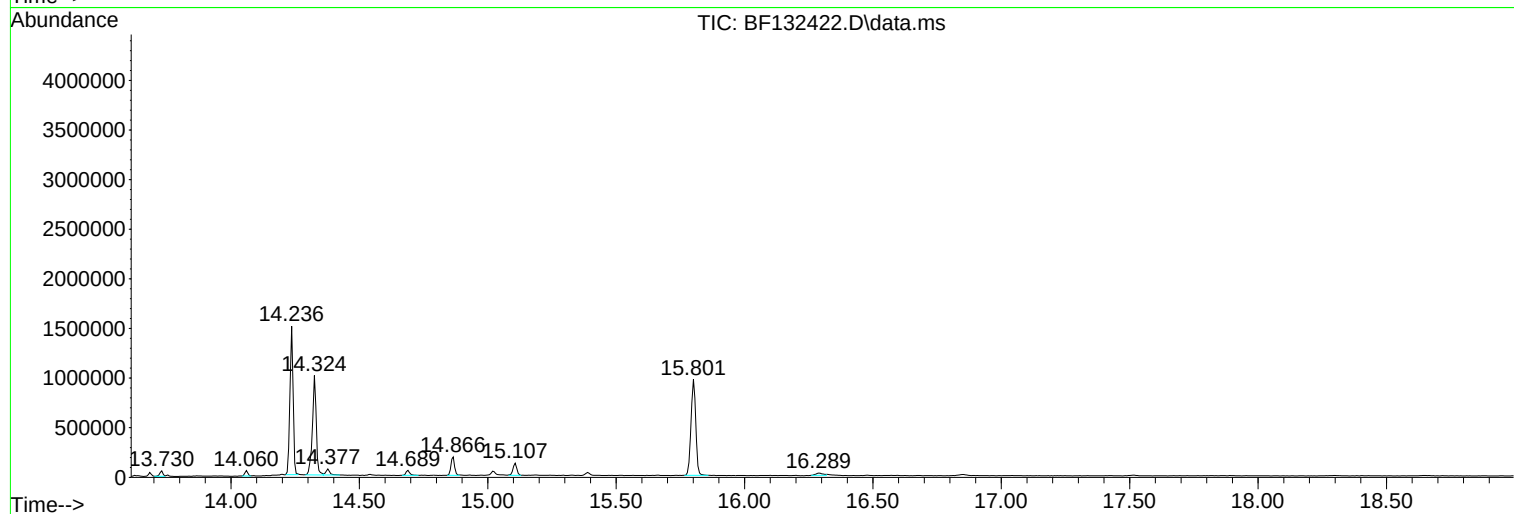
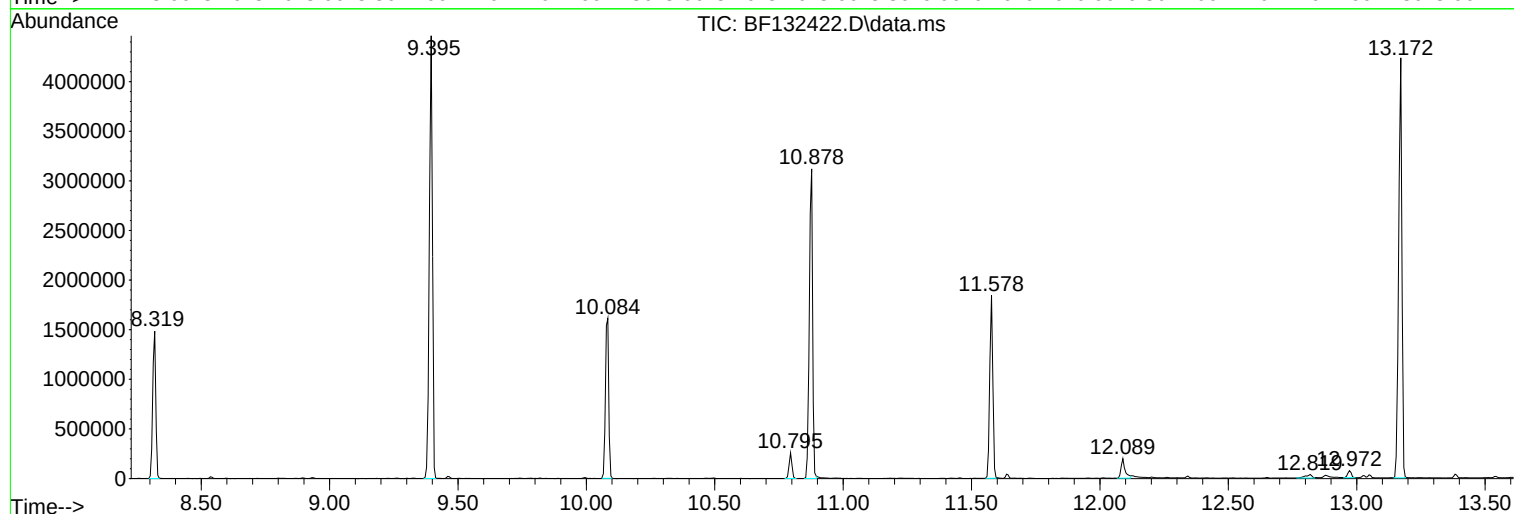
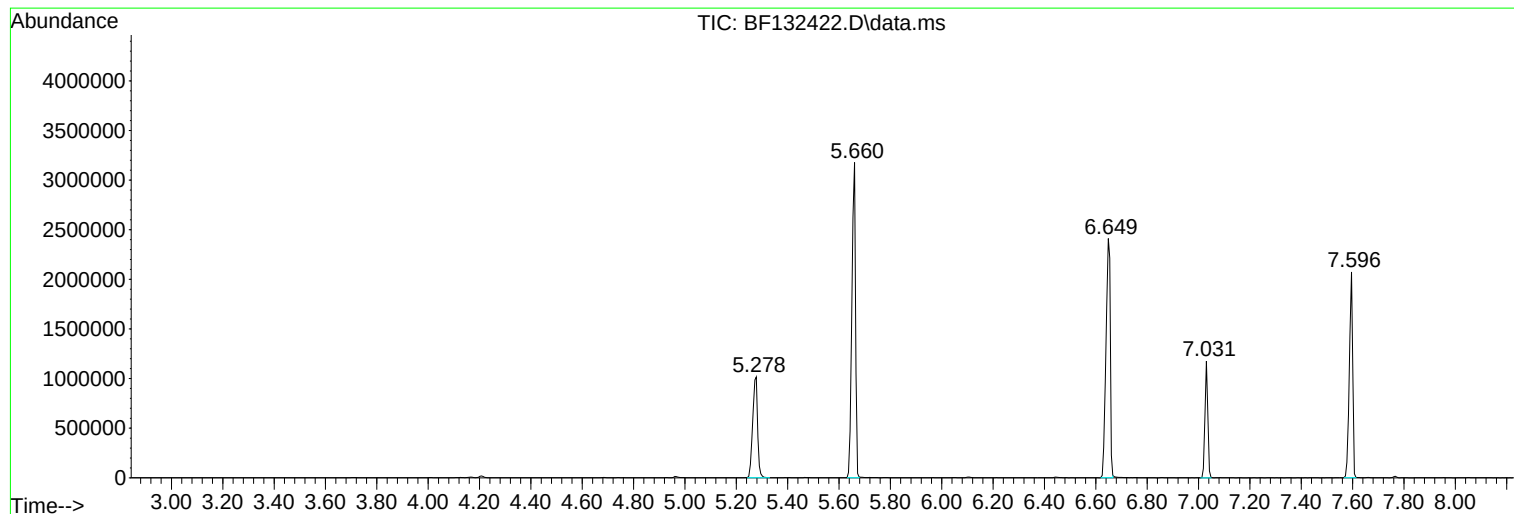
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ClientSampleId :
COMP-9-BORING-2-28-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021323.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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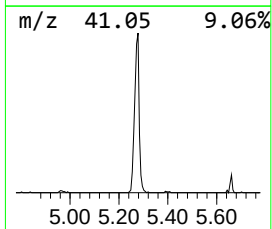
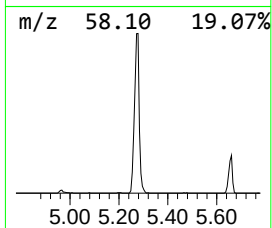
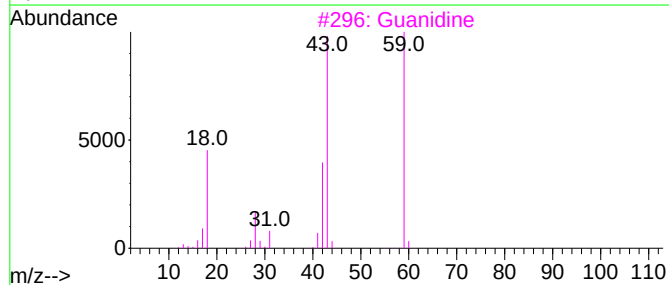
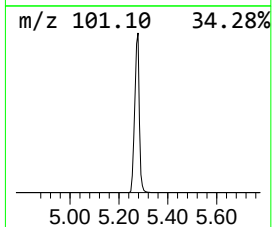
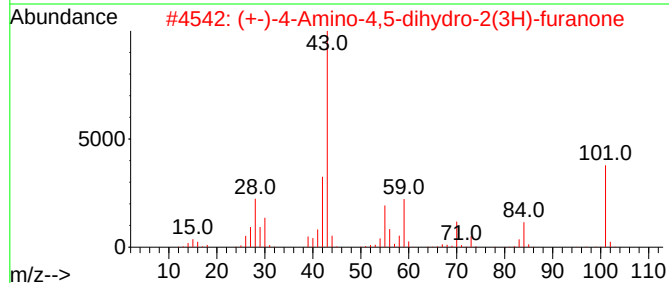
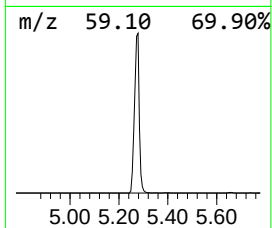
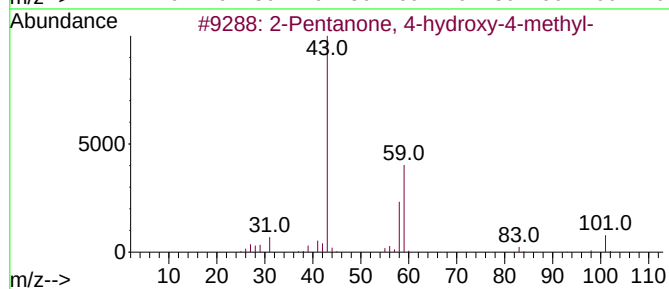
