

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
 Data File : BF132460.D
 Acq On : 17 Feb 2023 20:38
 Operator : CG\JU
 Sample : 01595-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-655-3

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132460.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.672	308	312	319	rBV	155496	158825	1.96%	0.302%
2	5.266	408	413	425	rVB	1928500	2572184	31.66%	4.897%
3	5.654	473	479	482	rBV	5018013	5575443	68.64%	10.615%
4	6.643	641	647	650	rBV	4894044	6093418	75.01%	11.601%
5	7.019	708	711	715	rBV	1824349	1512659	18.62%	2.880%
6	7.584	801	807	810	rBV	3557530	3751066	46.18%	7.142%
7	8.307	926	930	933	rBV	2374397	1948904	23.99%	3.710%
8	9.384	1107	1113	1116	rBV	6872128	6623040	81.53%	12.609%
9	10.072	1226	1230	1233	rVB	2488571	2244102	27.63%	4.273%
10	10.784	1343	1351	1355	rBV	495432	400002	4.92%	0.762%
11	10.866	1360	1365	1368	rBV	5191817	4939840	60.81%	9.405%
12	11.566	1480	1484	1487	rBV	2850234	2367488	29.14%	4.507%
13	12.078	1567	1571	1576	rBV	397081	438680	5.40%	0.835%
14	12.866	1700	1705	1718	rBV2	84015	151383	1.86%	0.288%
15	13.160	1750	1755	1758	rBV	7873167	8123280	100.00%	15.466%
16	14.042	1902	1905	1909	rBV	85310	97623	1.20%	0.186%
17	14.219	1931	1935	1939	rBV	2147551	1990307	24.50%	3.789%
18	14.307	1944	1950	1956	rBV	1005023	1171224	14.42%	2.230%
19	14.360	1956	1959	1966	rVB	89997	94776	1.17%	0.180%
20	14.672	2008	2012	2019	rBV	94744	96164	1.18%	0.183%
21	15.001	2065	2068	2075	rVB	74640	84111	1.04%	0.160%
22	15.089	2079	2083	2087	rVB	179625	182875	2.25%	0.348%
