

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
 Data File : BF133512.D
 Acq On : 26 May 2023 22:09
 Operator : CG\JU
 Sample : 02908-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB10A

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133512.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	10	rVB	330566	336829	12.90%	1.547%
2	2.222	19	23	29	rVB	50361	64457	2.47%	0.296%
3	4.210	356	361	373	rBV3	59707	124178	4.76%	0.570%
4	5.051	499	504	511	rVB	166008	187442	7.18%	0.861%
5	5.445	566	571	575	rBV	2453331	2504191	95.92%	11.504%
6	6.457	738	743	746	rBV	2436097	2533920	97.06%	11.640%
7	6.834	804	807	811	rBV	1003626	824101	31.57%	3.786%
8	7.398	898	903	906	rBV	1937618	1594211	61.07%	7.324%
9	8.122	1022	1026	1029	rBV	1247093	1053977	40.37%	4.842%
10	8.692	1118	1123	1130	rBV4	21789	46052	1.76%	0.212%
11	8.963	1166	1169	1176	rVB	81910	89544	3.43%	0.411%
12	9.198	1205	1209	1212	rVB	3094930	2610604	100.00%	11.993%
13	9.875	1320	1324	1327	rBV	1386458	1081272	41.42%	4.967%
14	10.527	1432	1435	1439	rBV	54960	49266	1.89%	0.226%
15	10.586	1442	1445	1449	rBV	312266	239528	9.18%	1.100%
16	10.663	1453	1458	1461	rBV	1809365	1704415	65.29%	7.830%
17	11.363	1573	1577	1579	rBV	1239907	1132081	43.36%	5.201%
18	11.892	1663	1667	1671	rBV	250640	232572	8.91%	1.068%
19	12.569	1777	1782	1786	rBV	155089	149083	5.71%	0.685%
20	12.674	1796	1800	1806	rBV4	50526	61137	2.34%	0.281%
21	12.798	1815	1821	1824	rBV	147527	144690	5.54%	0.665%
22	12.951	1843	1847	1850	rBV	2649763	2292299	87.81%	10.530%
23	13.857	1996	2001	2017	rBV2	119861	211722	8.11%	0.973%
24	13.998	2020	2025	2028	rVV	873075	893557	34.23%	4.105%
25	14.027	2028	2030	2035	rVB	61589	56265	2.16%	0.258%
26	14.480	2104	2107	2109	rBV2	37696	33645	1.29%	0.155%
27	14.792	2153	2160	2167	rBV2	34384	53558	2.05%	0.246%
28	15.033	2196	2201	2204	rBV2	62703	98870	3.79%	0.454%
29	15.127	2213	2217	2222	rBV3	39164	55471	2.12%	0.255%
30	15.333	2248	2252	2257	rVB	40386	48566	1.86%	0.223%
