

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133282.D
 Acq On : 06 May 2023 00:59
 Operator : CG\JU
 Sample : 02624-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WZ-2B

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	476	480	492	rVB	462706	550183	16.96%	1.982%
2	5.340	548	553	556	rBV	3207936	2893123	89.18%	10.420%
3	6.369	723	728	731	rBV	3023933	2923516	90.11%	10.529%
4	6.722	785	788	792	rBV	1419631	1112102	34.28%	4.005%
5	7.287	880	884	887	rBV	2178650	1858280	57.28%	6.693%
6	8.010	1003	1007	1010	rBV	1812711	1512106	46.61%	5.446%
7	9.081	1186	1189	1193	rBV	3697667	3244213	100.00%	11.684%
8	9.757	1300	1304	1308	rBV	2001194	1674590	51.62%	6.031%
9	10.469	1422	1425	1429	rBV	624617	512886	15.81%	1.847%
10	10.545	1434	1438	1441	rBV	2288754	1933426	59.60%	6.963%
11	10.669	1456	1459	1466	rVB2	35968	45459	1.40%	0.164%
12	11.239	1552	1556	1559	rBV	2059659	1681780	51.84%	6.057%
13	11.263	1559	1560	1563	rVB	117018	61991	1.91%	0.223%
14	11.775	1643	1647	1656	rBV3	232242	283044	8.72%	1.019%
15	12.339	1737	1743	1746	rVB4	22514	37097	1.14%	0.134%
16	12.445	1758	1761	1767	rBV	105290	110118	3.39%	0.397%
17	12.557	1778	1780	1790	rBV3	50960	91673	2.83%	0.330%
18	12.674	1794	1800	1803	rVV	113828	104039	3.21%	0.375%
19	12.822	1821	1825	1829	rBV	2951925	2878167	88.72%	10.366%
20	13.004	1850	1856	1860	rVB6	21218	37670	1.16%	0.136%
21	13.069	1863	1867	1870	rVB2	43033	45916	1.42%	0.165%
22	13.404	1922	1924	1927	rBV	51045	42624	1.31%	0.154%
23	13.733	1976	1980	1991	rBV	174663	265746	8.19%	0.957%
24	13.869	1999	2003	2007	rBV	1134693	1124915	34.67%	4.051%