23	15.783	2194	2201	2210	rBV	1363482	1906840	23.47%	3.630%

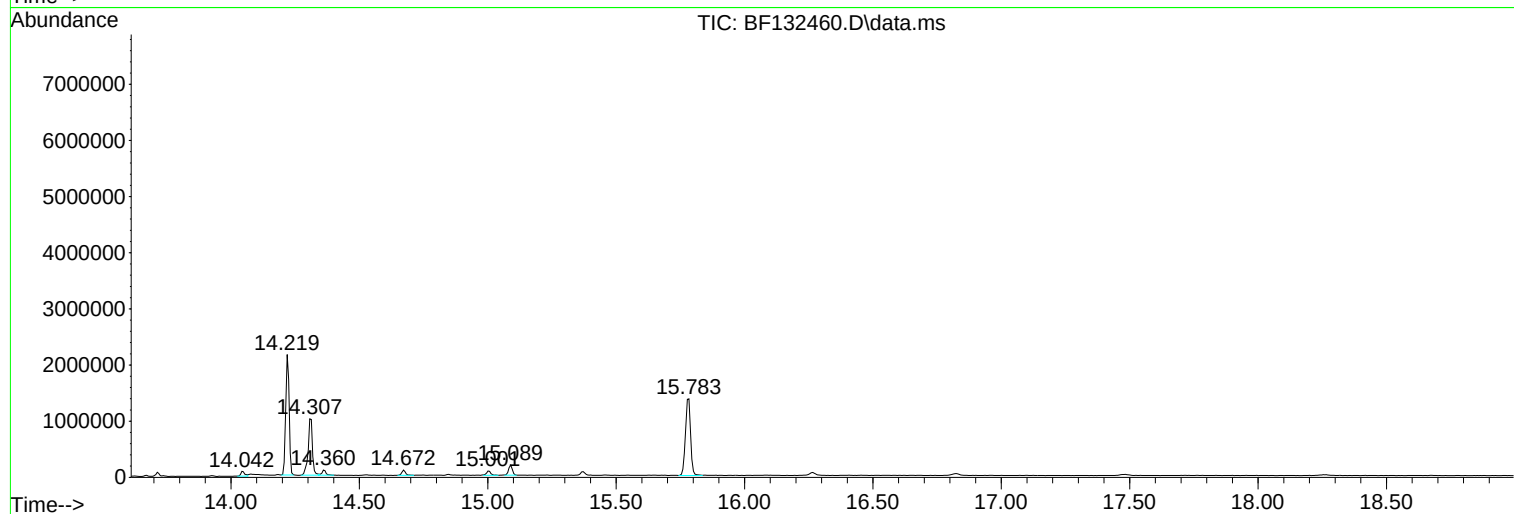
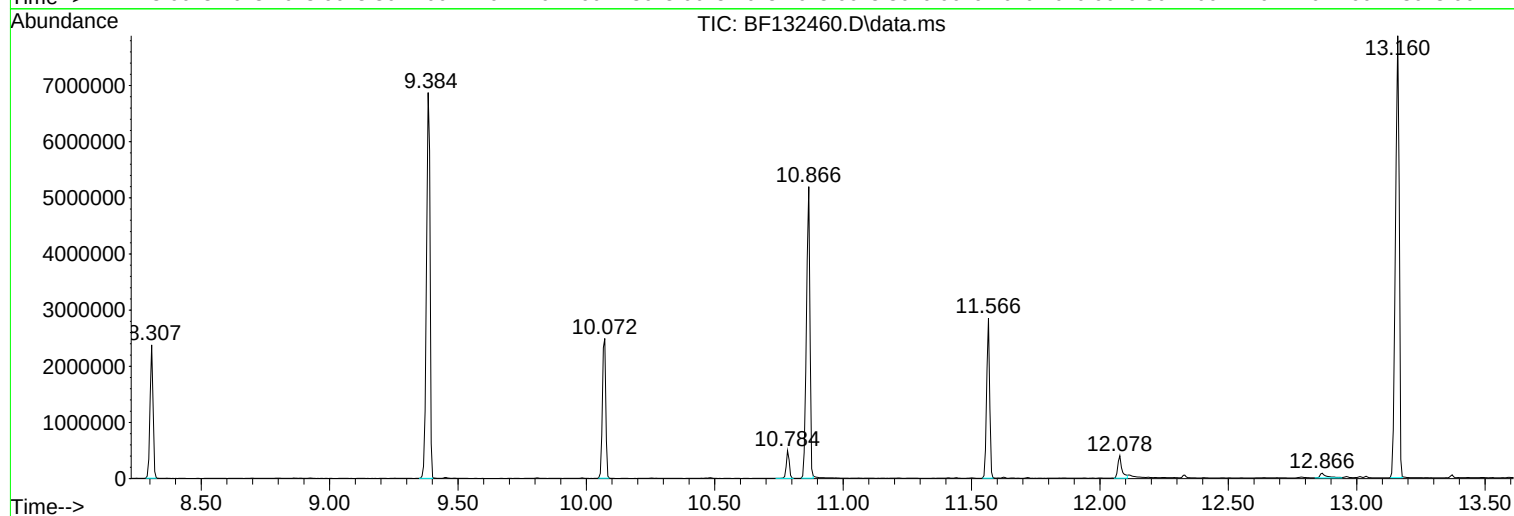
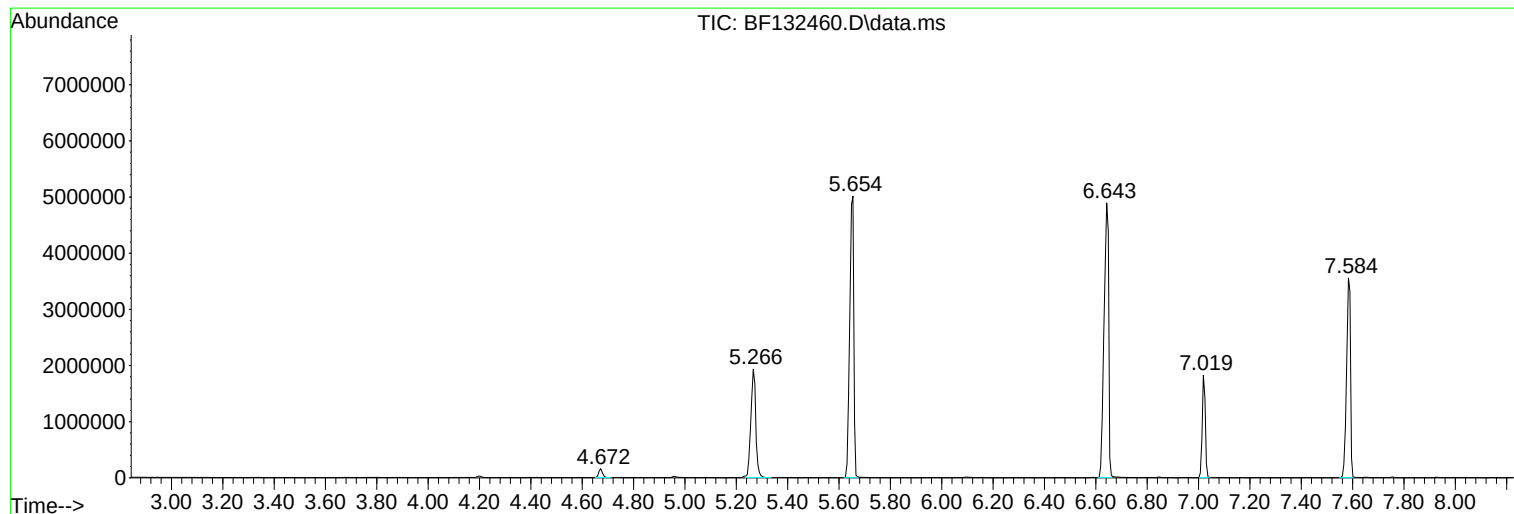
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Instrument :
BNA_F
ClientSampleId :
S-655-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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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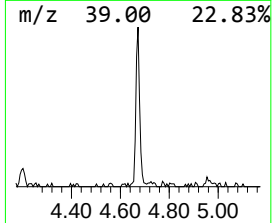
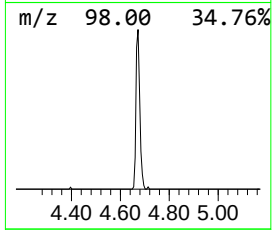
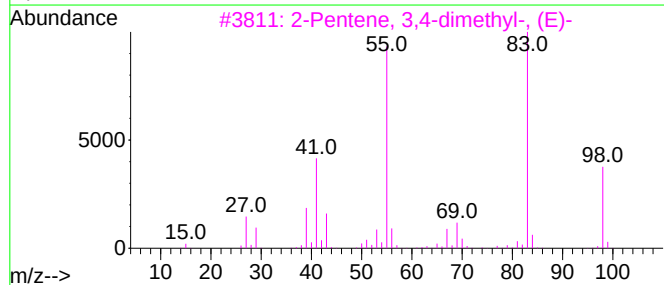
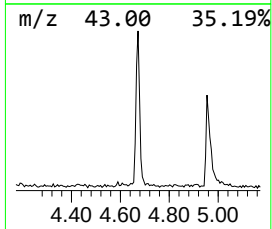
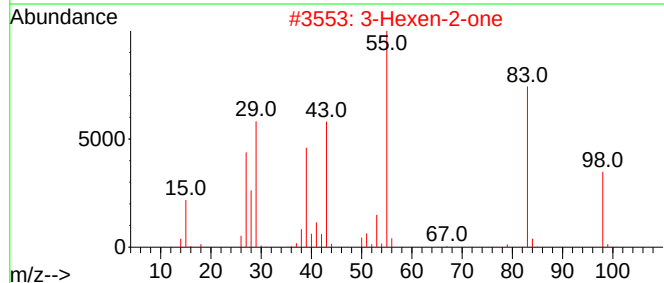
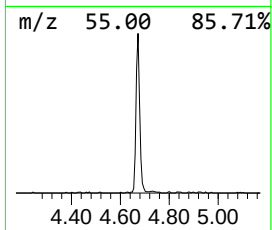
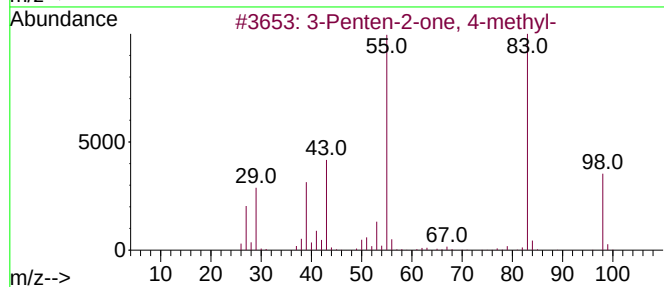
