

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
 Data File : BF132552.D
 Acq On : 27 Feb 2023 14:54
 Operator : CG\JU
 Sample : 01669-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-08-022323

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.237	403	408	416	rVB	1292249	1545627	48.48%	5.773%
2	5.631	470	475	478	rBV	2796433	2703229	84.78%	10.097%
3	6.019	537	541	547	rBV	42912	39985	1.25%	0.149%
4	6.625	640	644	647	rBV	2872892	2755981	86.44%	10.294%
5	7.001	704	708	712	rBV	1294704	1002947	31.46%	3.746%
6	7.566	799	804	807	rBV	2174258	1834303	57.53%	6.852%
7	8.289	923	927	930	rBV	1509178	1274621	39.98%	4.761%
8	9.366	1106	1110	1113	rBV	3623191	3188493	100.00%	11.910%
9	9.430	1119	1121	1126	rVB	44103	34865	1.09%	0.130%
10	10.048	1223	1226	1230	rVB	1712463	1424297	44.67%	5.320%
11	10.766	1344	1348	1351	rBV	1379205	1174150	36.82%	4.386%
12	10.842	1357	1361	1365	rBV	2269688	1971511	61.83%	7.364%
13	11.072	1397	1400	1404	rBV	156383	124932	3.92%	0.467%
14	11.542	1476	1480	1483	rBV	1515428	1354662	42.49%	5.060%
15	11.566	1483	1484	1488	rVB	80781	55254	1.73%	0.206%
16	12.054	1564	1567	1582	rBV3	281350	331686	10.40%	1.239%
17	12.160	1582	1585	1591	rVB3	25476	44132	1.38%	0.165%
18	12.766	1684	1688	1692	rBV	189426	185652	5.82%	0.693%
19	12.842	1699	1701	1707	rBV4	40039	49846	1.56%	0.186%
20	12.995	1724	1727	1729	rBV	176716	126028	3.95%	0.471%
21	13.136	1746	1751	1754	rBV	2477110	2315800	72.63%	8.650%
22	13.354	1785	1788	1790	rBV	45982	41645	1.31%	0.156%
23	13.695	1843	1846	1848	rBV	58983	50443	1.58%	0.188%
24	14.024	1899	1902	1915	rVB2	166065	302107	9.47%	1.128%
25	14.160	1923	1925	1928	rBV	58083	55784	1.75%	0.208%
26	14.201	1928	1932	1935	rVV	1073584	1038913	32.58%	3.881%
