

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
 Data File : BF133904.D
 Acq On : 22 Jun 2023 16:37
 Operator : CG\JU
 Sample : 03320-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-19

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133904.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	18	rVB	306656	391281	15.00%	2.168%
2	3.434	227	229	239	rBV	52307	102850	3.94%	0.570%
3	4.481	404	407	413	rBV	29149	36140	1.39%	0.200%
4	5.098	507	512	523	rBV	419550	557434	21.37%	3.089%
5	5.498	575	580	583	rBV	2318190	2217333	84.99%	12.288%
6	6.498	745	750	753	rBV	2266585	2249601	86.23%	12.467%
7	6.857	808	811	820	rBV	745900	612302	23.47%	3.393%
8	7.422	902	907	910	rBV	1700707	1423786	54.57%	7.890%
9	8.139	1025	1029	1041	rBV	928642	785687	30.11%	4.354%
10	9.216	1208	1212	1215	rBV	3304363	2608973	100.00%	14.458%
11	9.898	1324	1328	1334	rBV	894232	770679	29.54%	4.271%
12	10.616	1446	1450	1453	rBV	308899	259631	9.95%	1.439%
13	10.692	1458	1463	1475	rBV	1578098	1582065	60.64%	8.767%
14	11.392	1578	1582	1585	rBV	736609	669883	25.68%	3.712%
15	11.916	1668	1671	1676	rBV	149172	155003	5.94%	0.859%
16	12.710	1803	1806	1816	rBV3	34309	51254	1.96%	0.284%
17	12.986	1849	1853	1857	rBV	2477587	2268692	86.96%	12.572%
18	13.898	2004	2008	2017	rBV3	89706	198701	7.62%	1.101%
19	14.051	2028	2034	2040	rBV	624089	651247	24.96%	3.609%
20	15.557	2285	2290	2295	rBV	356794	452529	17.35%	2.508%