31	15.392	2258	2262	2267	rVV	60883	74247	2.84%	0.341%
32	15.457	2268	2273	2278	rVV	621676	758159	29.04%	3.483%
33	15.510	2279	2282	2292	rVB	41111	60570	2.32%	0.278%
34	15.757	2320	2324	2331	rBV	42490	72837	2.79%	0.335%
35	15.945	2353	2356	2361	rVB2	35171	47153	1.81%	0.217%
36	16.457	2437	2443	2449	rBV2	26163	52245	2.00%	0.240%

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Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.898	2514	2518	2526	rVB2	25495	48350	1.85%	0.222%
38	17.056	2539	2545	2552	rBV7	16093	41784	1.60%	0.192%
39	17.339	2588	2593	2600	rVB2	21766	41765	1.60%	0.192%
40	17.545	2620	2628	2630	rBV9	25503	63769	2.44%	0.293%

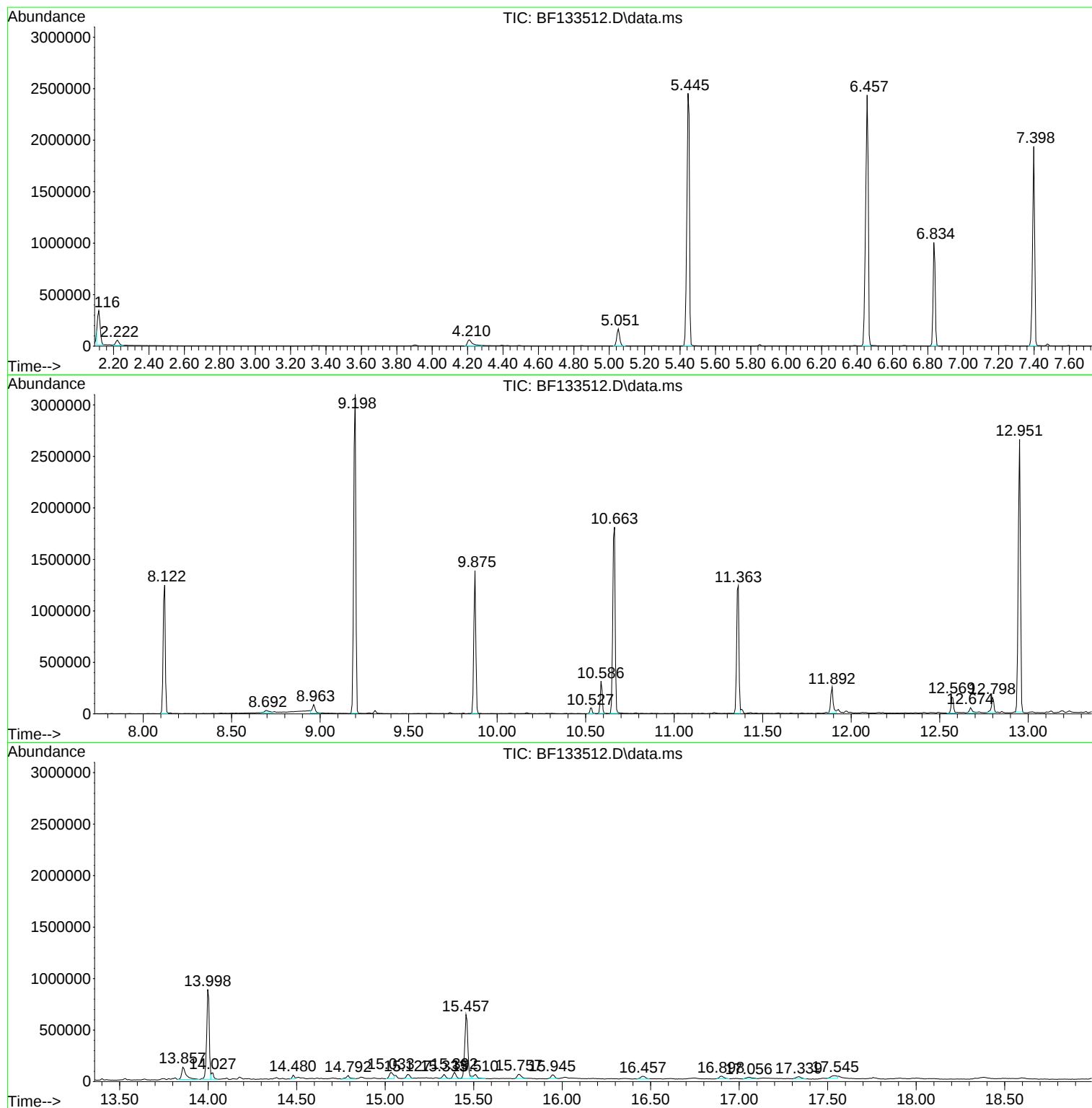
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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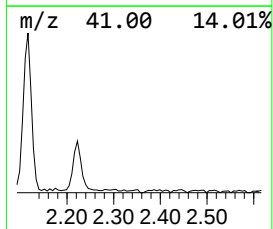
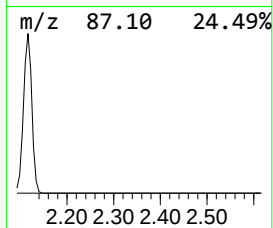
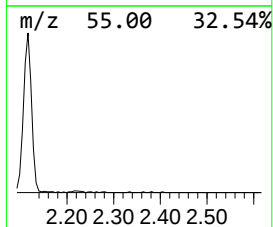
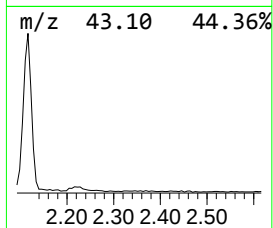
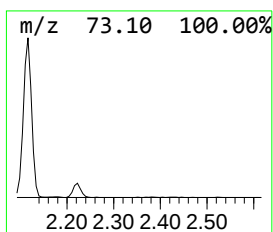