27	14.224	1935	1936	1944	rVB	105947	79833	2.50%	0.298%
28	14.342	1954	1956	1959	rBV	63265	54064	1.70%	0.202%
29	14.654	2006	2009	2012	rBV2	72113	68723	2.16%	0.257%
30	14.983	2062	2065	2068	rVB	48817	47329	1.48%	0.177%
31	15.283	2113	2116	2120	rBV	88466	137159	4.30%	0.512%
32	15.348	2124	2127	2130	rVB	53745	55998	1.76%	0.209%
33	15.618	2170	2173	2178	rVB	58301	71557	2.24%	0.267%
34	15.683	2181	2184	2190	rVV	70050	88873	2.79%	0.332%
35	15.754	2191	2196	2204	rVV	743943	1007062	31.58%	3.762%
36	16.512	2323	2325	2334	rVB4	86941	134506	4.22%	0.502%

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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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

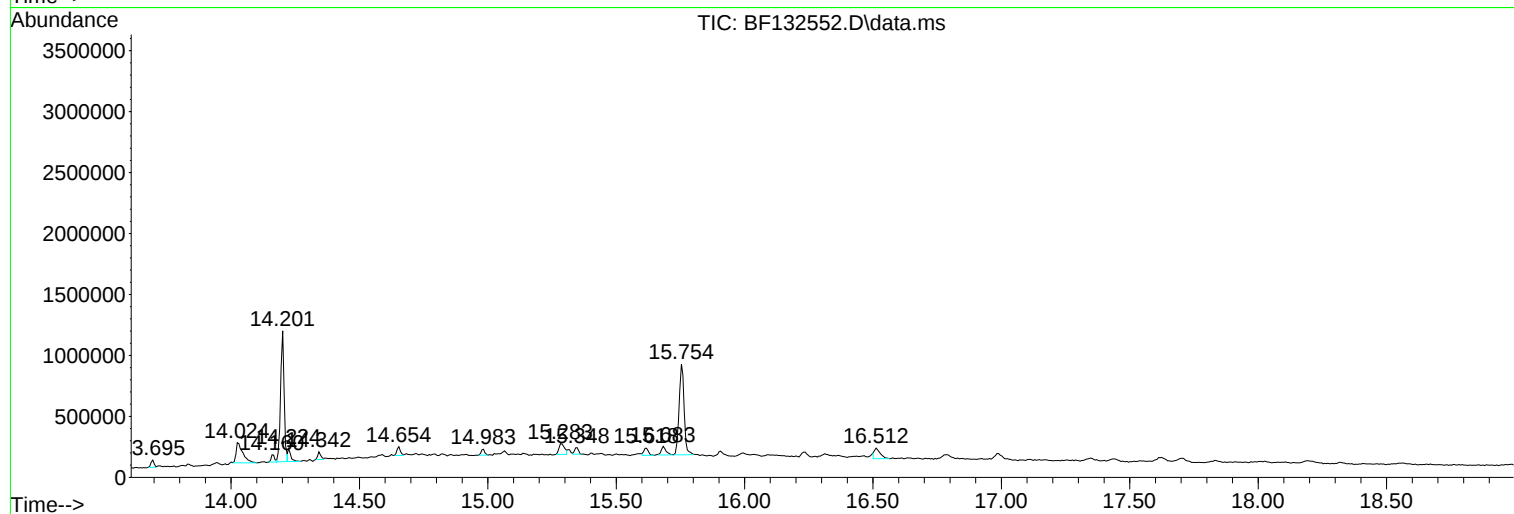
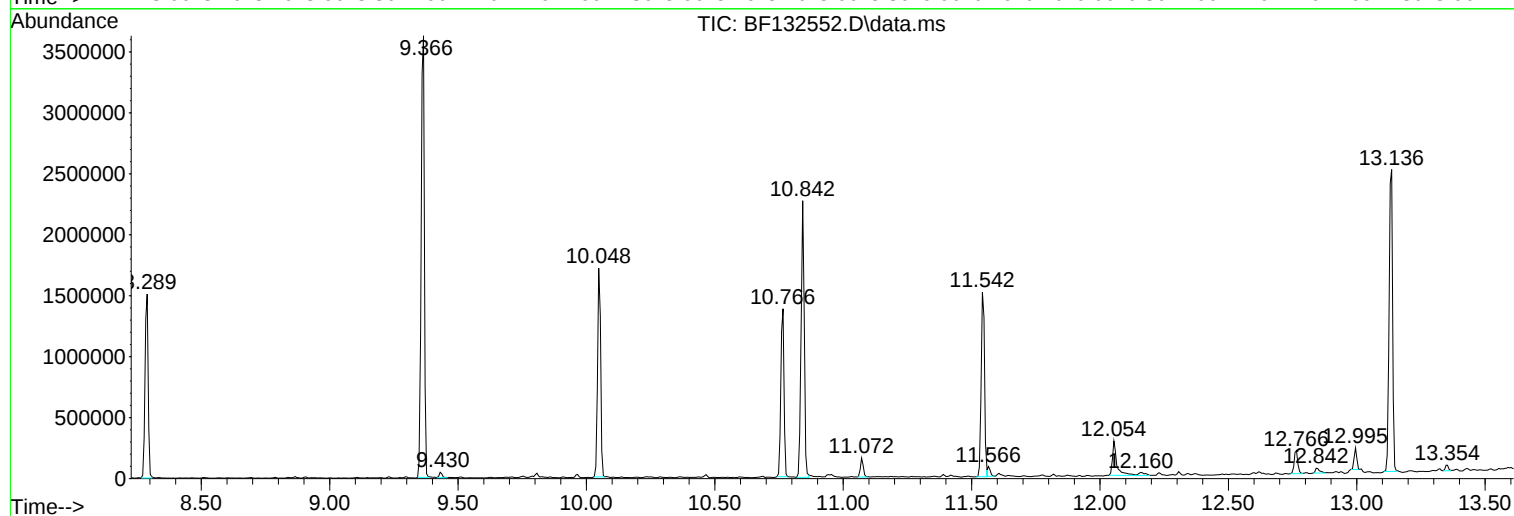
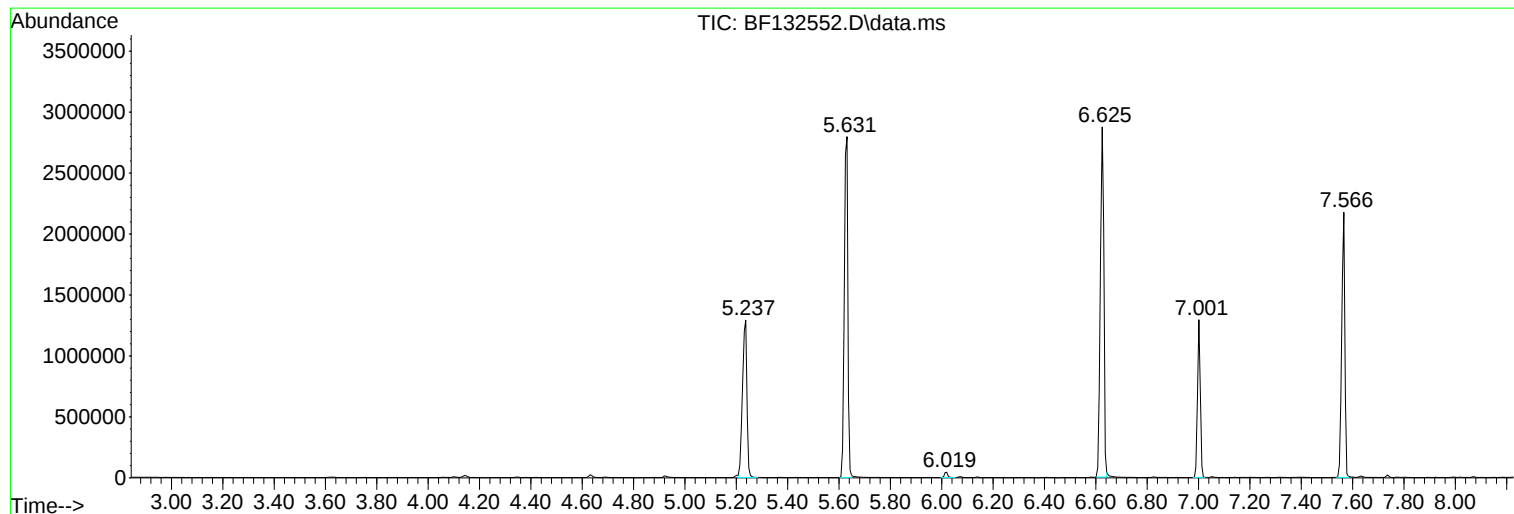