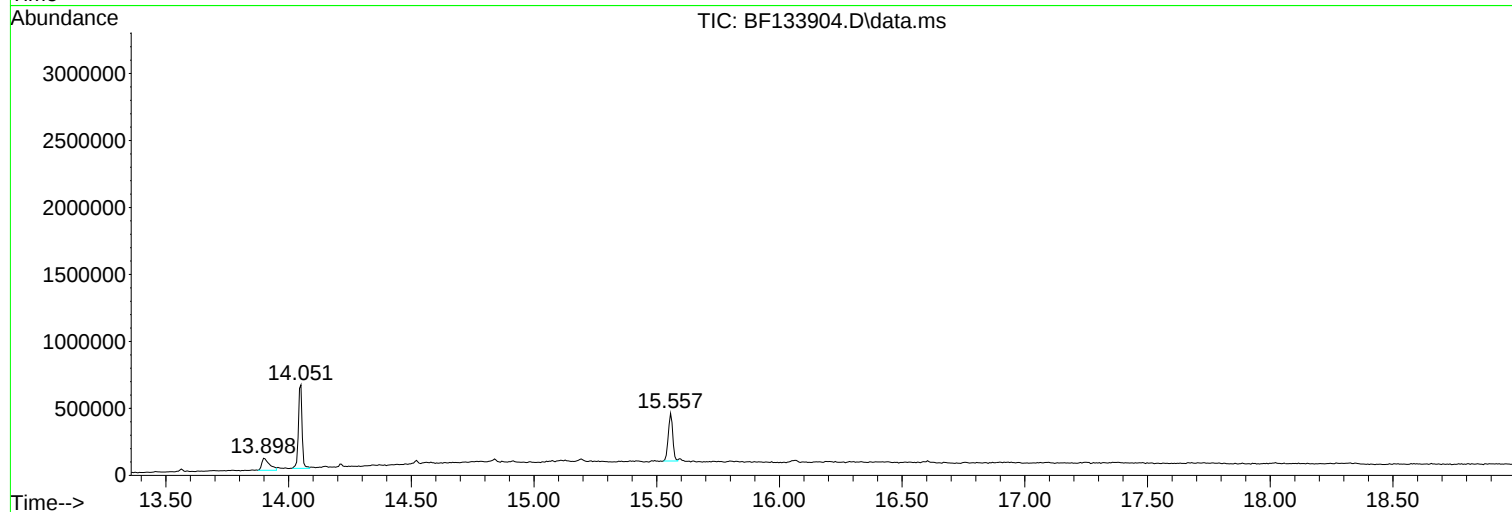
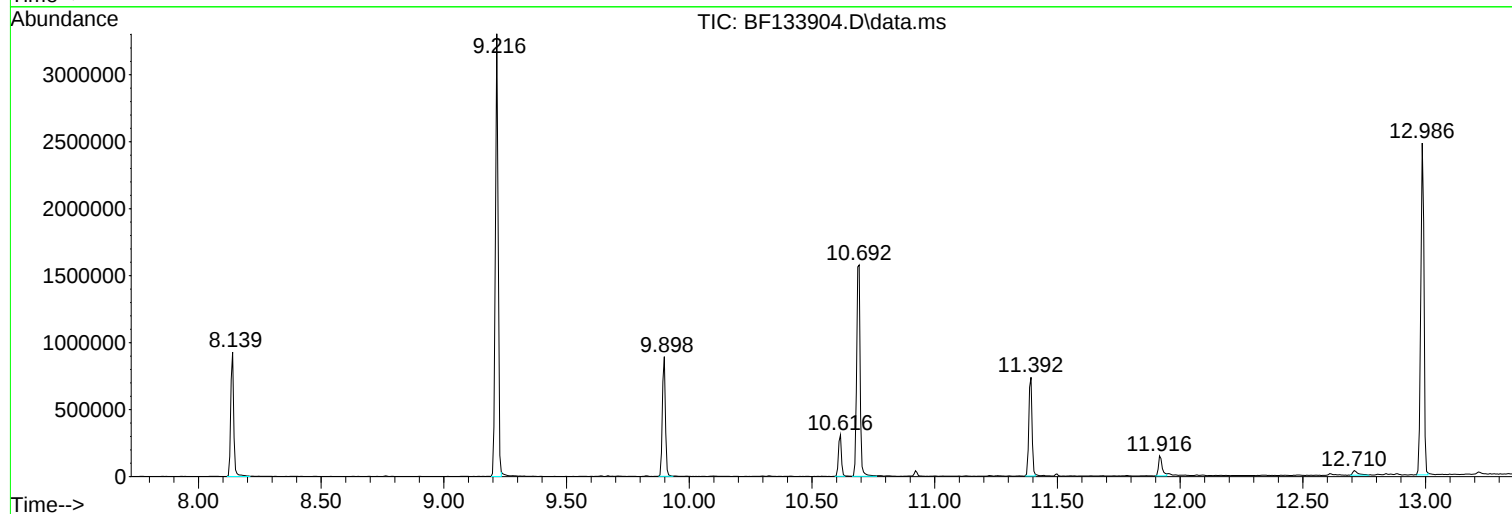
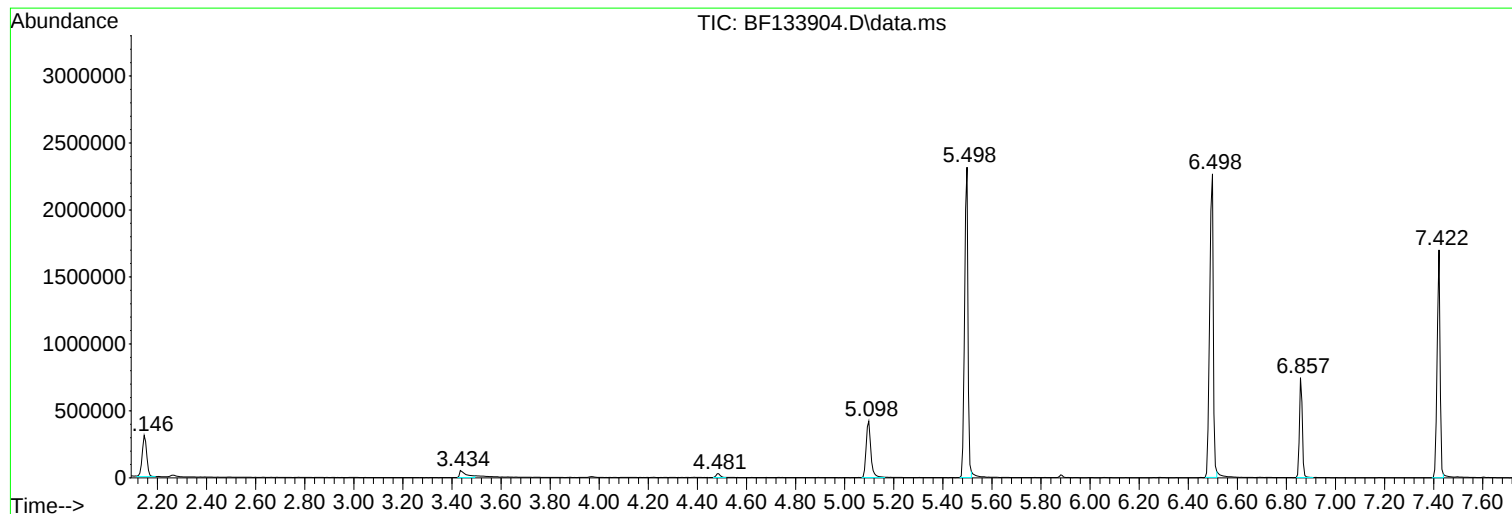
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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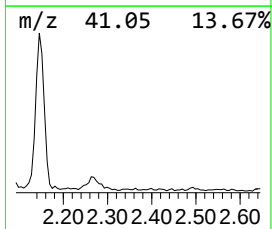
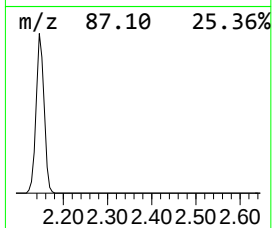
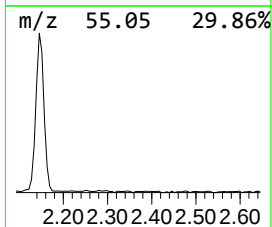
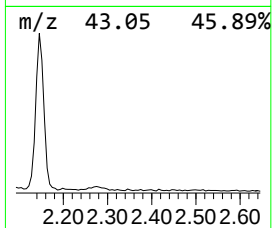
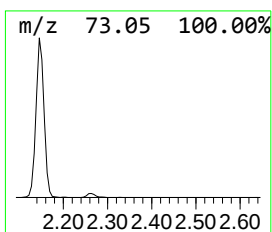
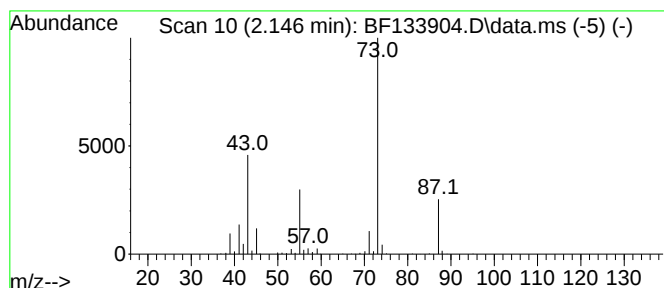
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	12.78 ng	391281	1,4-Dichlorobenzene-d4	6.857

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	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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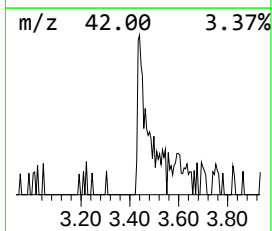