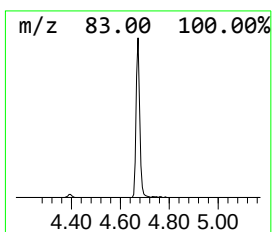
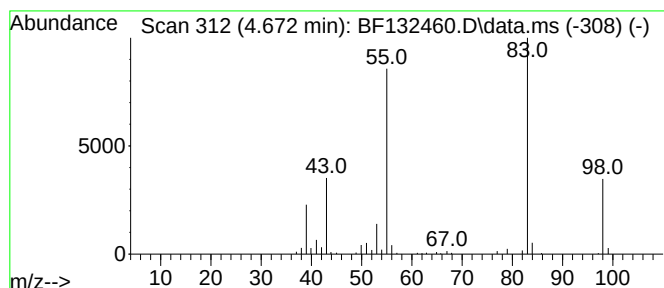
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.672	2.10 ng	158825	1,4-Dichlorobenzene-d4	7.019

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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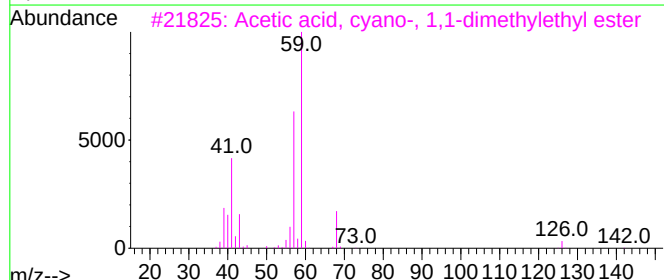
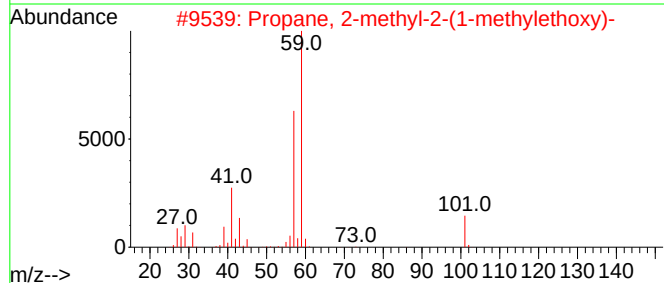
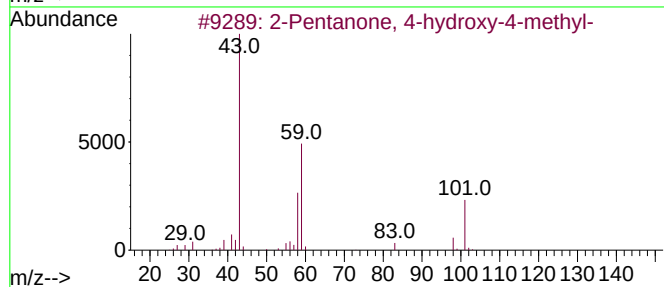
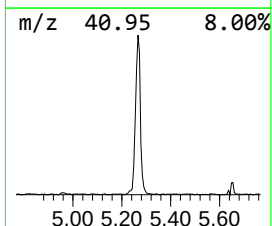
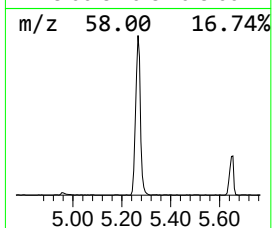
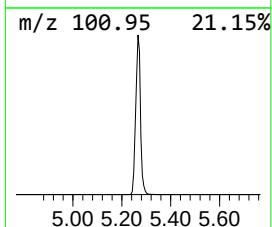
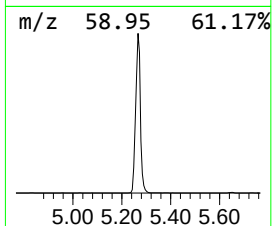
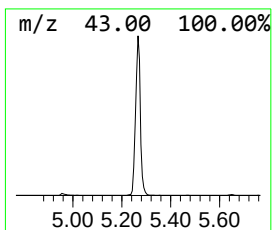
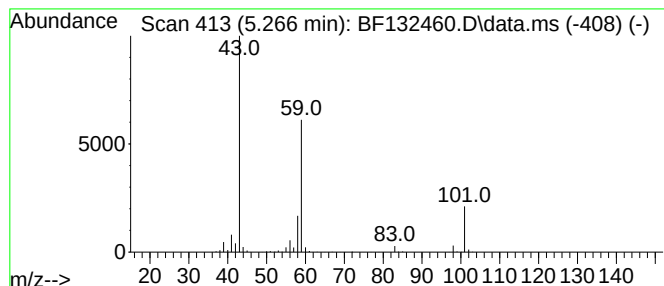
Instrument :
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ClientSampleId :
S-655-3