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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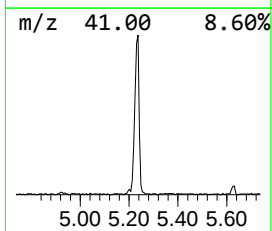
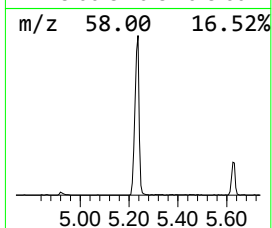
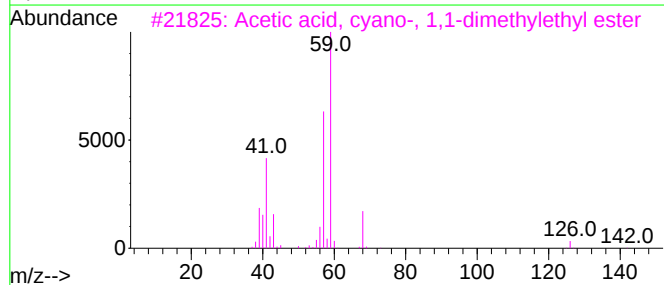
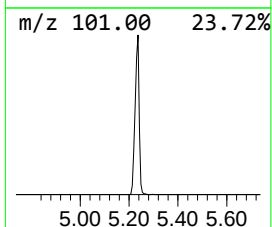
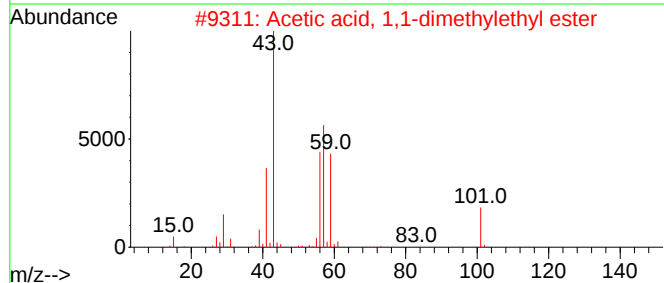
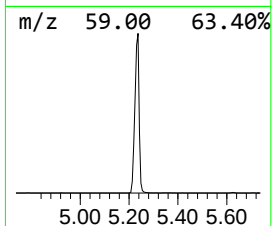
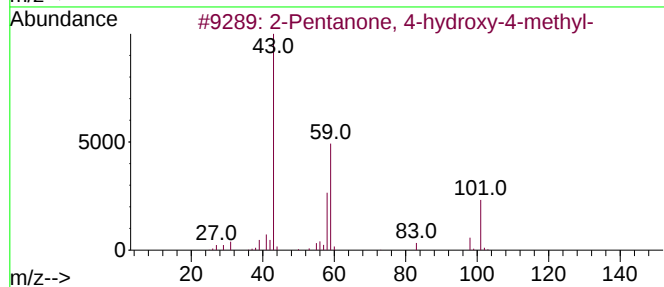
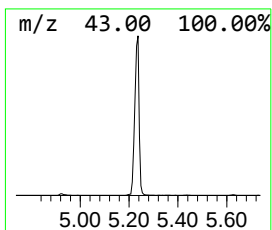
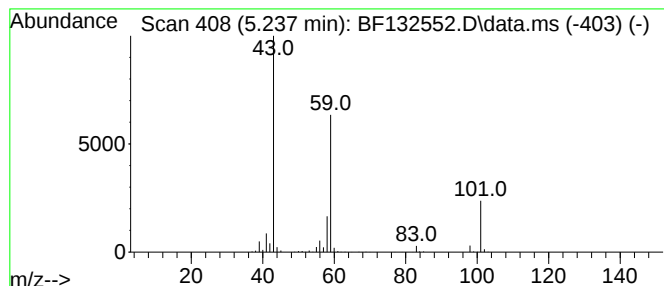
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.237	30.82 ng	1545630	1,4-Dichlorobenzene-d4	7.001	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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Instrument :
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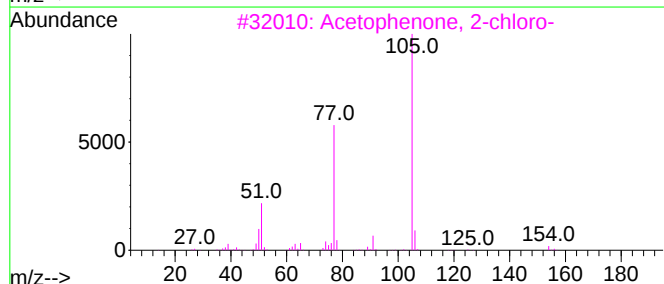
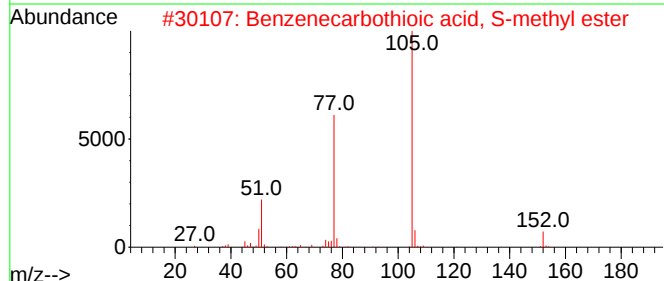