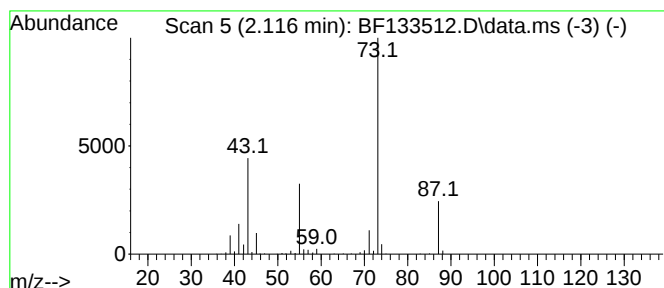
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	8.17 ng	336829	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23



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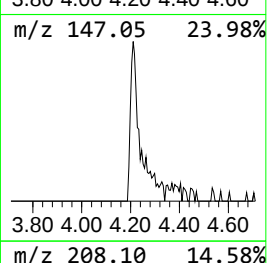
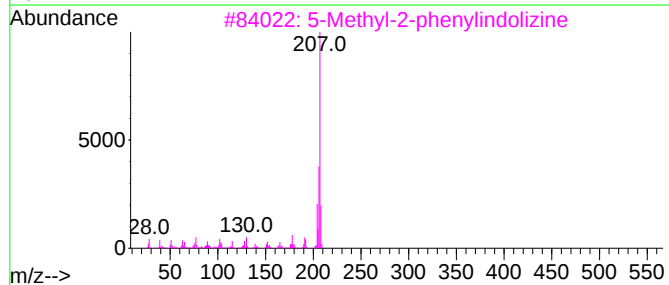
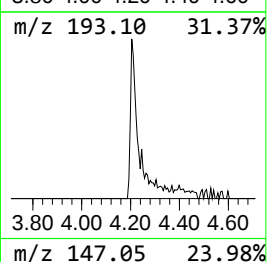
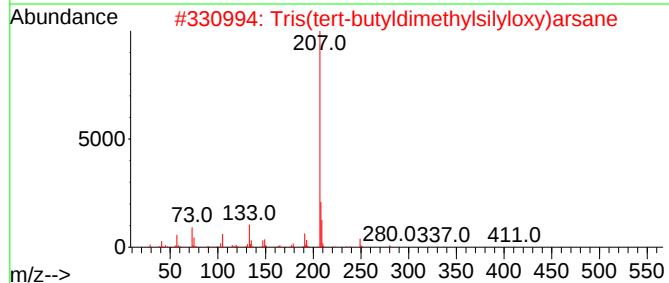
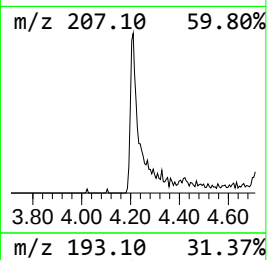
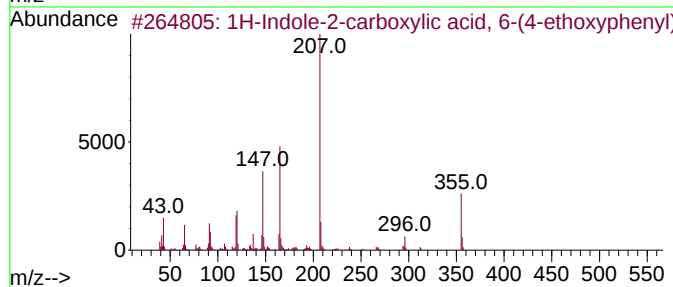
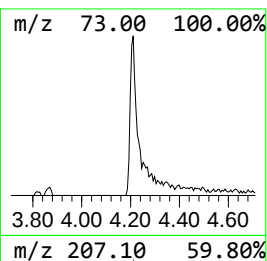
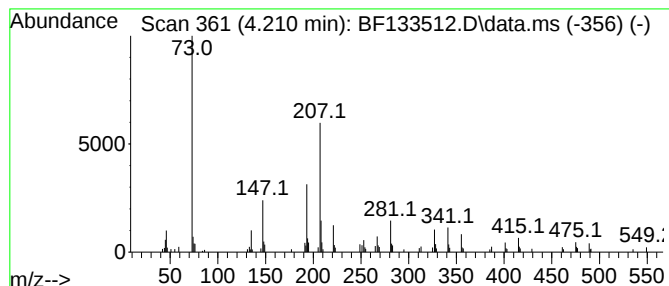
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown4.210 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.210	3.01 ng	124178	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole-2-carboxylic acid, 6-(...	355	C21H25NO4	1010316-17-5	27
2			Tris(tert-butyldimethylsilyloxy)...	468	C18H45AsO3Si3	1000366-57-5	27
3			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	27
4			N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	27