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.266	34.01 ng	2572180	1,4-Dichlorobenzene-d4			7.019
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	10
5	Guanidine	59	CH5N3		000113-00-8	9



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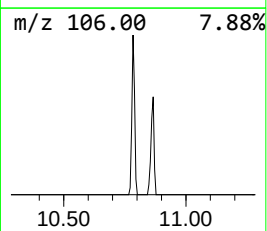
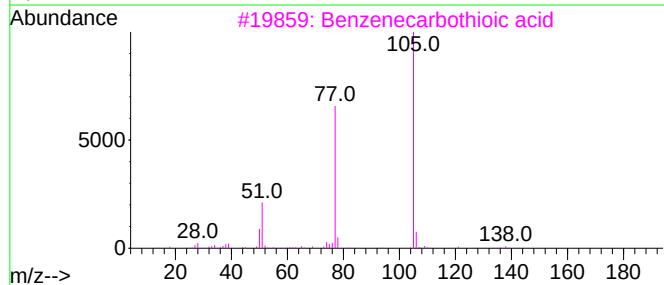
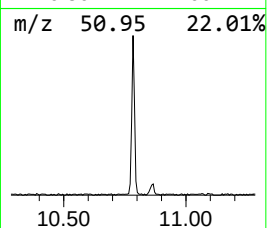
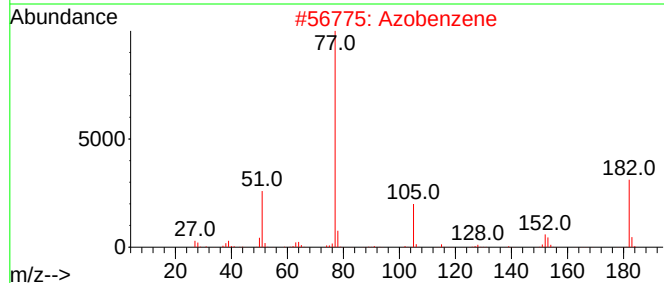
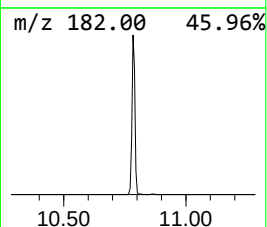
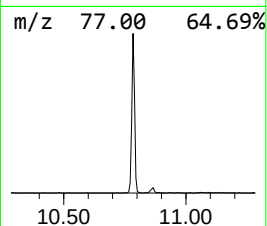
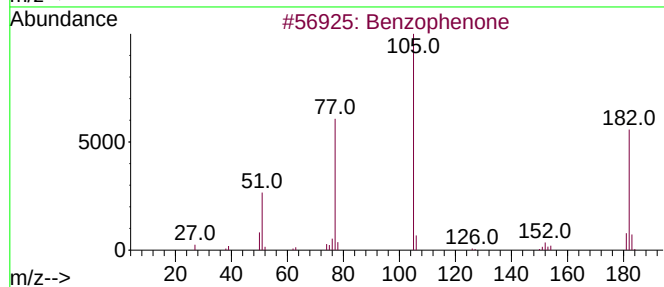
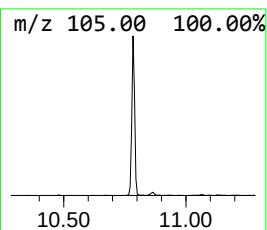
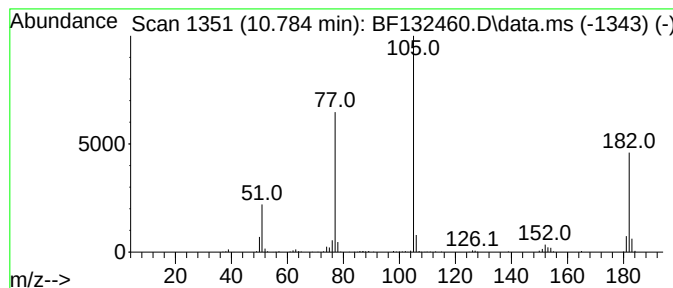
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.784	3.56 ng	400002	Acenaphthene-d10	10.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47