25	13.968	2014	2020	2026	rBV	966569	1039564	32.04%	3.744%
26	14.051	2031	2034	2038	rVB	69753	66445	2.05%	0.239%
27	14.357	2082	2086	2089	rBV	78163	88038	2.71%	0.317%
28	14.651	2133	2136	2140	rBV	67037	60463	1.86%	0.218%
29	14.721	2145	2148	2155	rVB2	35581	51845	1.60%	0.187%
30	14.886	2173	2176	2184	rVB	31166	52605	1.62%	0.189%
31	14.974	2187	2191	2196	rBV	79787	99562	3.07%	0.359%
32	15.286	2239	2244	2248	rBV	812818	1007641	31.06%	3.629%
33	15.333	2249	2252	2257	rVB	68042	93430	2.88%	0.336%
34	15.739	2317	2321	2326	rBV2	68831	94358	2.91%	0.340%
35	16.215	2397	2402	2408	rVB2	49001	86823	2.68%	0.313%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

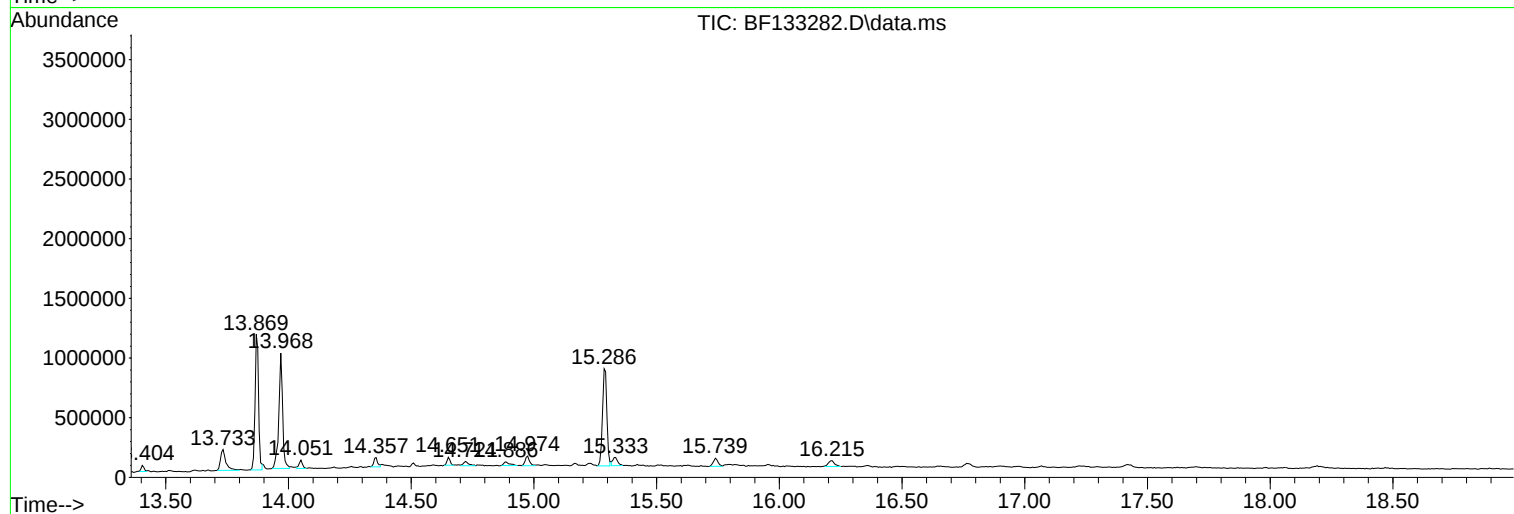
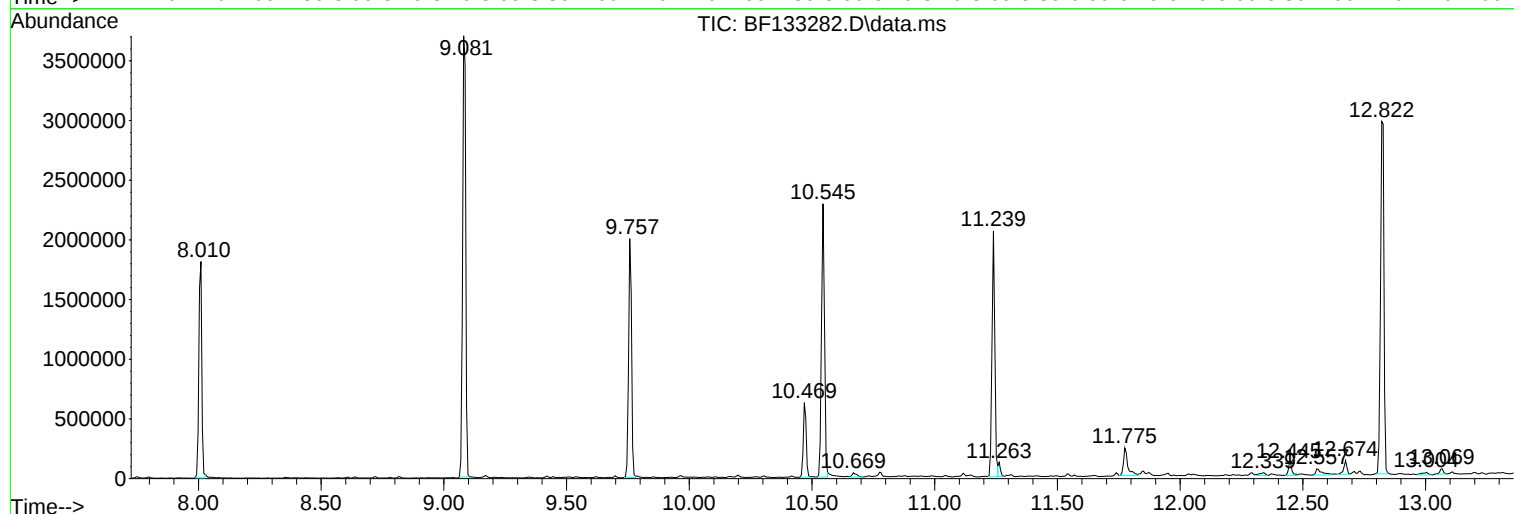
