

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
 Data File : BF132464.D
 Acq On : 17 Feb 2023 22:48
 Operator : CG\JU
 Sample : 01595-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-322-3

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: BF132464.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.266	408	413	426	rVB	1900158	2376658	41.81%	4.981%
2	5.648	473	478	481	rBV	4678431	4757101	83.68%	9.970%
3	6.643	641	647	650	rBV	4422953	4793270	84.32%	10.046%
4	7.019	707	711	715	rBV	1817446	1464252	25.76%	3.069%
5	7.584	801	807	810	rBV	3491951	3166406	55.70%	6.636%
6	8.307	925	930	933	rBV	2345696	1893930	33.32%	3.969%
7	9.384	1107	1113	1116	rBV	6099796	5515979	97.03%	11.561%
8	10.072	1226	1230	1233	rVB	2549614	2176135	38.28%	4.561%
9	10.783	1347	1351	1355	rBV	2756986	2502352	44.02%	5.245%
10	10.866	1360	1365	1368	rBV	3782782	3633244	63.91%	7.615%
11	11.095	1400	1404	1411	rBV	439573	402718	7.08%	0.844%
12	11.160	1411	1415	1418	rBV	253666	240255	4.23%	0.504%
13	11.413	1447	1458	1461	rBV10	27079	78150	1.37%	0.164%
14	11.460	1463	1466	1469	rVB	160947	122151	2.15%	0.256%
15	11.566	1480	1484	1487	rBV	2694044	2307305	40.59%	4.836%
16	12.077	1567	1571	1588	rBV	727080	890185	15.66%	1.866%
17	12.330	1610	1614	1617	rVB	197712	174451	3.07%	0.366%
18	12.636	1659	1666	1669	rBV	35367	65201	1.15%	0.137%
19	12.866	1701	1705	1718	rBV	116112	201369	3.54%	0.422%
20	13.160	1750	1755	1758	rBV	5537745	5684908	100.00%	11.915%
21	14.048	1902	1906	1907	rBV2	95920	102522	1.80%	0.215%