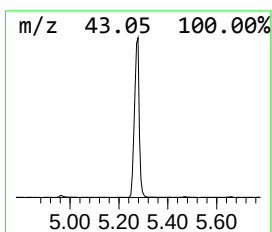
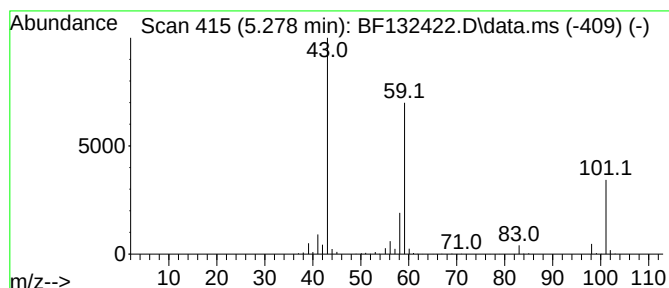
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.278	29.87 ng	1347560	1,4-Dichlorobenzene-d4	7.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Guanidine	59	CH5N3	000113-00-8	38
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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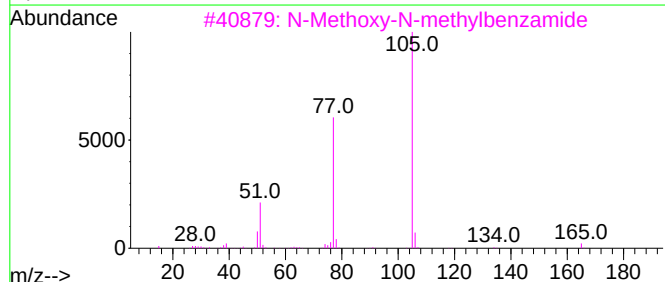
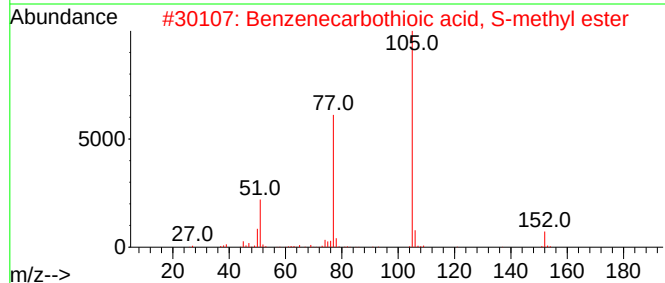
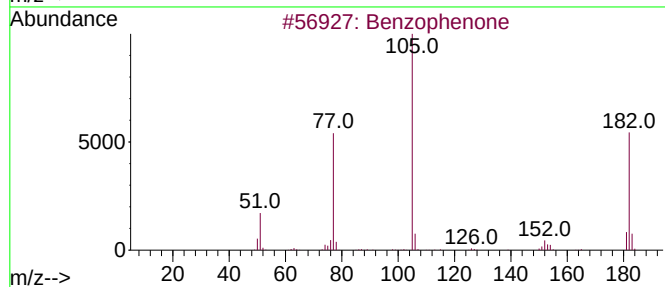
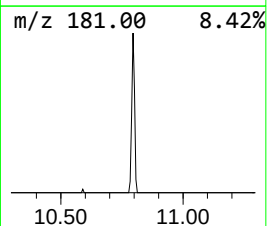
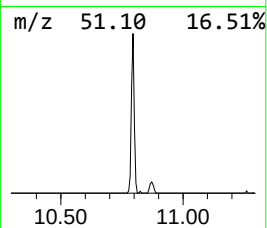
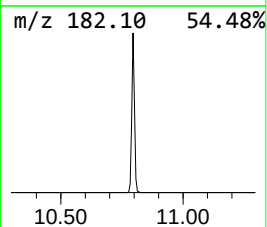
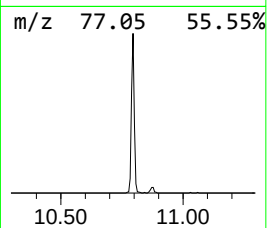