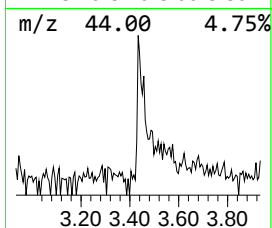
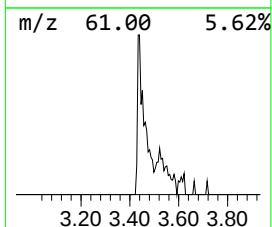
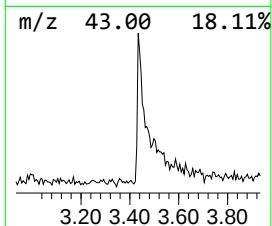
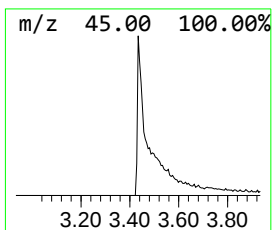
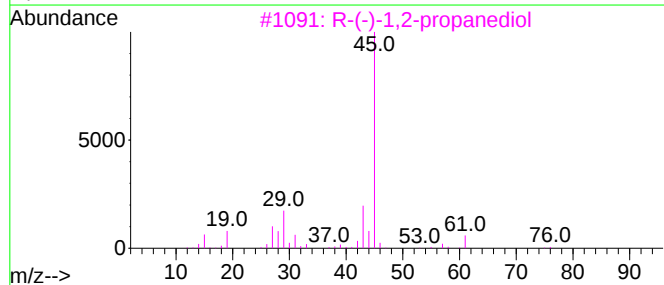
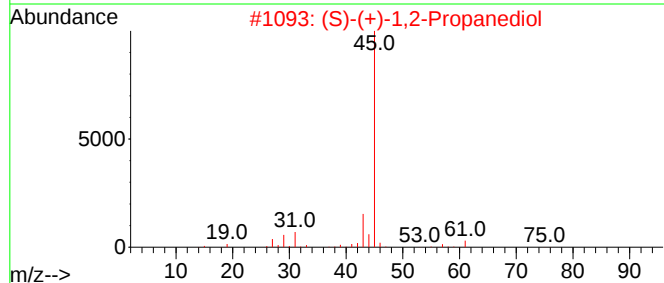
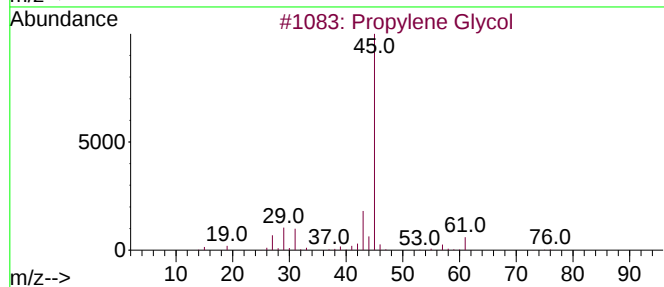
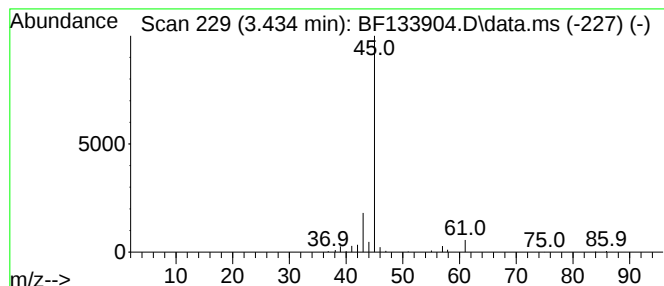
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Peak Number 2 unknown3.434 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.434	3.36 ng	102850	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	43
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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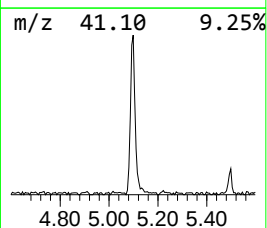