5			N-(2-Hydroxyethyl)-N'-(2-methoxy...	354	C16H30N2O3Si2	1000501-33-3	27



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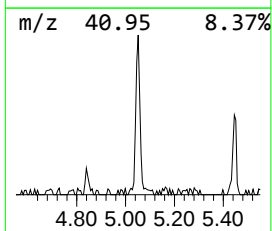
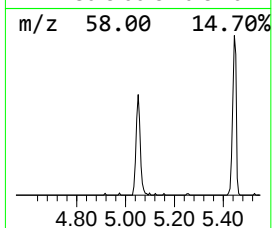
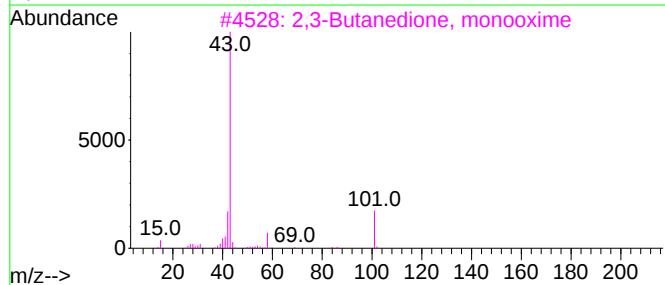
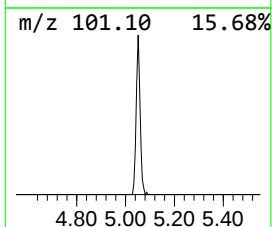
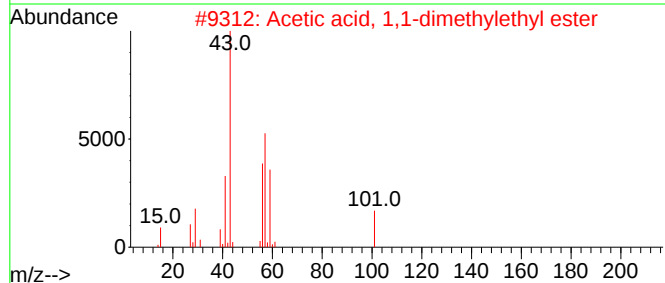
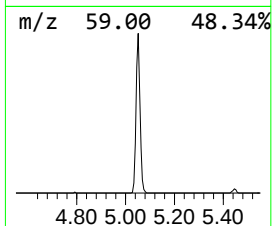
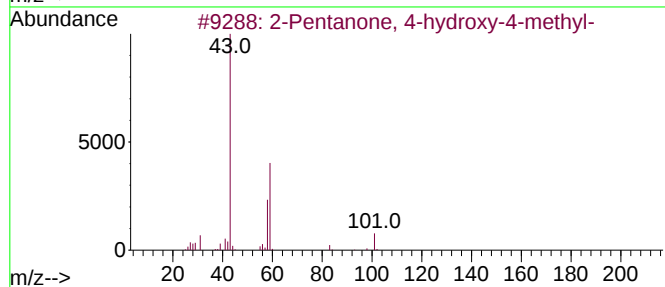
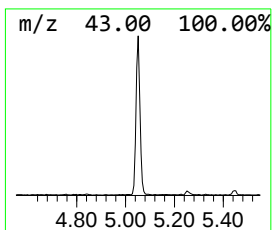
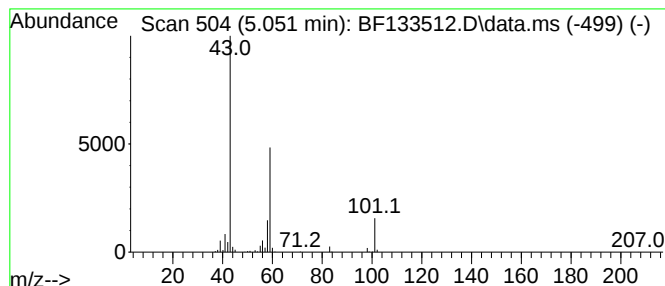
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	4.55 ng	187442	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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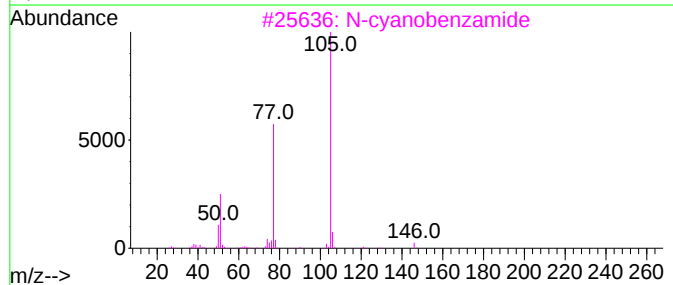
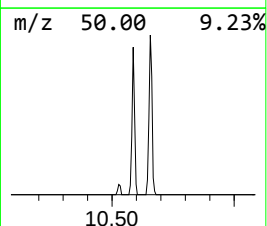
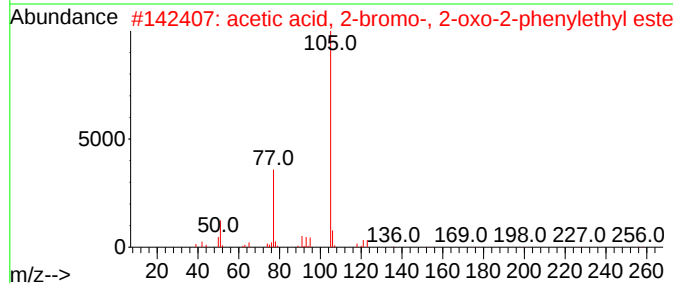
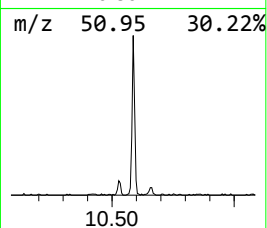
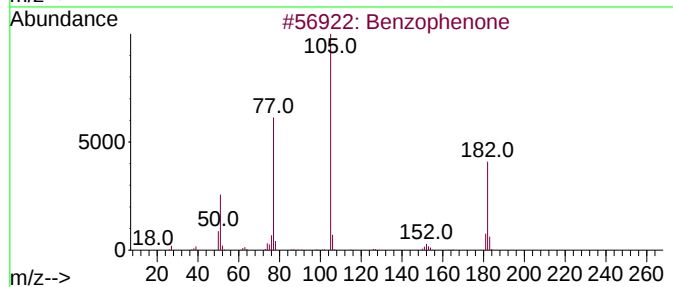
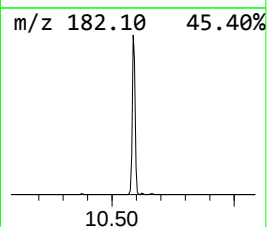
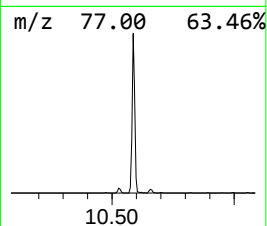
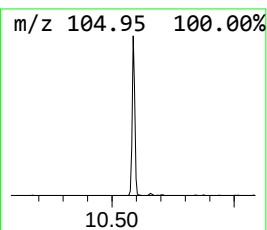