4			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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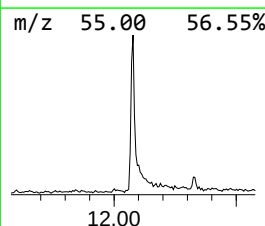
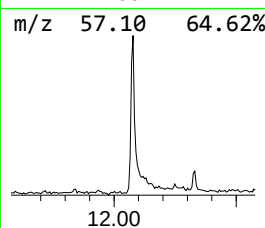
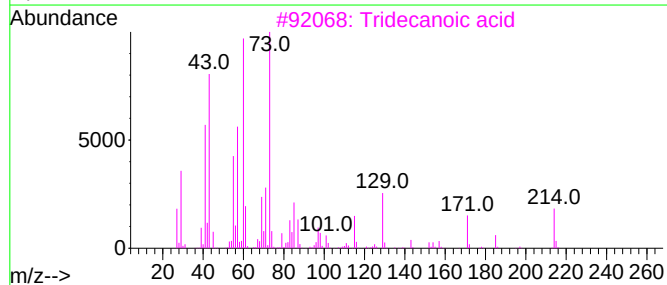
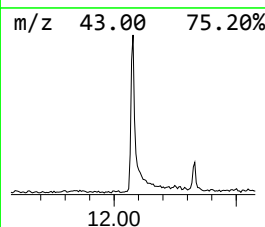
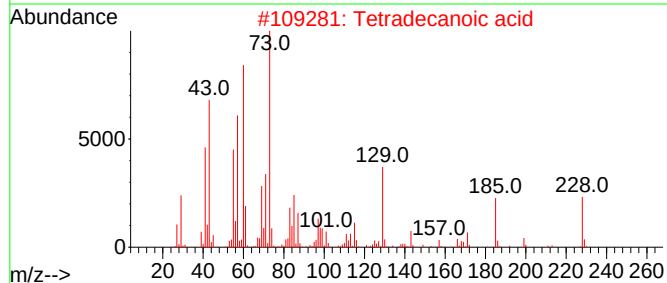
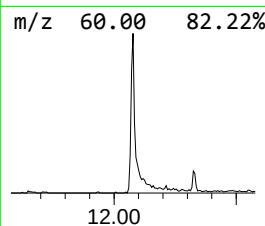
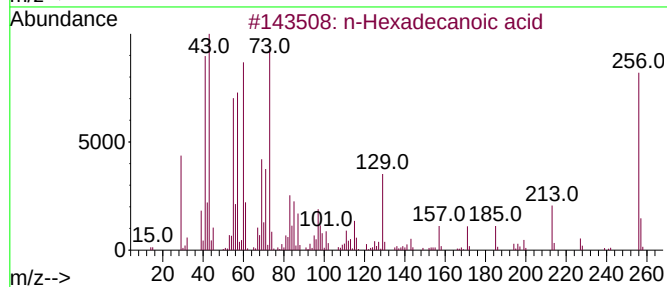
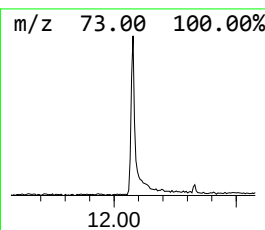
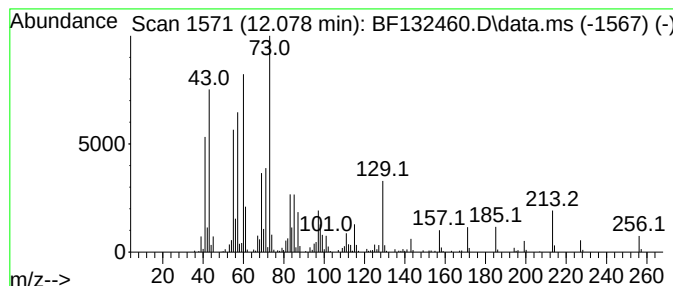
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.078	3.71 ng	438680	Phenanthrene-d10	11.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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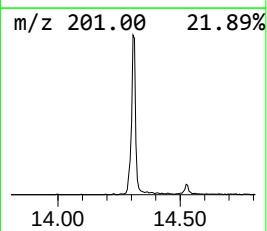
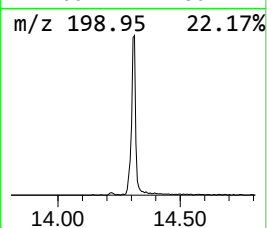