22	14.219	1931	1935	1939	rBV	2093541	1847710	32.50%	3.872%
23	14.307	1944	1950	1956	rBV	1056788	1141014	20.07%	2.391%
24	14.671	2009	2012	2020	rBV	66783	71763	1.26%	0.150%
25	15.001	2064	2068	2075	rVB	63237	78457	1.38%	0.164%
26	15.083	2079	2082	2090	rVB	132913	153220	2.70%	0.321%
27	15.366	2126	2130	2137	rVB	63180	82037	1.44%	0.172%
28	15.777	2194	2200	2211	rBV2	1197592	1594938	28.06%	3.343%
29	16.265	2278	2283	2289	rVB	79736	132057	2.32%	0.277%
30	16.818	2372	2377	2383	rBV2	35076	64065	1.13%	0.134%

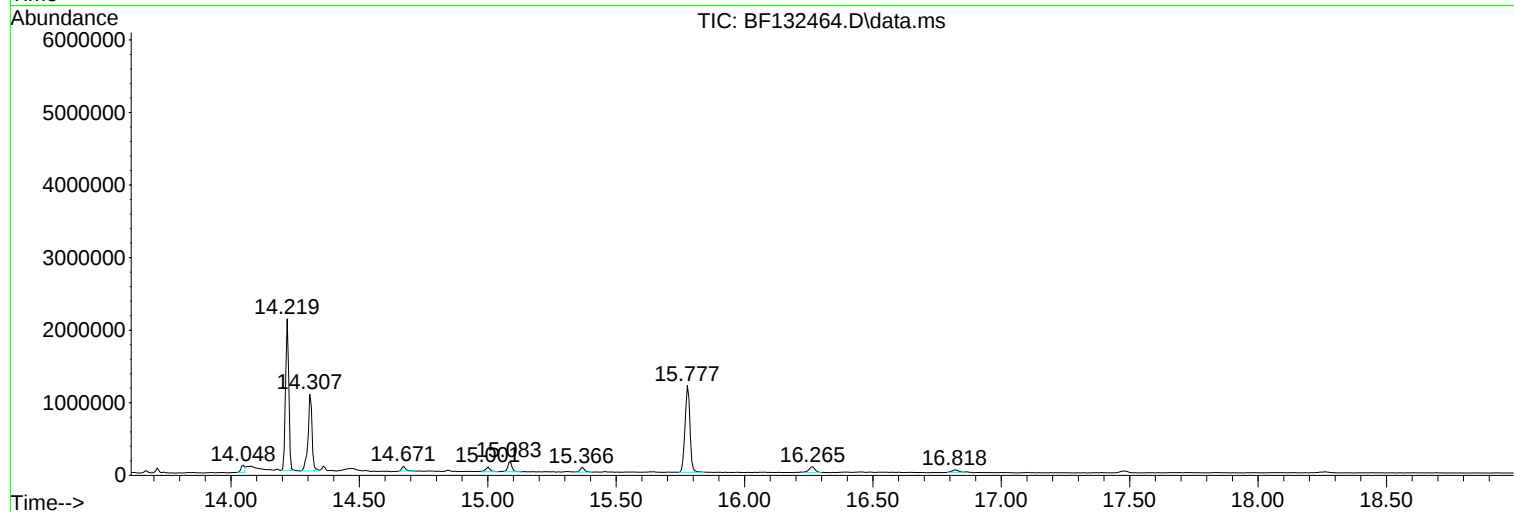
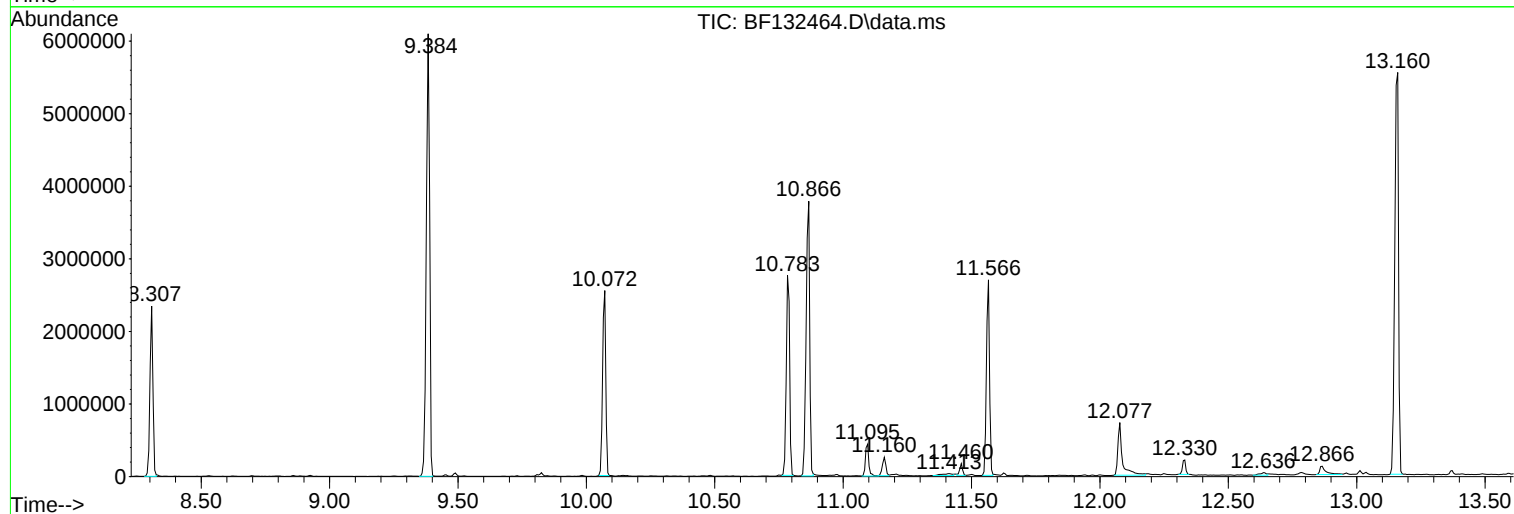
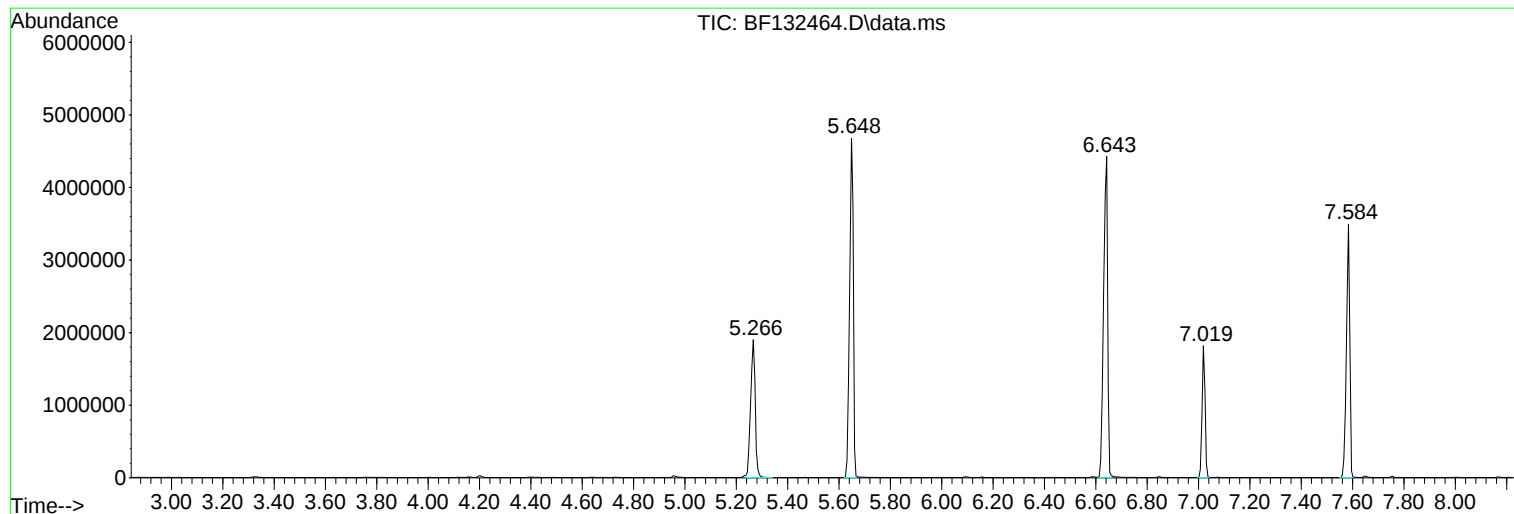
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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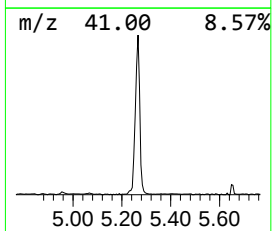