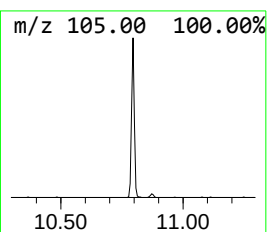
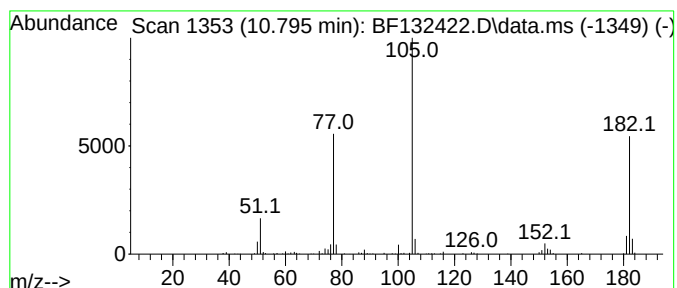
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.795	2.70 ng	196129	Acenaphthene-d10	10.084

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	46
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43



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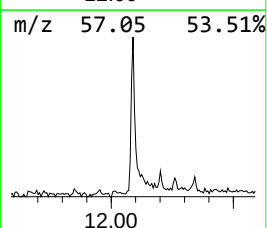
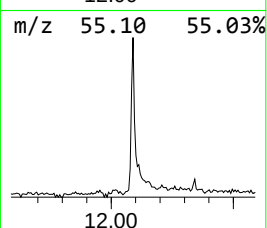
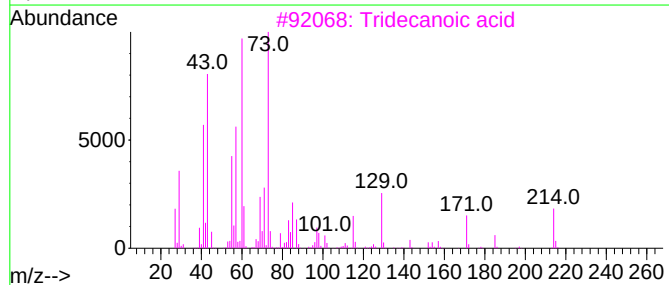
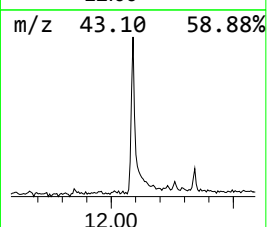
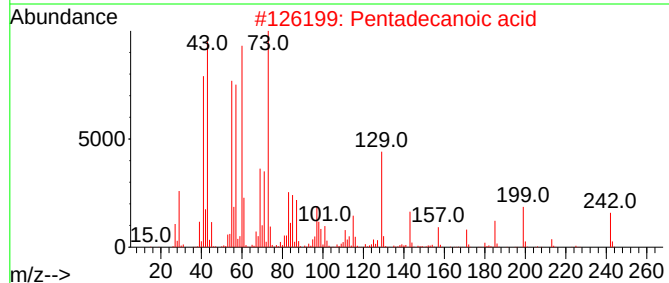
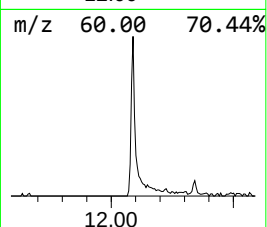
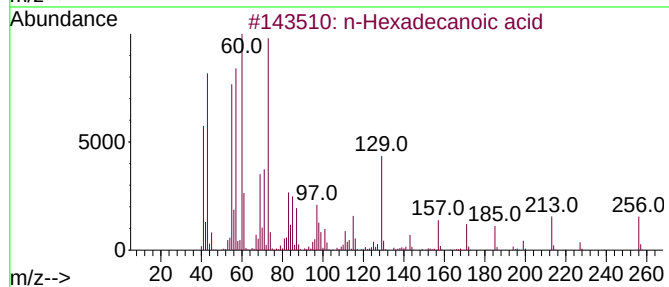