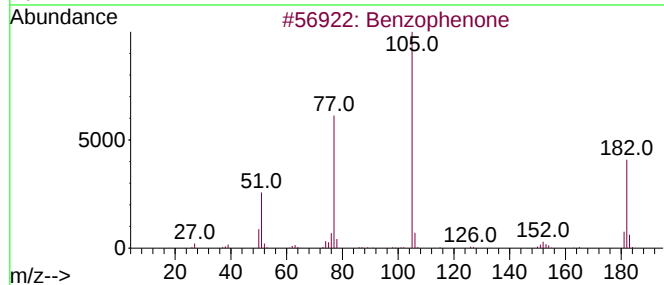
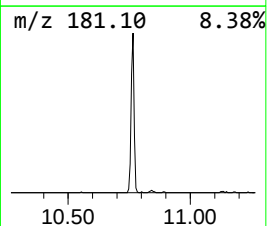
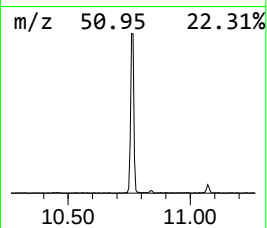
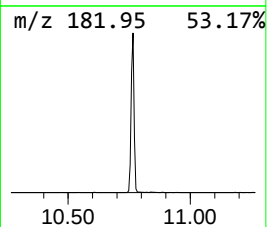
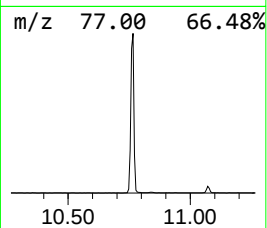
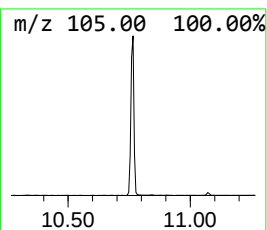
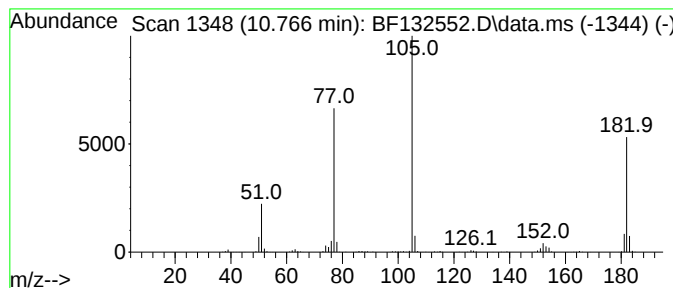
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.766	16.49 ng	1174150	Acenaphthene-d10	10.048

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	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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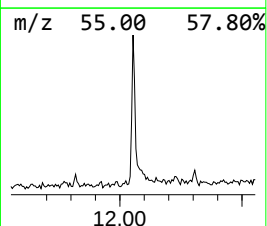
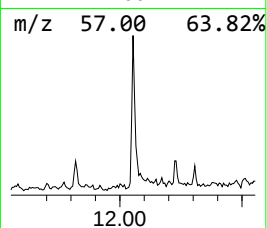
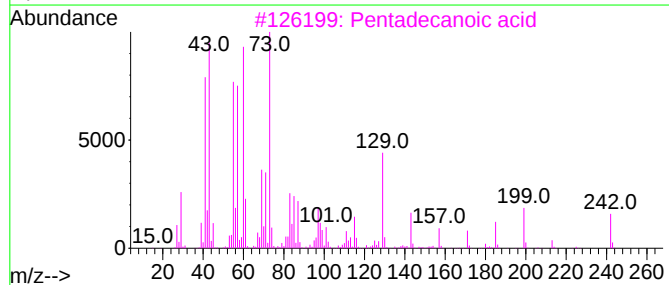
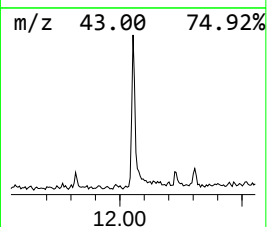
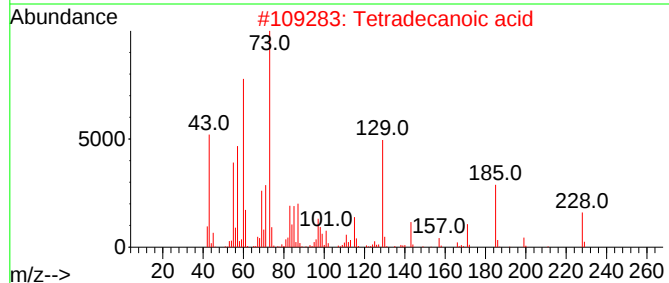
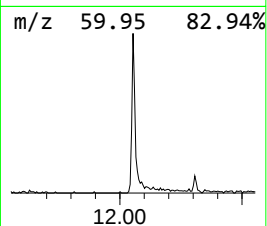
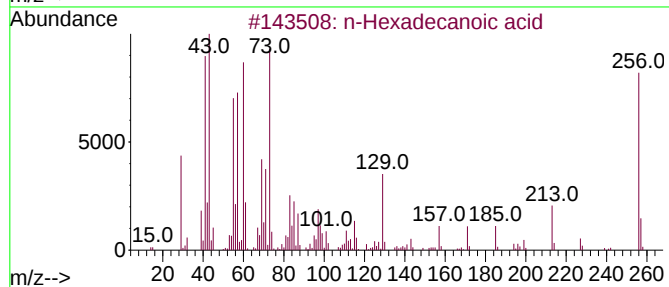