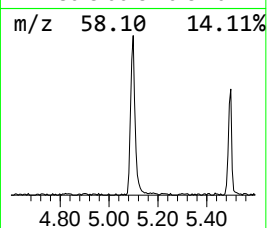
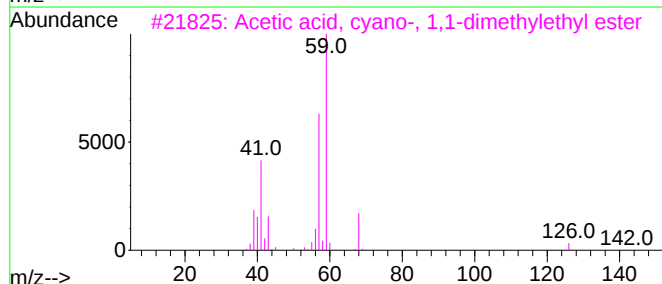
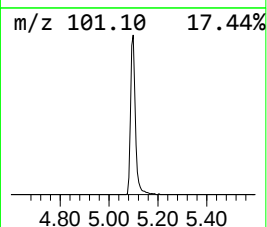
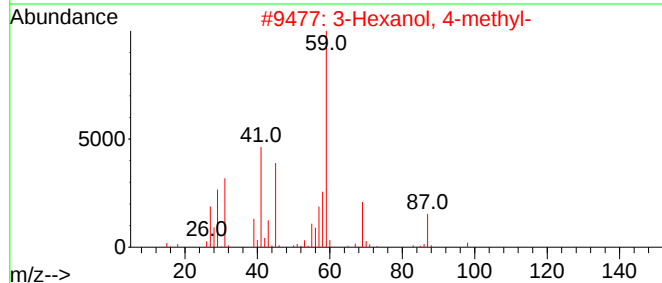
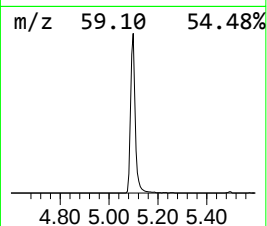
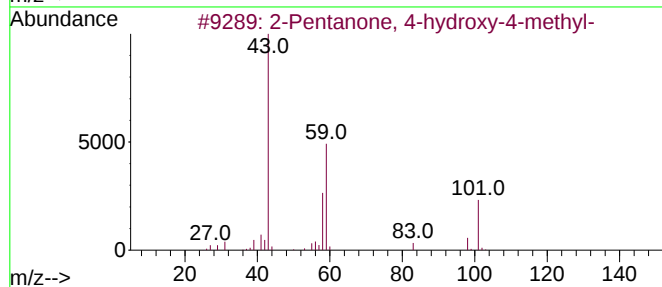
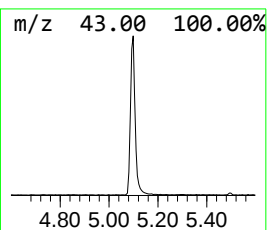
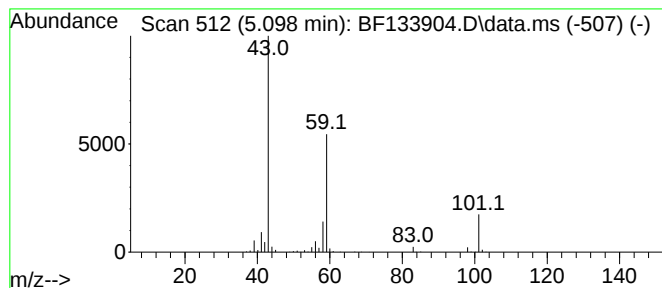
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	18.21 ng	557434	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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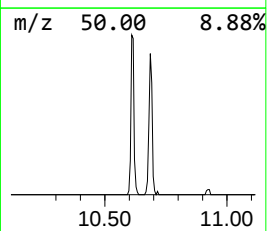
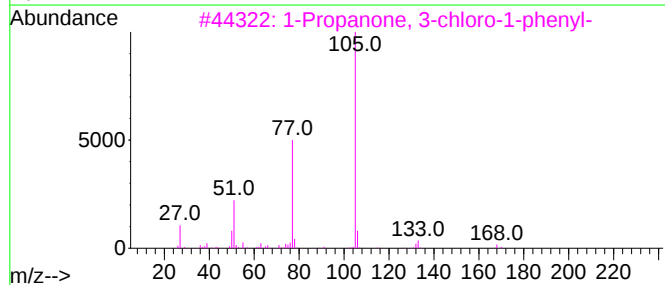
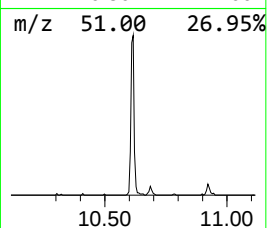
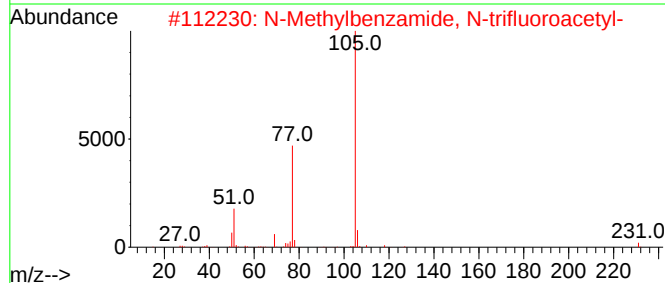
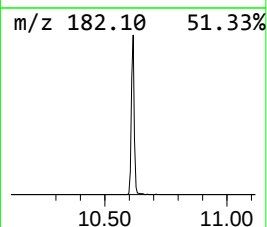