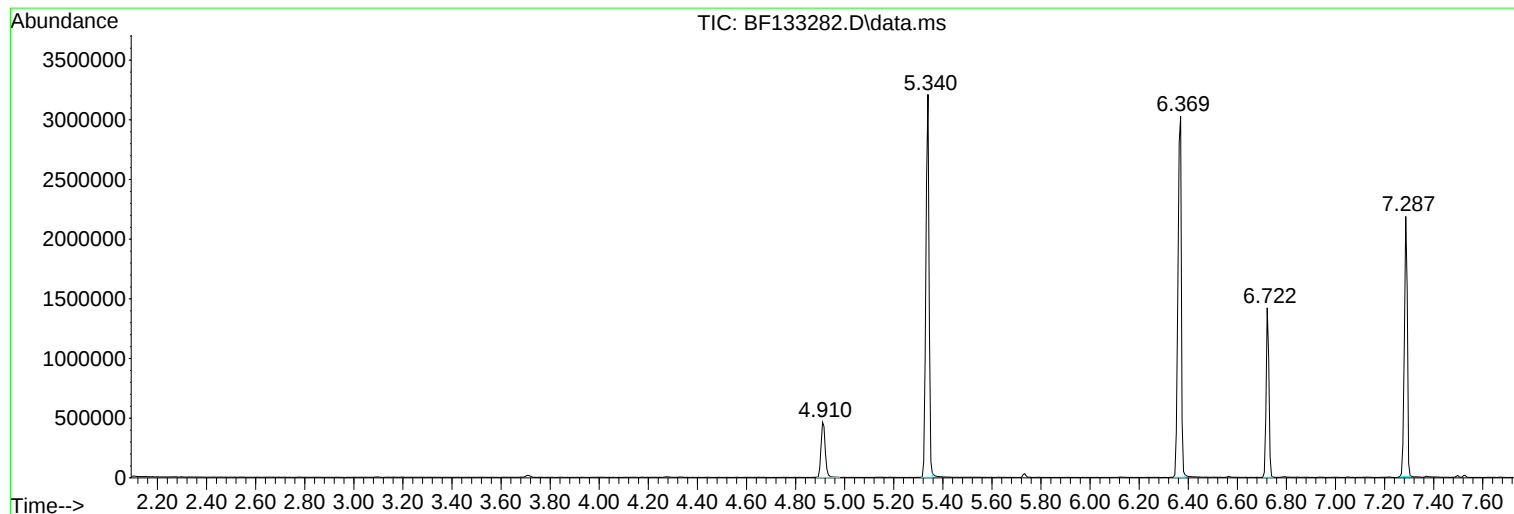
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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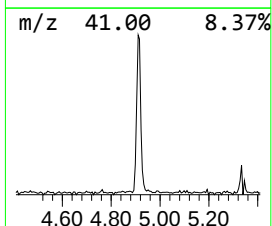
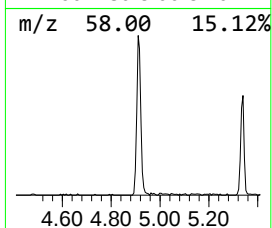
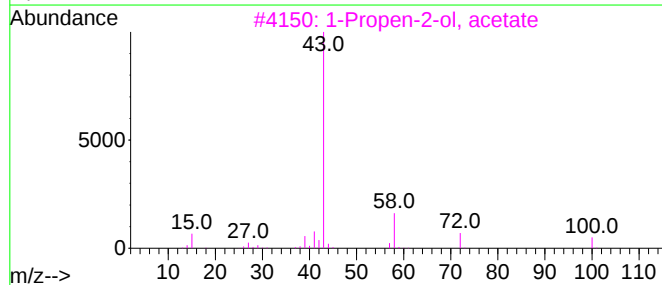
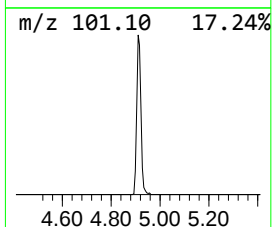
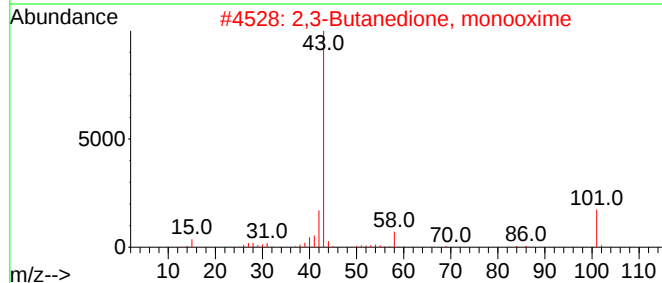
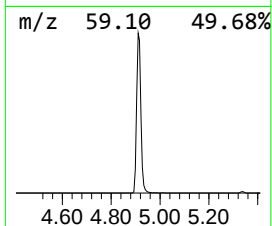
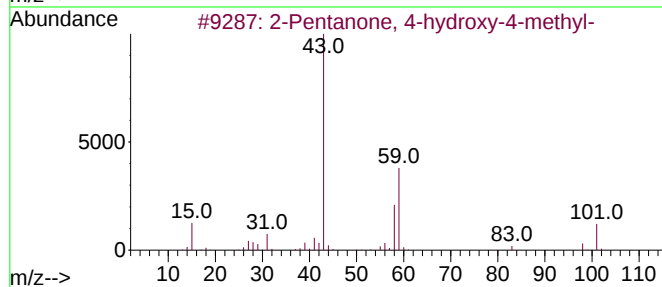
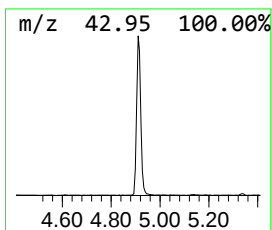
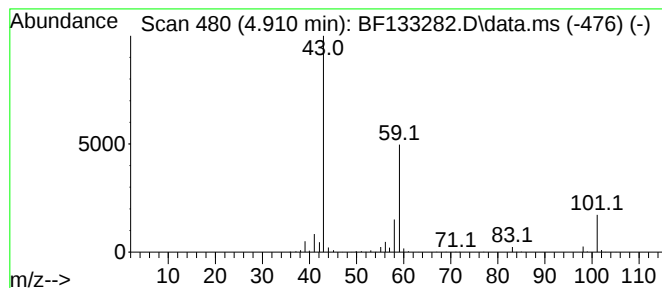
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	9.89 ng	550183	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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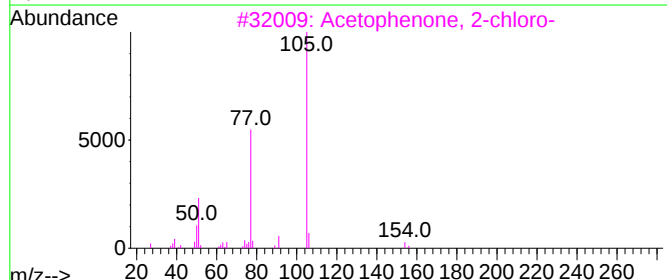
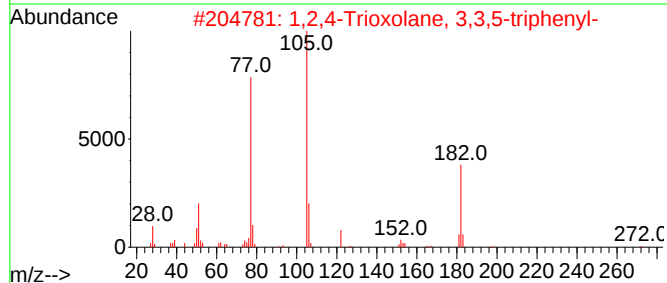