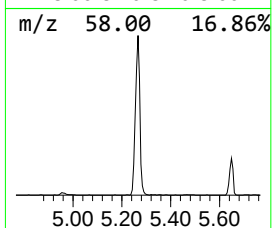
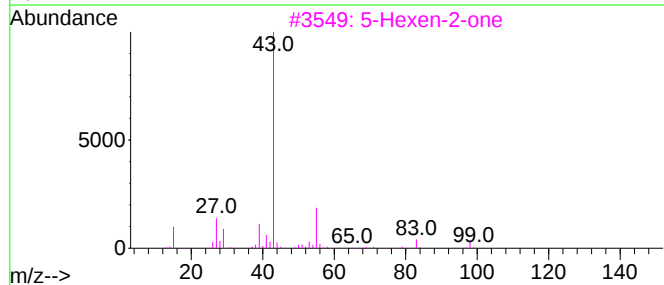
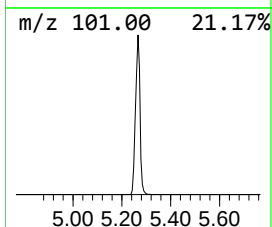
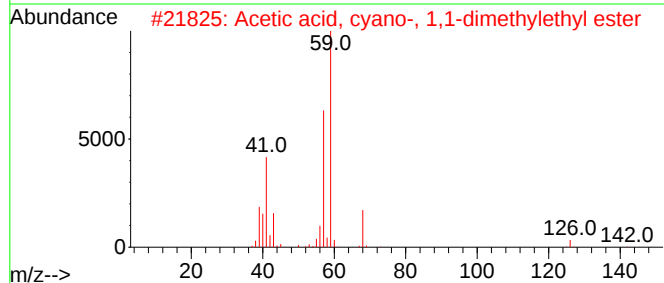
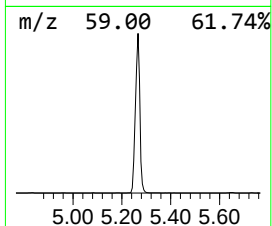
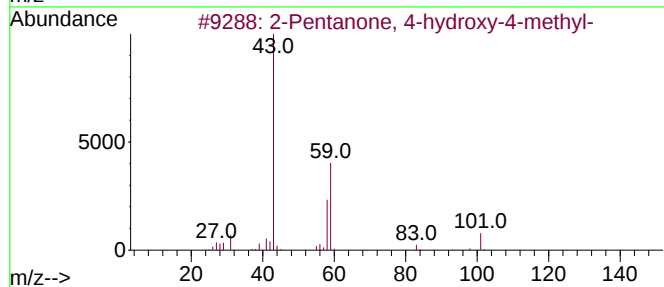
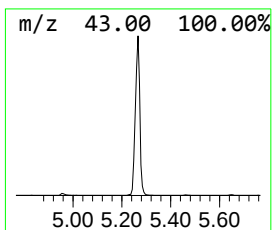
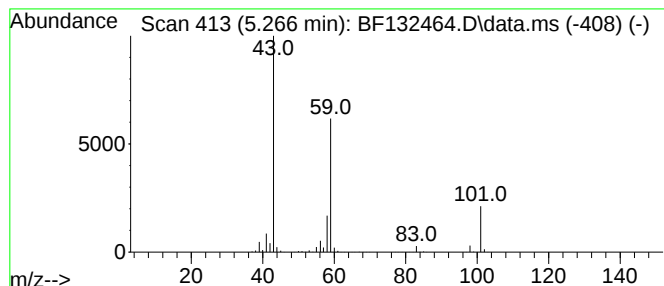
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.266	32.46 ng	2376660	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	Acetone	58	C3H6O	000067-64-1	9		



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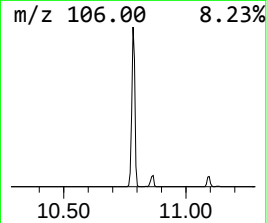
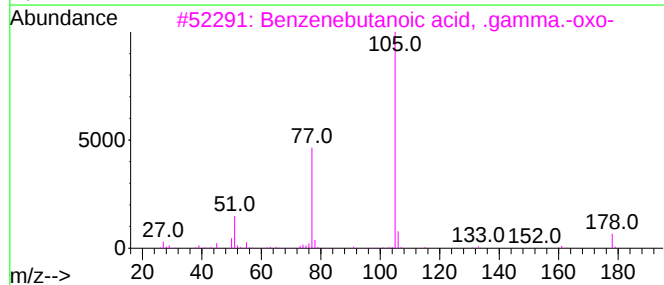
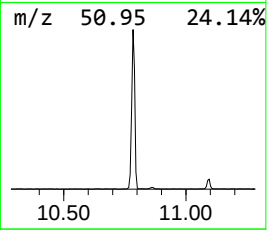
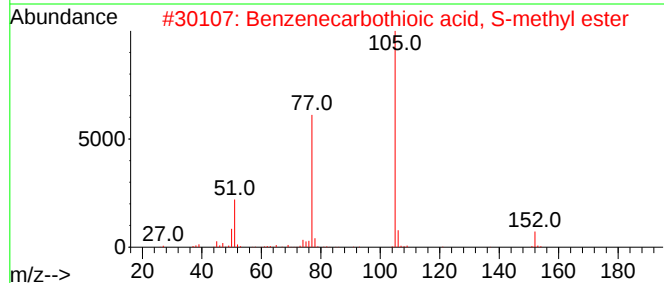
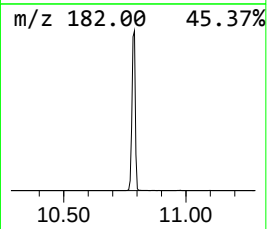