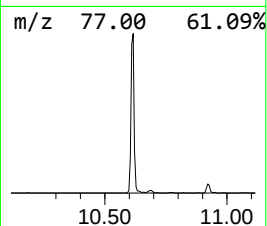
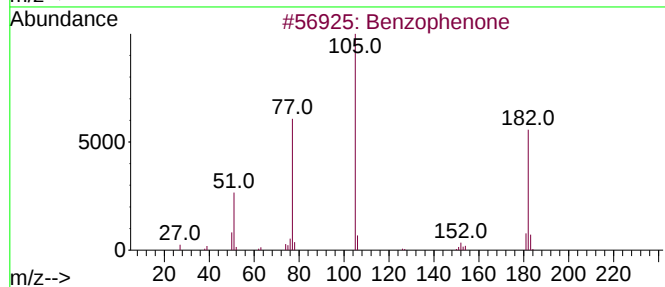
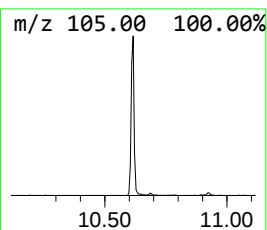
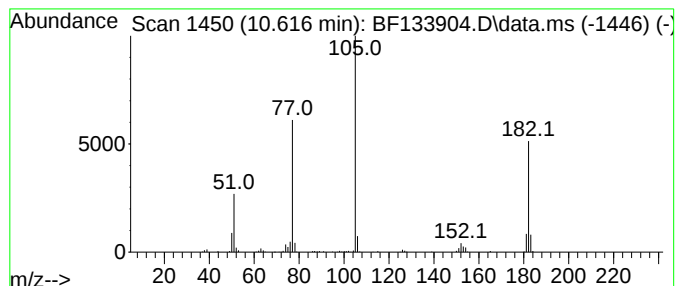
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	6.74 ng	259631	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



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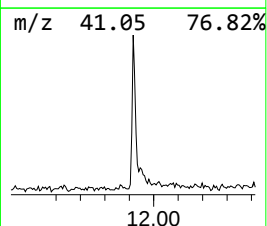
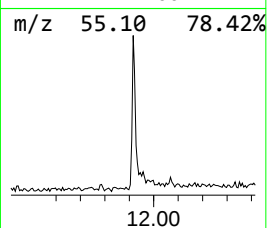
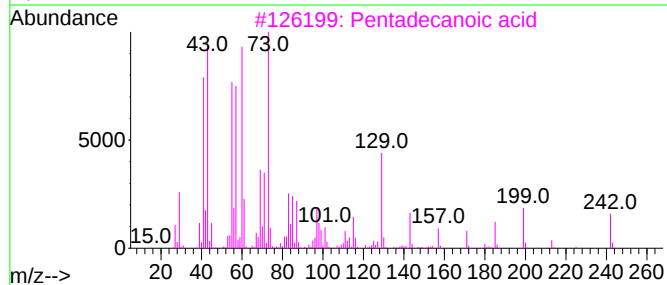
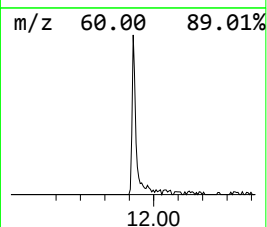
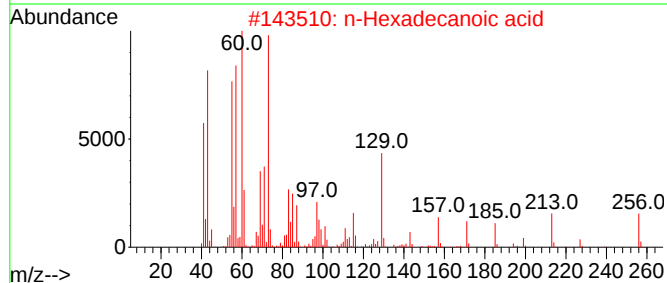
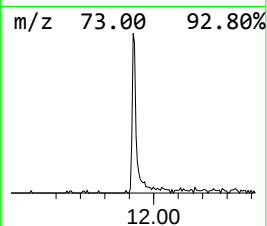
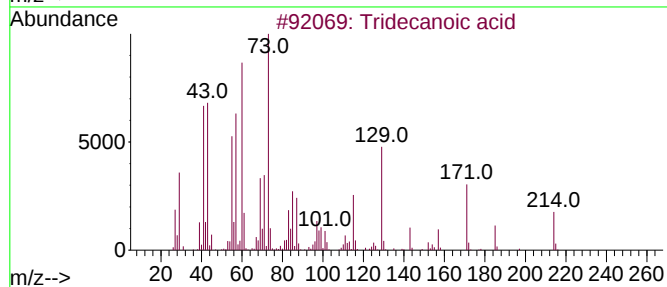
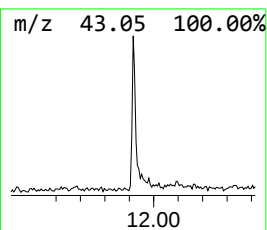