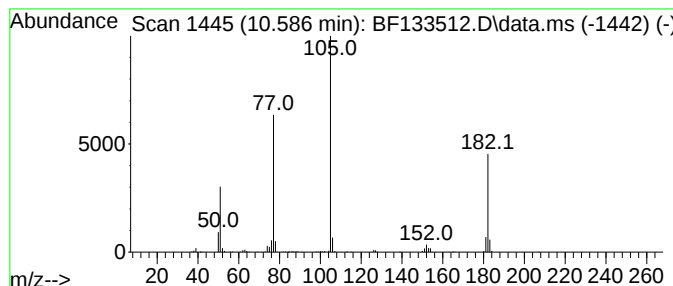
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	4.43 ng	239528	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
3			N-cyanobenzamide	146	C8H6N2O	015150-25-1	50
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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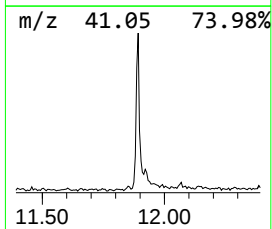
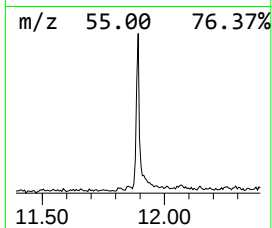
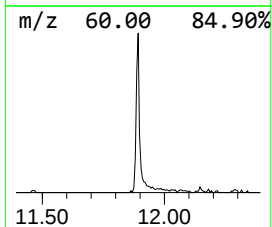
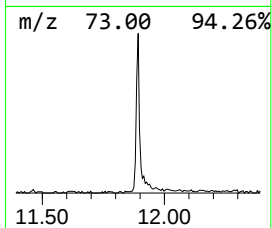
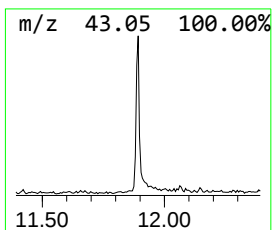
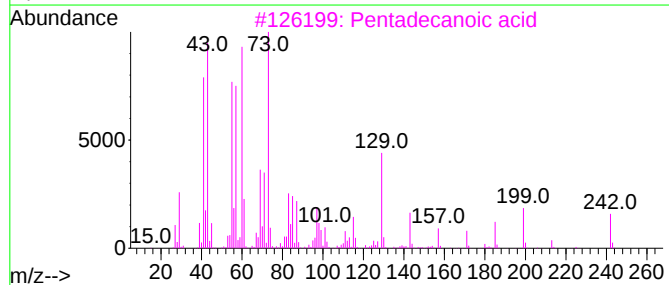
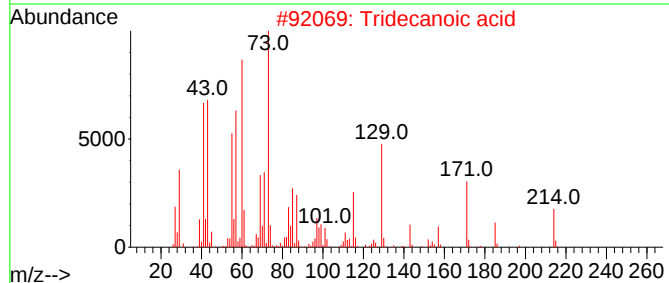
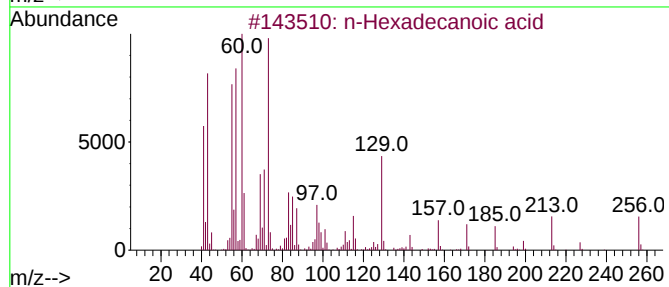
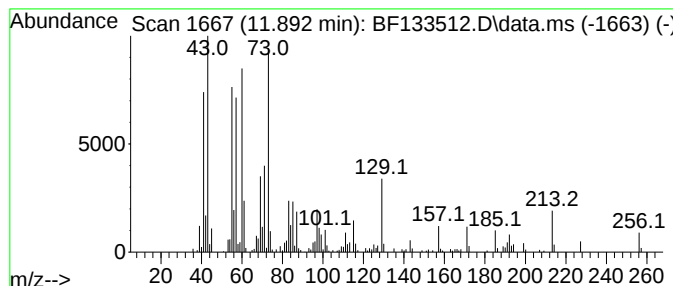
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.892	4.11 ng	232572	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62



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ClientSampleId :
SB10A

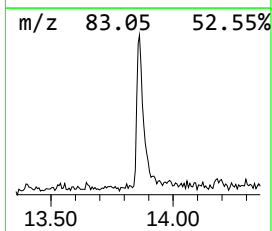
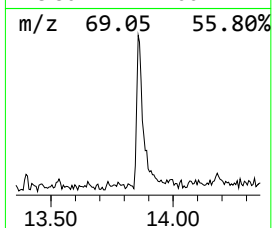