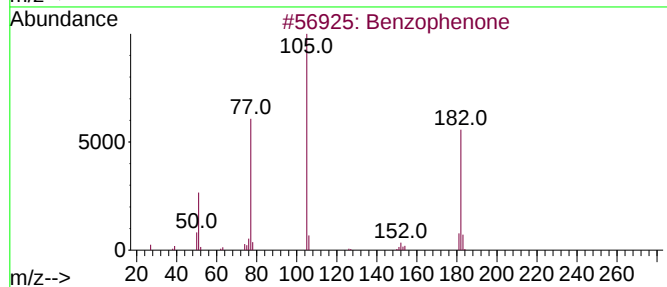
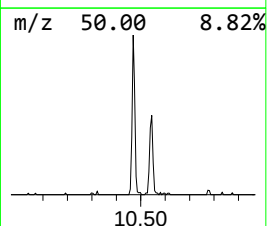
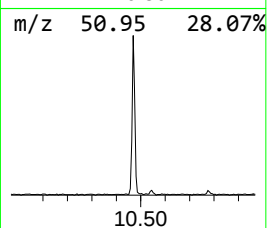
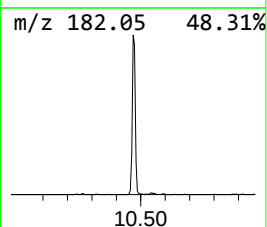
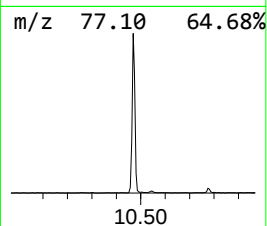
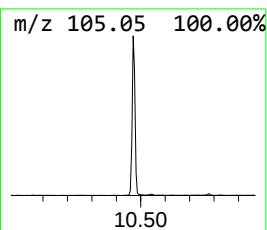
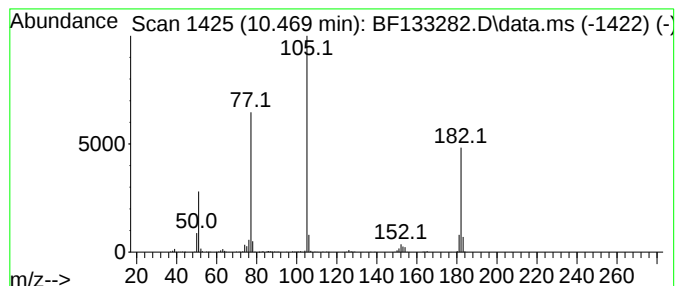
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	6.13 ng	512886	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



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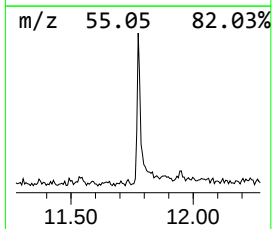
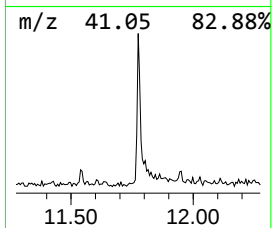
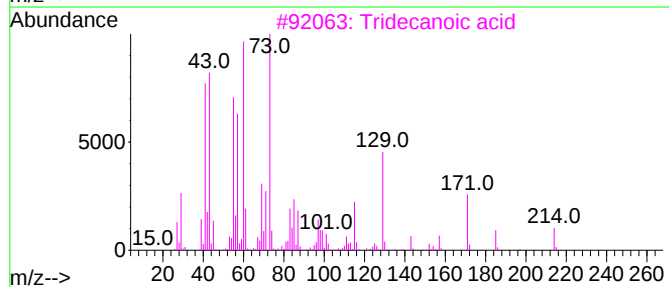
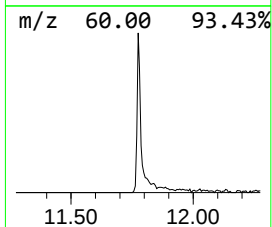
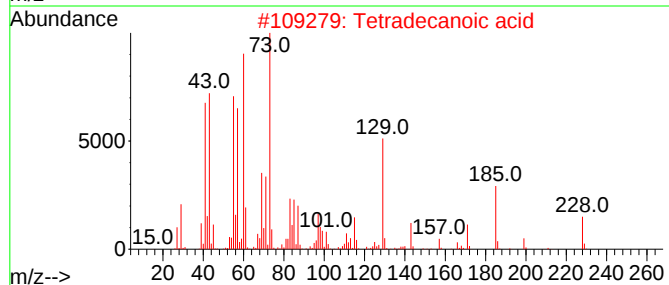
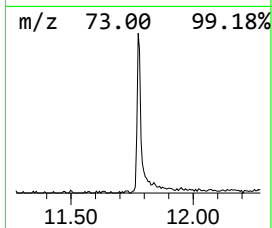
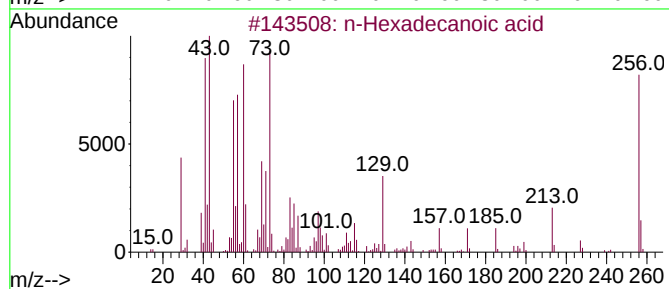
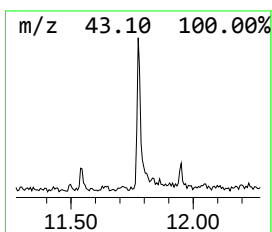