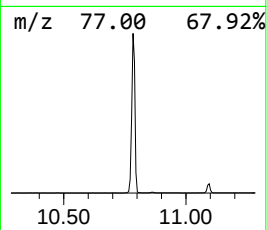
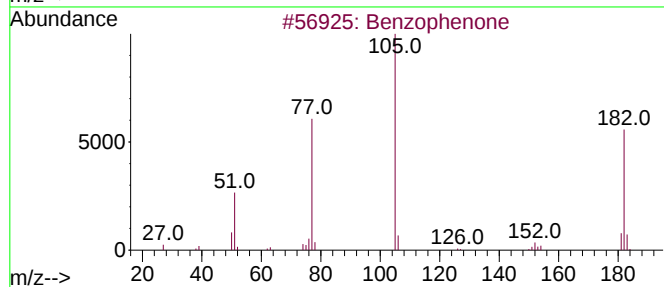
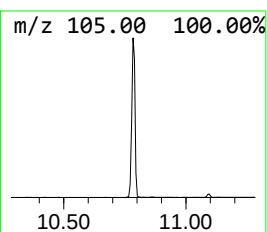
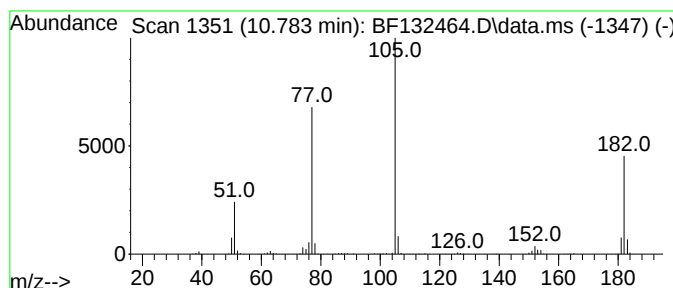
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.784	23.00 ng	2502350	Acenaphthene-d10	10.072

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	50
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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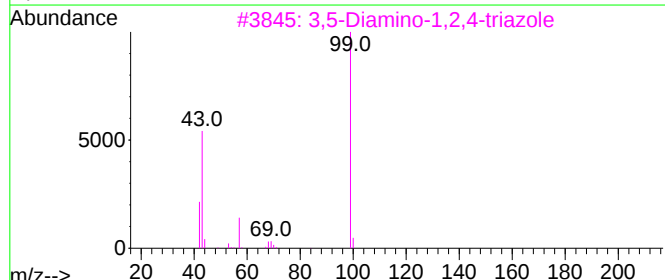
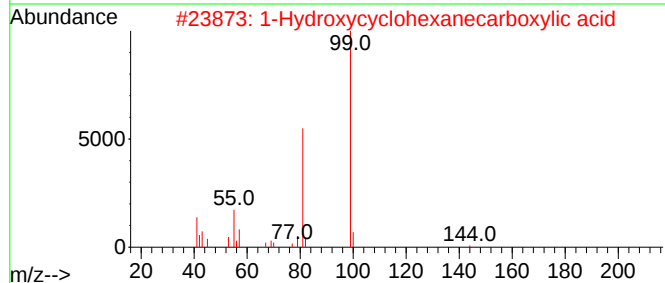
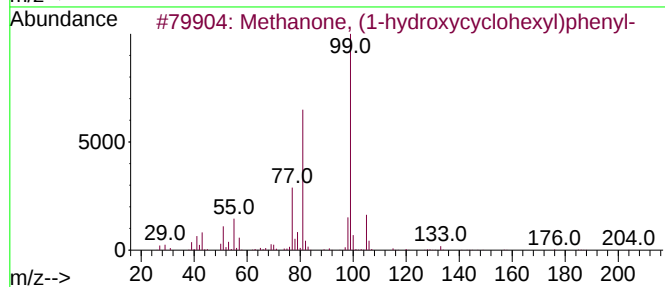
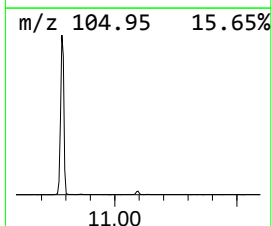
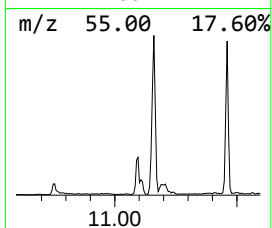
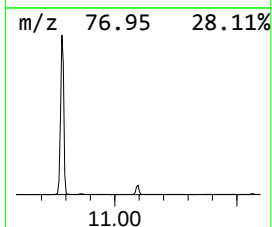
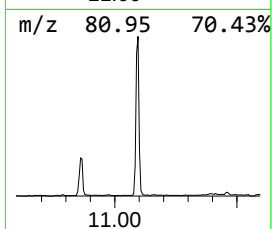
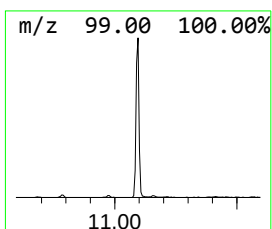