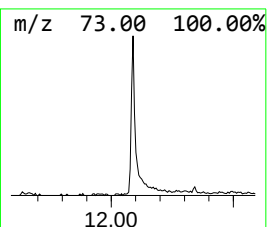
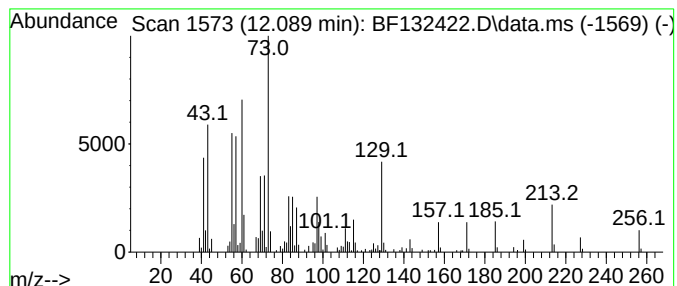
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.089	2.82 ng	217041	Phenanthrene-d10	11.578

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	76
3			Tridecanoic acid	214	C13H26O2	000638-53-9	60
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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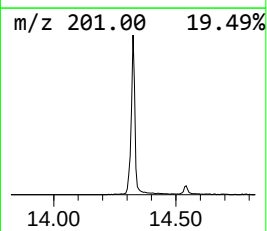
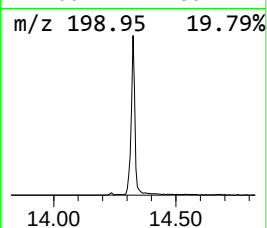
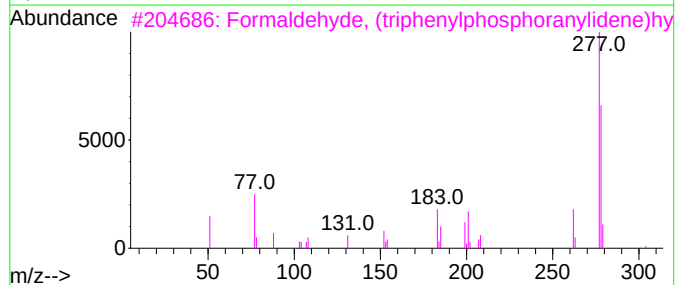
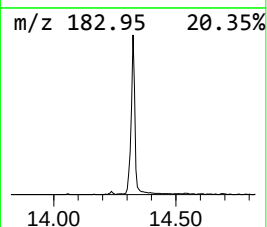
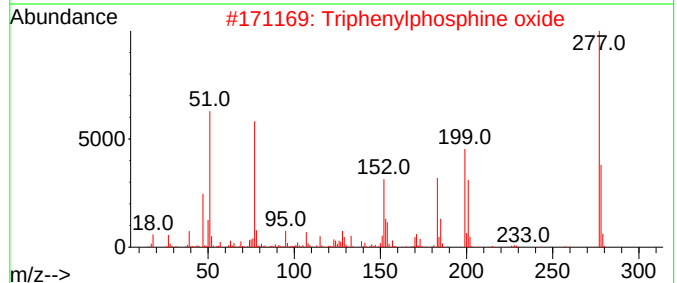
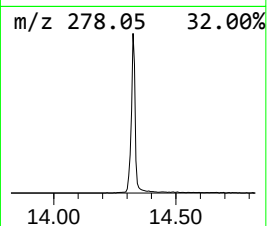
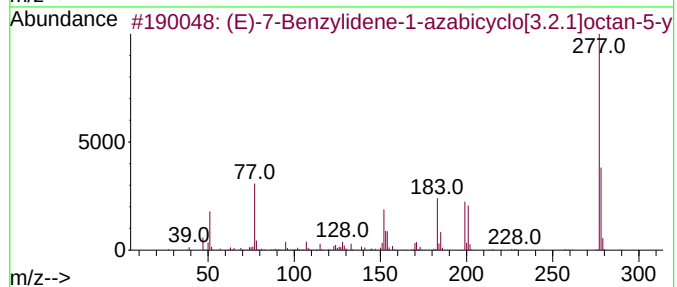