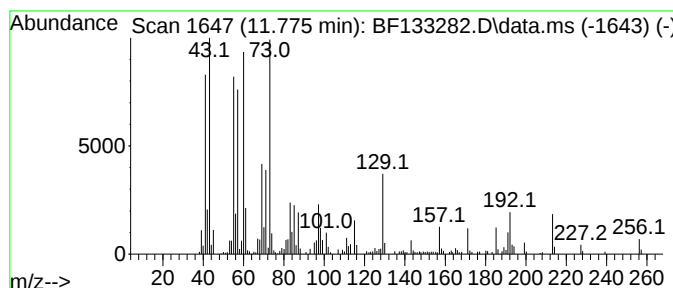
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.775	3.37 ng	283044	Phenanthrene-d10	11.239	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Undecanoic acid	186	C11H22O2	000112-37-8	74



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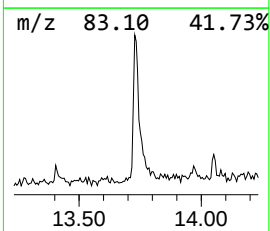
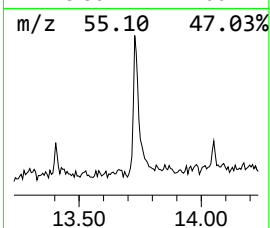
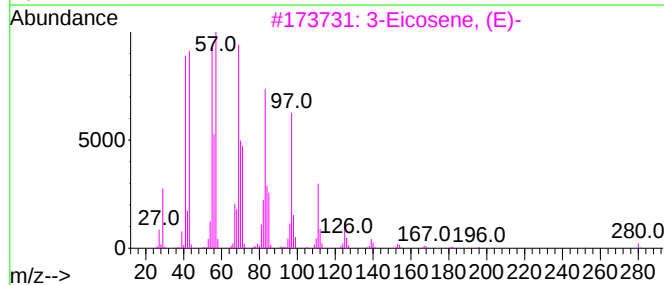
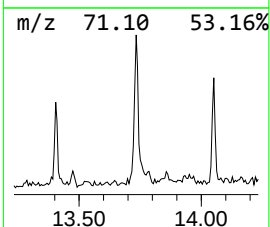
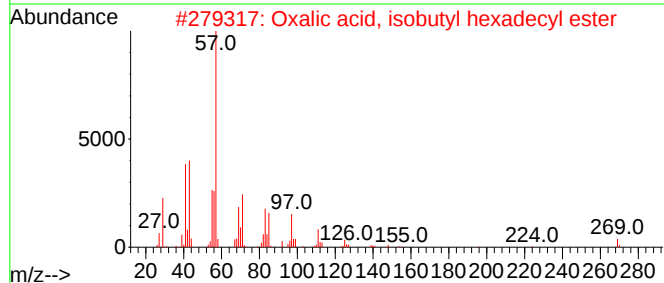
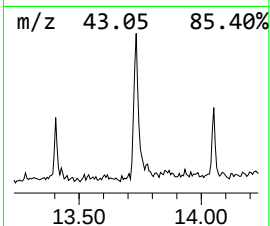
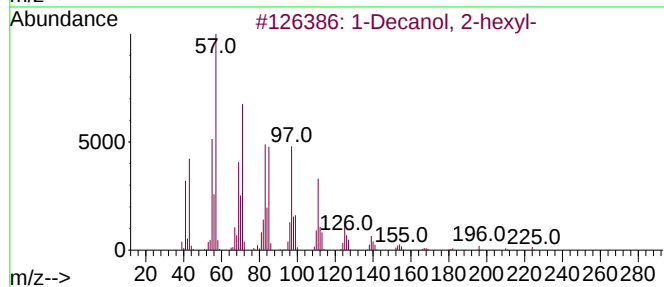
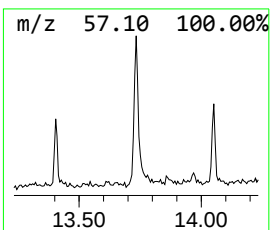
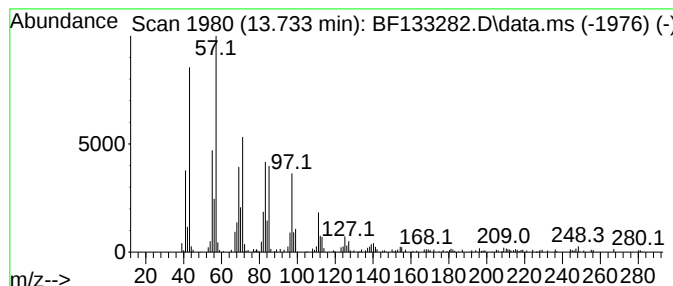
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	4.72 ng	265746	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	91