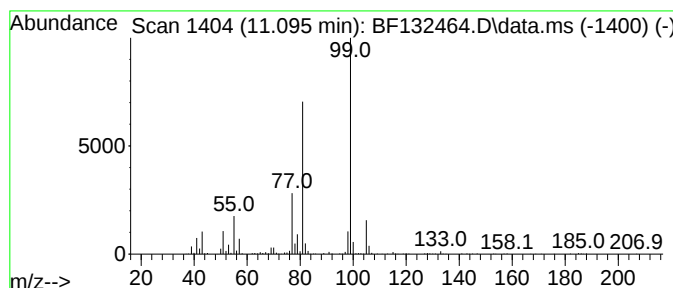
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.095	3.49 ng	402718	Phenanthrene-d10		11.566	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...		204	C13H16O2	000947-19-3	90
2	1-Hydroxycyclohexanecarboxylic acid		144	C7H12O3	001123-28-0	47
3	3,5-Diamino-1,2,4-triazole		99	C2H5N5	001455-77-2	43
4	Isothiazole, 3-methyl-		99	C4H5NS	000693-92-5	37
5	Cholestan-22(26)-isoeopoxy-3.beta...		402	C27H46O2	103099-02-1	25



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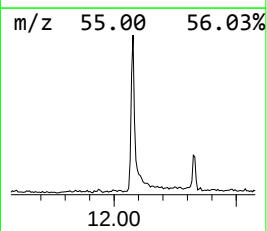
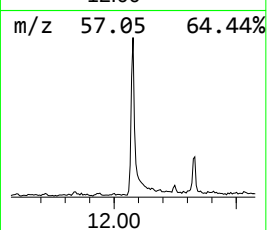
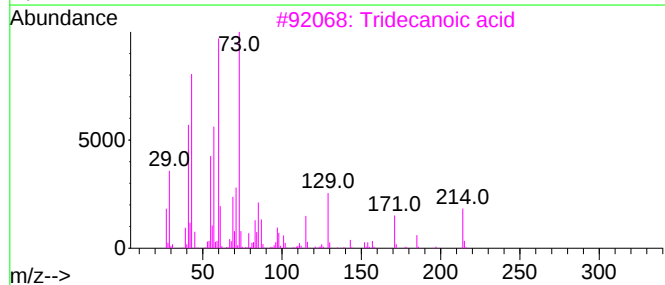
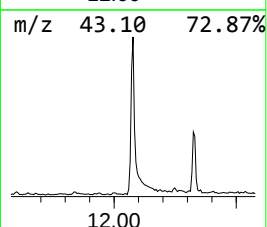
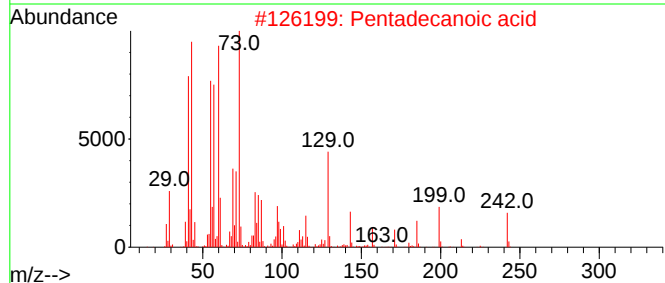
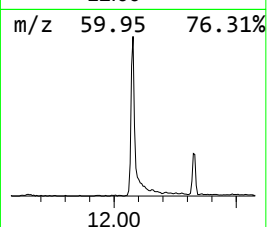