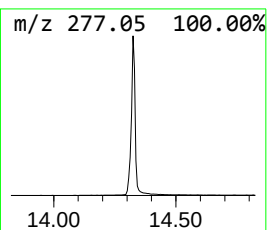
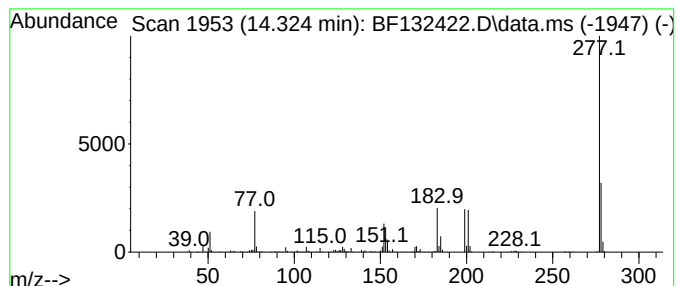
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.325	16.14 ng	1037590	Chrysene-d12	14.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl	293	C15H19NO3S	1000483-83-4	91		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	90		
3	Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	38		
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	28		
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	23		



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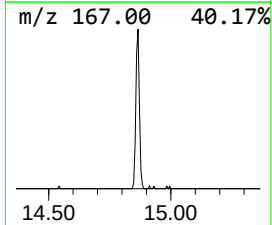
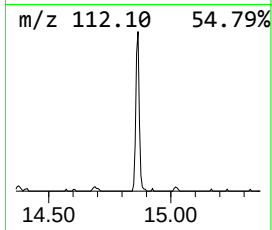