2	Oxalic acid, isobutyl hexadecyl ...			370	C22H42O4	1000309-38-1	91
3	3-Eicosene, (E)-			280	C20H40	074685-33-9	91
4	Ethanol, 2-(hexadecyloxy)-			286	C18H38O2	002136-71-2	91
5	Triacontyl pentafluoropropionate			584	C33H61F5O2	1000351-80-0	91



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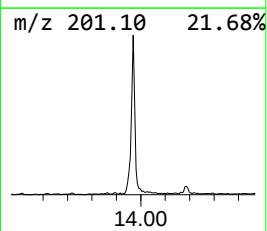
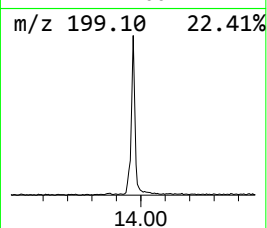
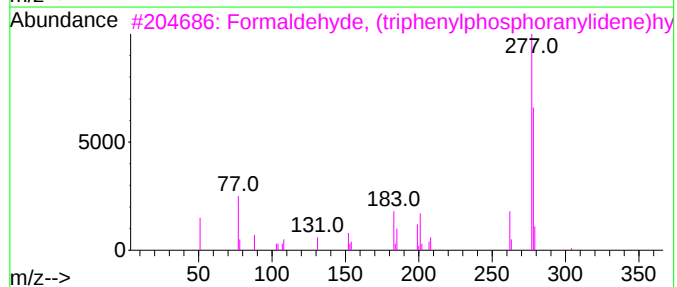
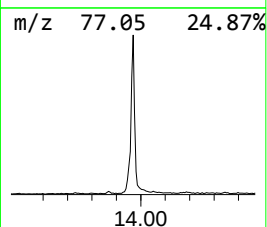
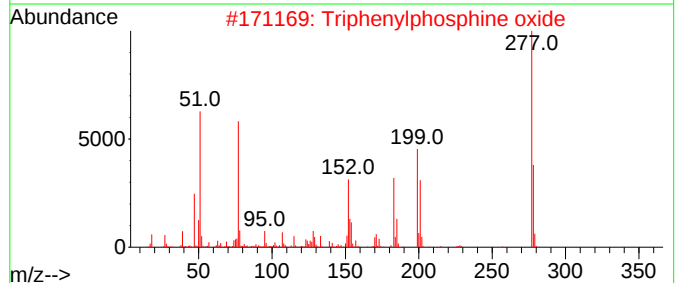
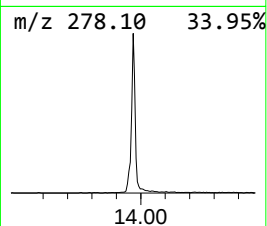
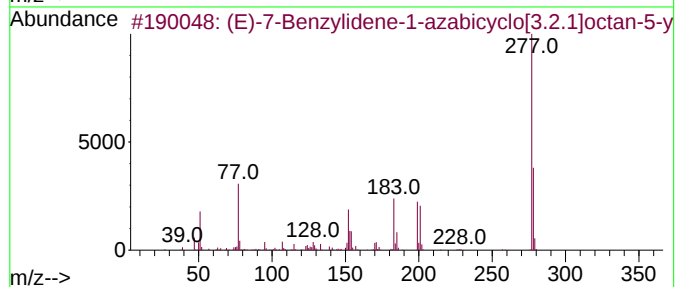
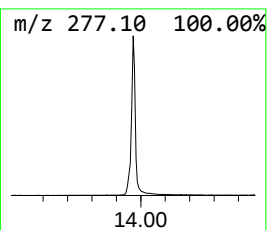
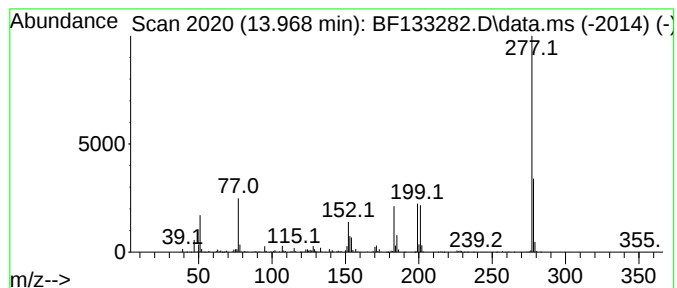
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	18.48 ng	1039560	Chrysene-d12	13.868

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	94		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93		
3	Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	64		
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	25		
5	Oxoprophines	277	C17H11NO3	1000128-51-1	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133282.D
Acq On : 06 May 2023 00:59
Operator : CG\JU
Sample : 02624-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WZ-2B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.910	9.9	ng	550183	1	6.722	1112100	20.0
Benzophenone	10.469	6.1	ng	512886	3	9.757	1674590	20.0
n-Hexadecanoic ...	11.775	3.4	ng	283044	4	11.239	1681780	20.0
1-Decanol, 2-he...	13.733	4.7	ng	265746	5	13.868	1124920	20.0
(E)-7-Benzylide...	13.969	18.5	ng	1039560	5	13.868	1124920	20.0