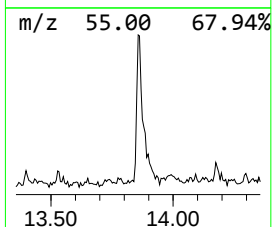
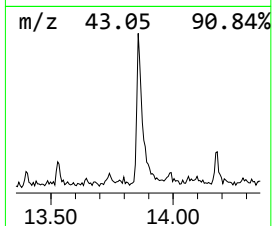
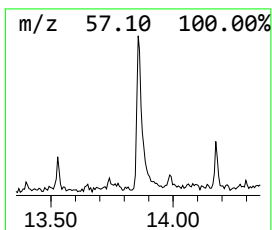
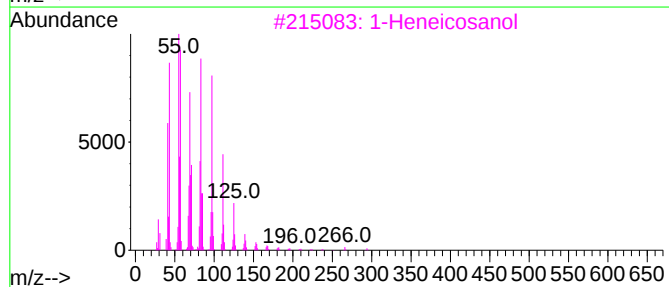
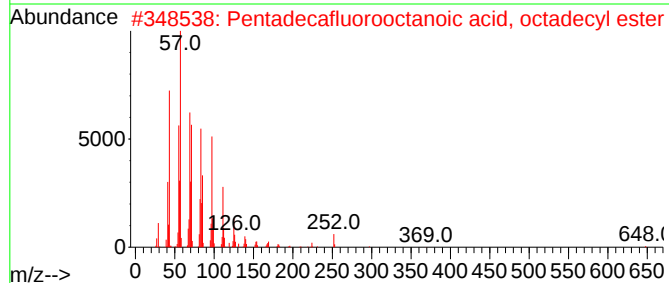
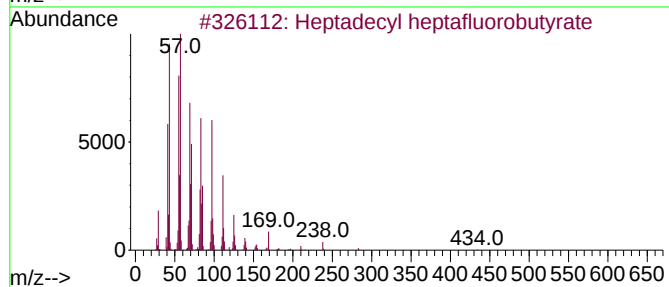
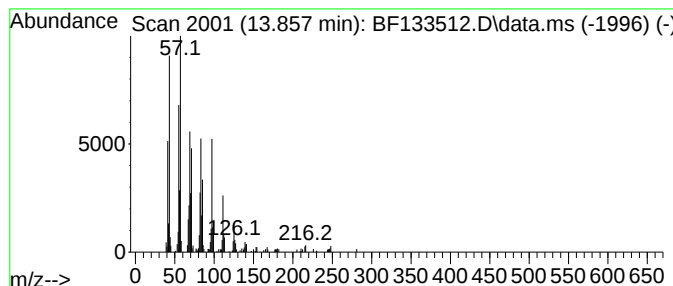
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	4.74 ng	211722	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
Data File : BF133512.D
Acq On : 26 May 2023 22:09
Operator : CG\JU
Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB10A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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
Butane, 2-metho...	2.116	8.2	ng	336829	1	6.834	824101	20.0
unknown4.210	4.210	3.0	ng	124178	1	6.834	824101	20.0
2-Pentanone, 4-...	5.051	4.5	ng	187442	1	6.834	824101	20.0
Benzophenone	10.586	4.4	ng	239528	3	9.875	1081270	20.0
n-Hexadecanoic ...	11.892	4.1	ng	232572	4	11.363	1132080	20.0
Heptadecyl hept...	13.857	4.7	ng	211722	5	13.998	893557	20.0