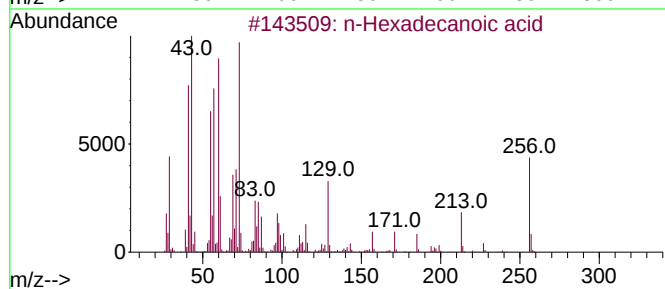
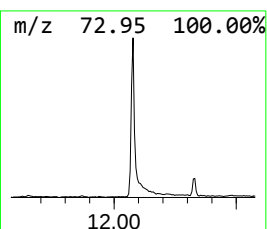
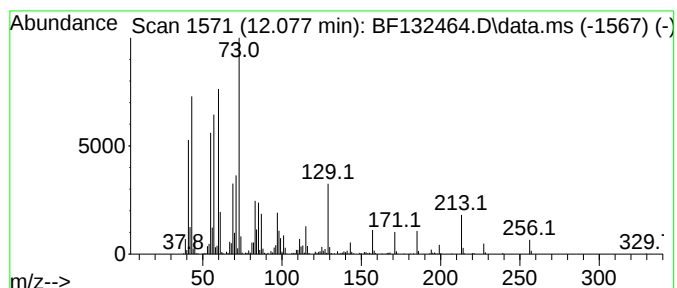
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.078	7.72 ng	890185	Phenanthrene-d10	11.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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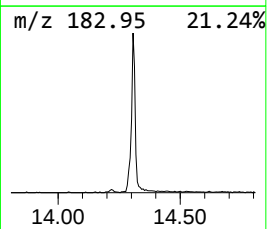
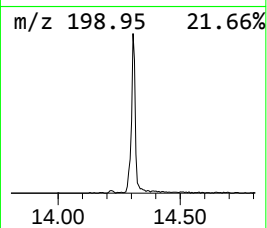
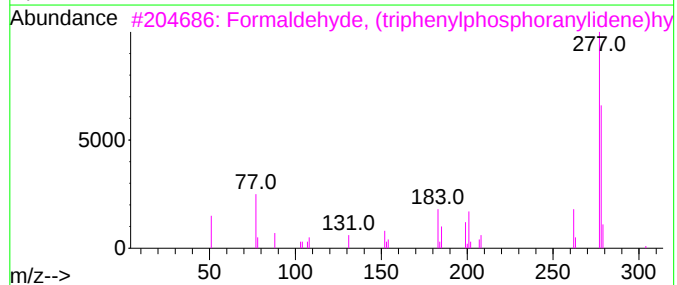
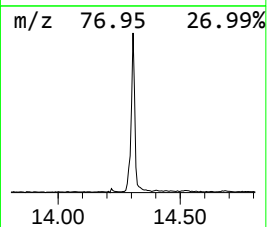
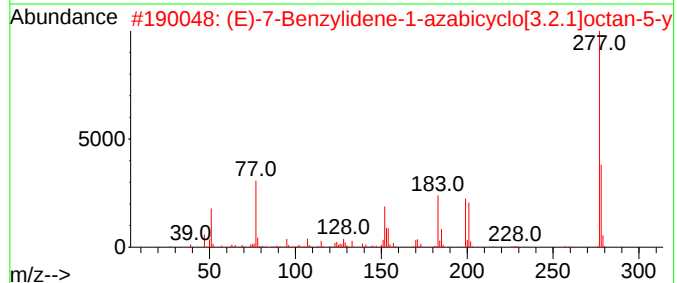
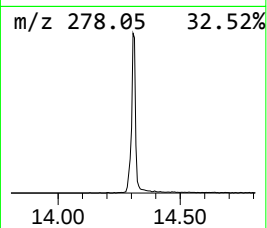
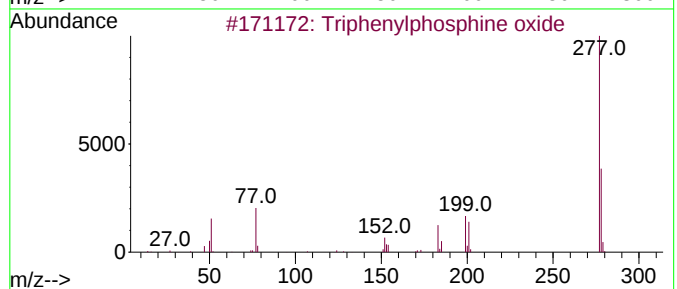
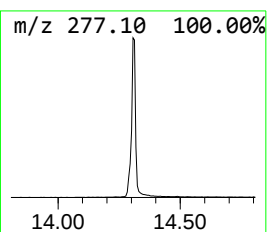
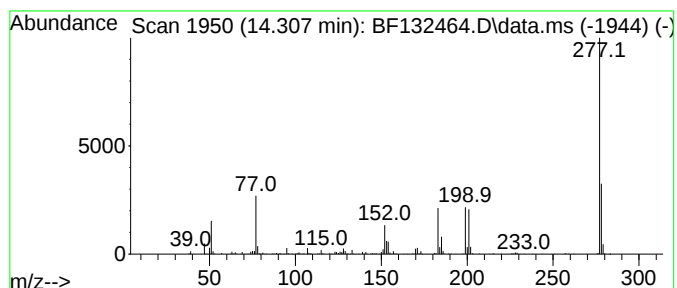
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Peak Number 6 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.307	12.35 ng	1141010	Chrysene-d12	14.219

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	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	46
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37



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ClientSampleId :
S-322-3

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.266	32.5	ng	2376660	1	7.019	1464250	20.0
Benzophenone	10.784	23.0	ng	2502350	3	10.072	2176140	20.0
Methanone, (1-h...	11.095	3.5	ng	402718	4	11.566	2307310	20.0
2-{2-[2-(Acrylo...	11.160	2.1	ng	240255	4	11.566	2307310	20.0
n-Hexadecanoic ...	12.078	7.7	ng	890185	4	11.566	2307310	20.0
Triphenylphosph...	14.307	12.4	ng	1141010	5	14.219	1847710	20.0