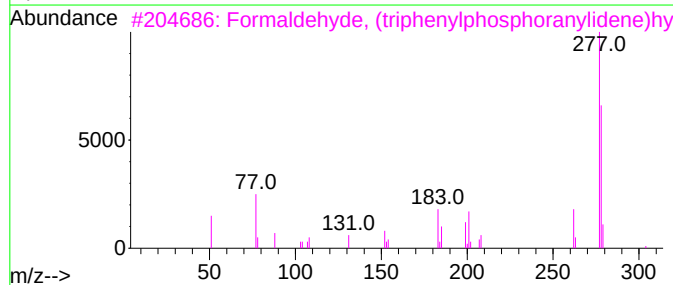
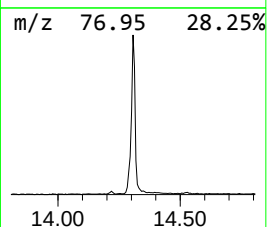
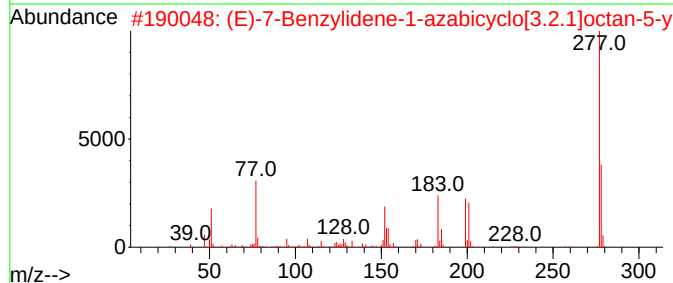
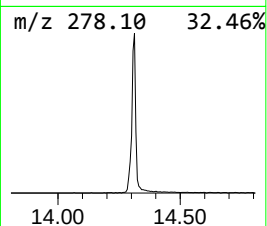
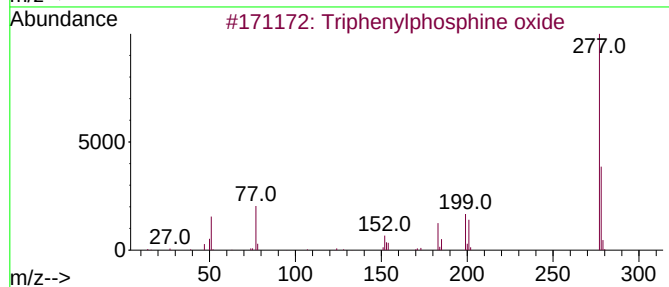
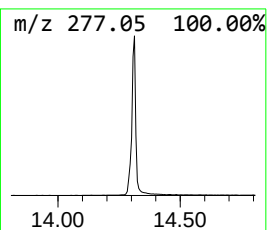
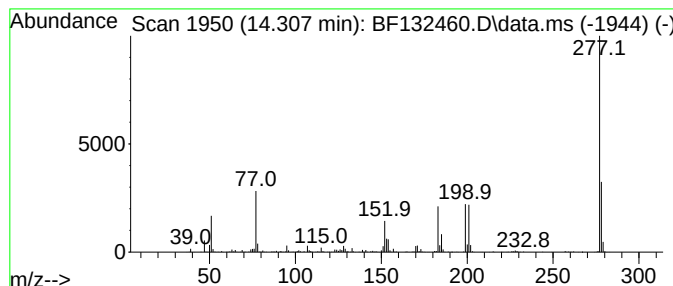
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.307	11.77 ng	1171220	Chrysene-d12	14.219

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	38
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.672	2.1	ng	158825	1	7.019	1512660	20.0
2-Pentanone, 4-...	5.266	34.0	ng	2572180	1	7.019	1512660	20.0
Benzophenone	10.784	3.6	ng	400002	3	10.072	2244100	20.0
n-Hexadecanoic ...	12.078	3.7	ng	438680	4	11.566	2367490	20.0
Triphenylphosph...	14.307	11.8	ng	1171220	5	14.219	1990310	20.0