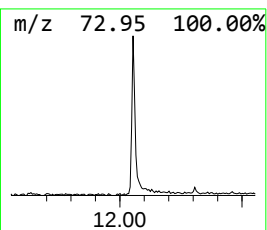
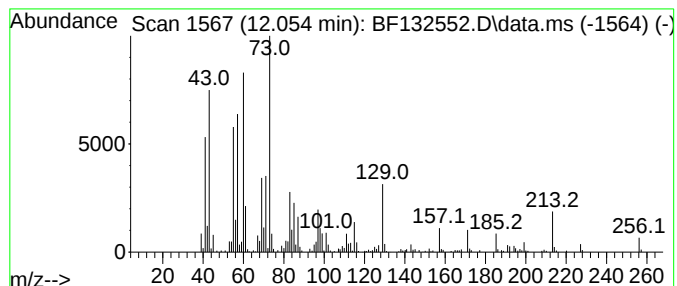
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.054	4.90 ng	331686	Phenanthrene-d10	11.542

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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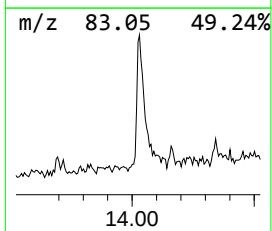
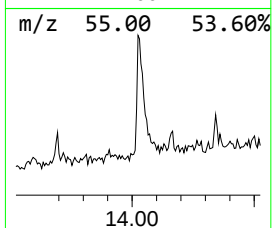
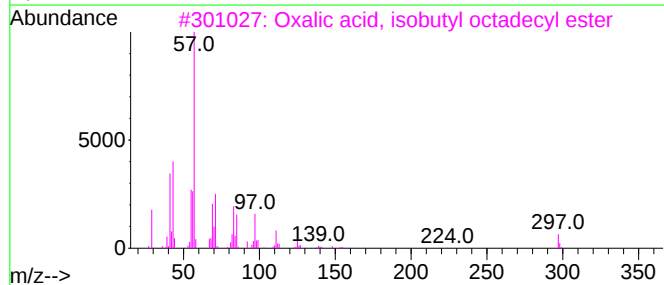
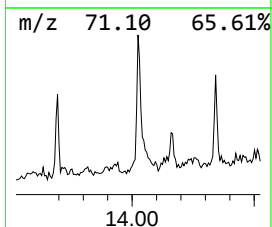
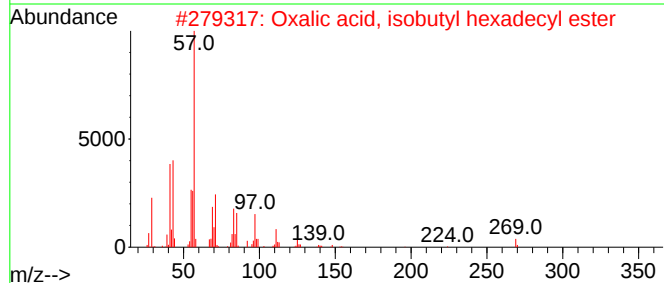
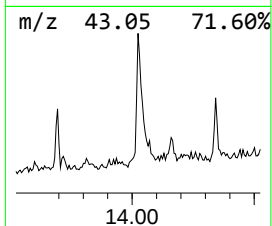
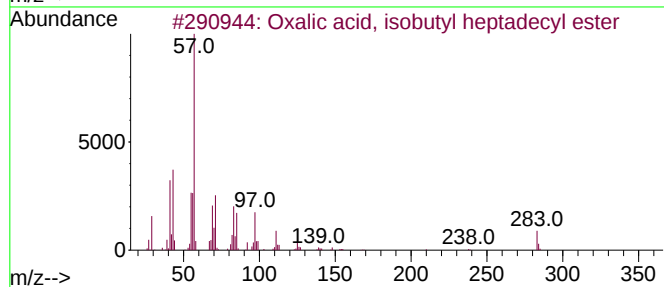
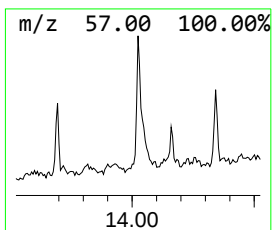
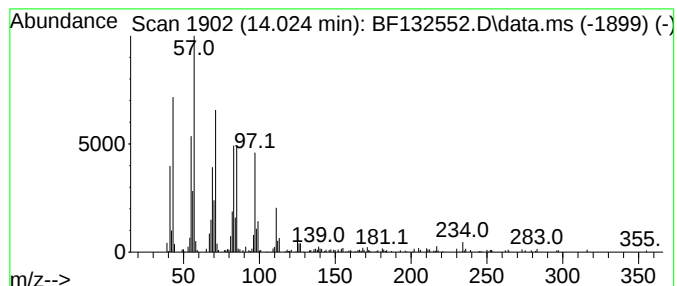
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Oxalic acid, isobutyl hepta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.024	5.82 ng	302107	Chrysene-d12	14.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	90