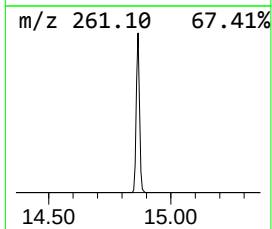
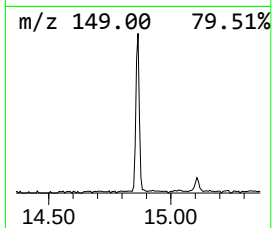
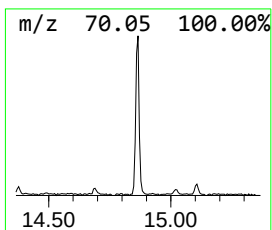
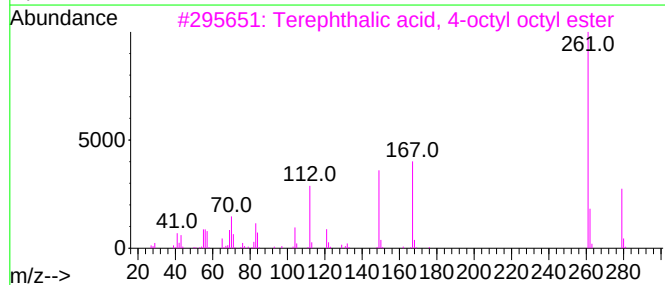
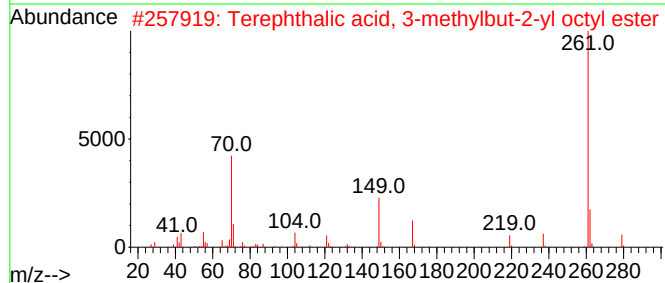
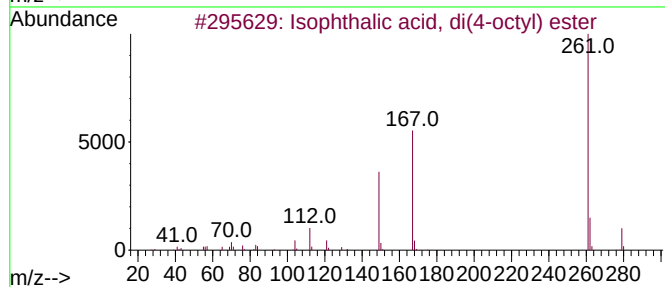
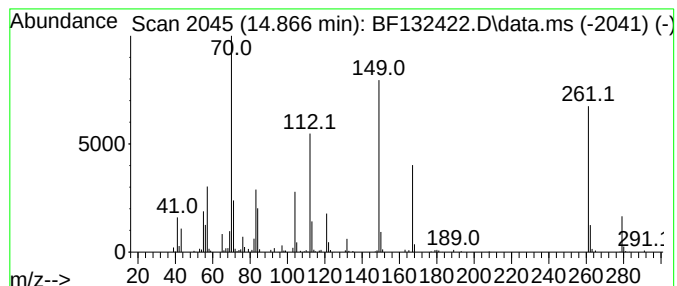
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Isophthalic acid, di(4-octyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.866	2.84 ng	182741	Chrysene-d12	14.236	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	87
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
3	Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	68
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58