3			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	90
4			Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	74
5			Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	74



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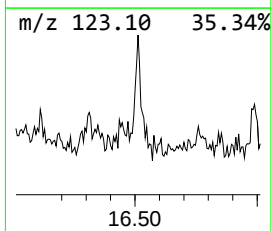
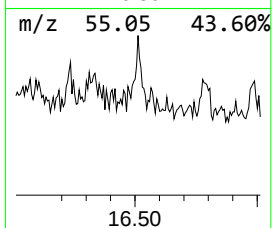
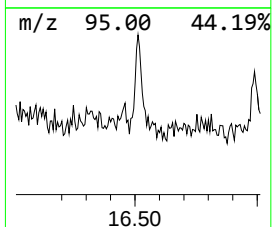
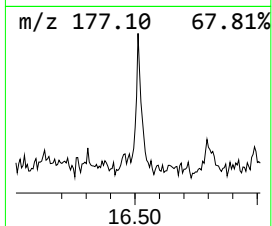
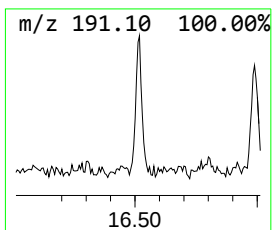
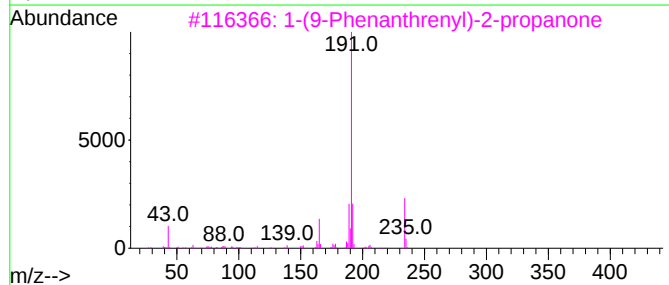
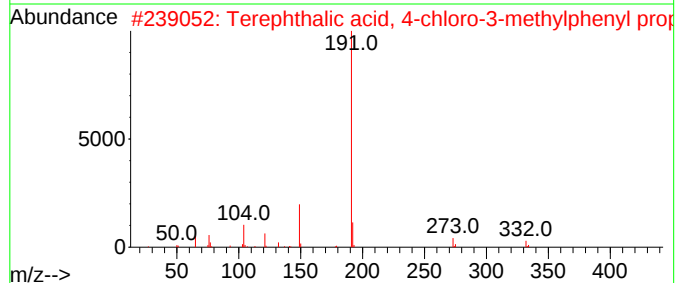
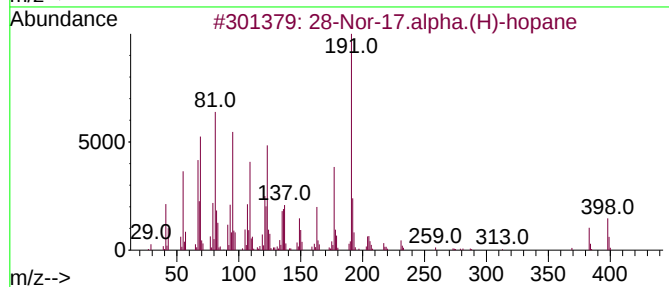
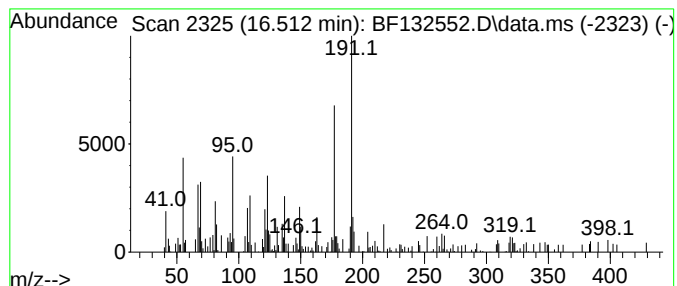
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown16.512 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.512	2.67 ng	134506	Perylene-d12	15.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane		398	C29H50	053584-60-4	41	
2	Terephthalic acid, 4-chloro-3-me...		332	C18H17ClO4	1000323-69-7	38	
3	1-(9-Phenanthrenyl)-2-propanone		234	C17H14O	1000326-08-9	30	
4	2-Amino-4-methyl-6-(2-thienyl)py...		191	C9H9N3S	026963-43-9	30	
5	2-Fluoro-3-trifluoromethylbenzoi...		332	C15H9ClF4O2	1010331-62-3	30	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132552.D
Acq On : 27 Feb 2023 14:54
Operator : CG\JU
Sample : 01669-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-022323

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.237	30.8	ng	1545630	1	7.001	1002950	20.0
Benzophenone	10.766	16.5	ng	1174150	3	10.048	1424300	20.0
n-Hexadecanoic ...	12.054	4.9	ng	331686	4	11.542	1354660	20.0
Oxalic acid, is...	14.024	5.8	ng	302107	5	14.201	1038910	20.0
unknown16.512	16.512	2.7	ng	134506	6	15.754	1007060	20.0