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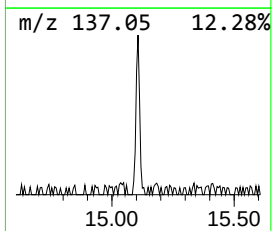
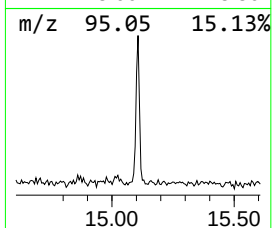
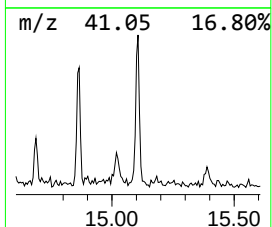
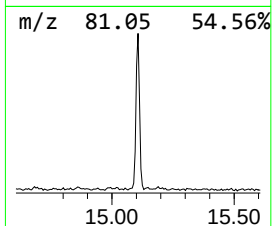
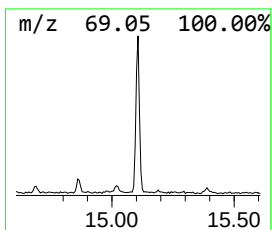
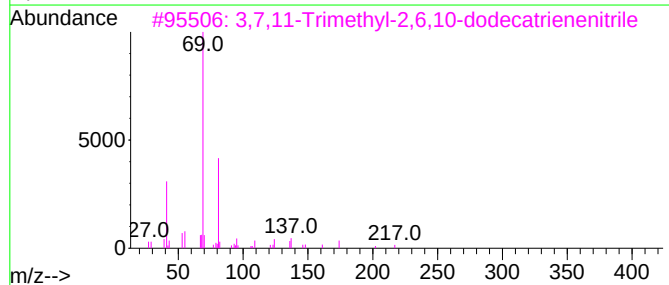
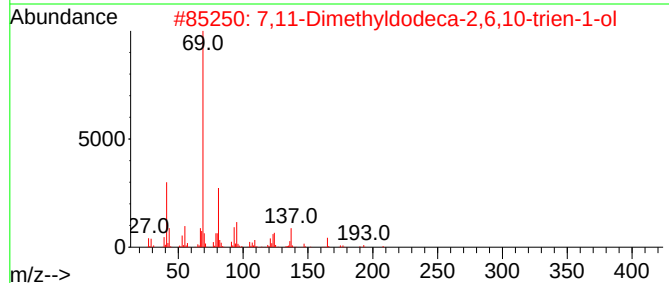
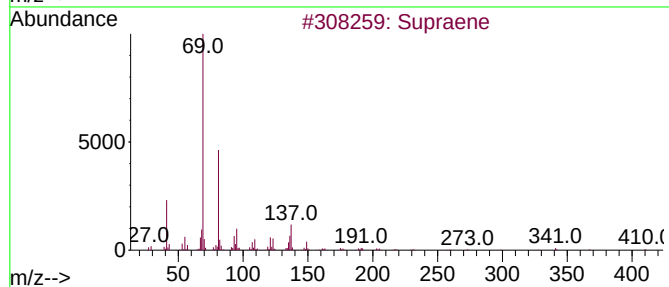
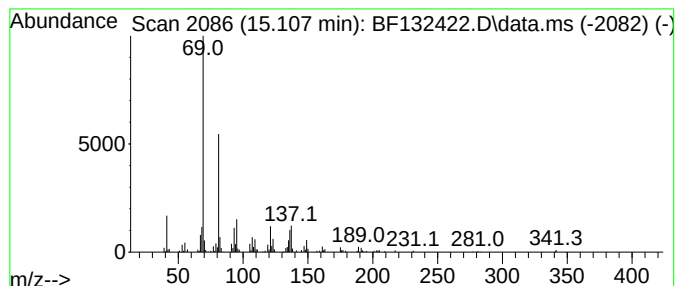
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.107	2.00 ng	124692	Perylene-d12	15.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
3			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	53
4			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021323\
Data File : BF132422.D
Acq On : 13 Feb 2023 21:51
Operator : CG\JU
Sample : 01329-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-9-BORING-2-28-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021323.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-...	5.278	29.9	ng	1347560	1	7.031	902331	20.0
Benzophenone	10.795	2.7	ng	196129	3	10.084	1454020	20.0
n-Hexadecanoic ...	12.089	2.8	ng	217041	4	11.578	1539030	20.0
(E)-7-Benzylide...	14.325	16.1	ng	1037590	5	14.236	1285680	20.0
Isophthalic aci...	14.866	2.8	ng	182741	5	14.236	1285680	20.0
Supraene	15.107	2.0	ng	124692	6	15.801	1243940	20.0