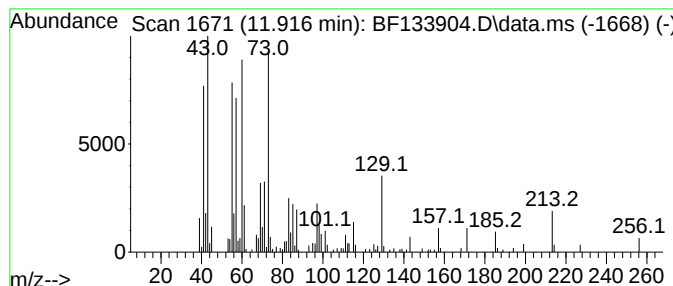
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Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.63 ng	155003	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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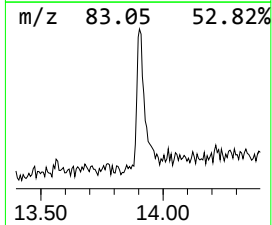
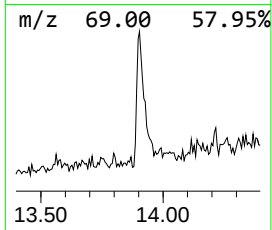
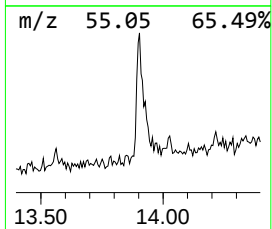
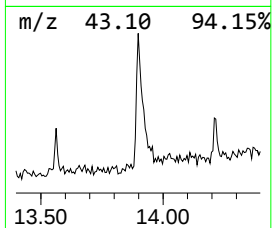
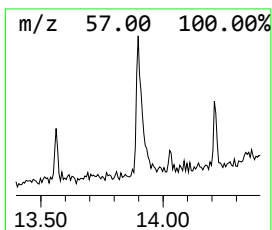
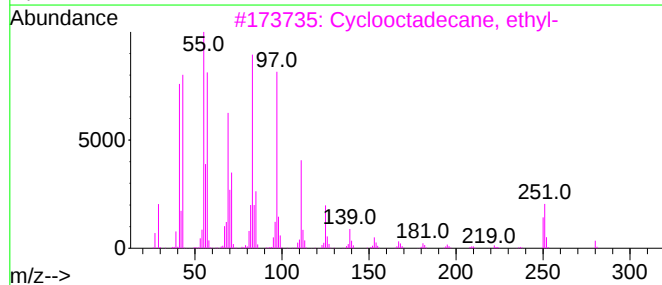
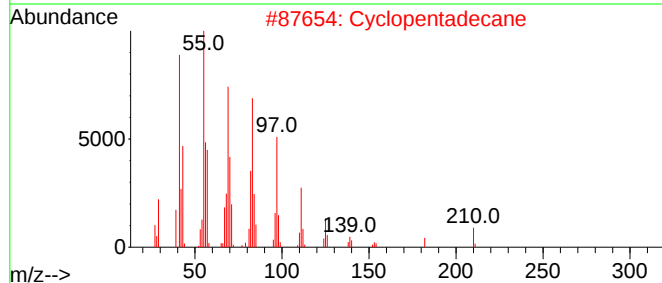
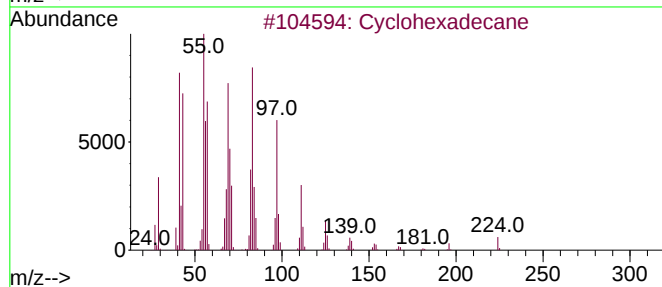
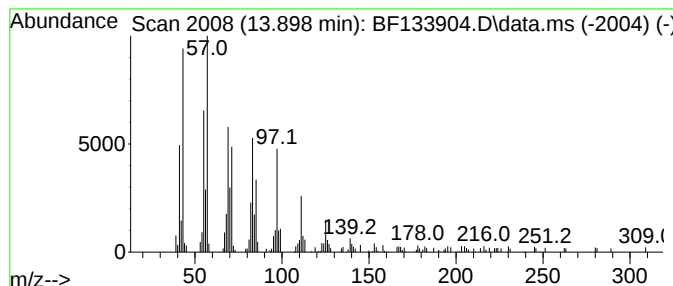
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	6.10 ng	198701	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	96
2			Cyclopentadecane	210	C15H30	000295-48-7	96
3			Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	96
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
5			1-Eicosene	280	C20H40	003452-07-1	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133904.D
Acq On : 22 Jun 2023 16:37
Operator : CG\JU
Sample : 03320-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-19

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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...	2.146	12.8	ng	391281	1	6.857	612302	20.0
unknown3.434	3.434	3.4	ng	102850	1	6.857	612302	20.0
2-Pentanone, 4-...	5.098	18.2	ng	557434	1	6.857	612302	20.0
Benzophenone	10.616	6.7	ng	259631	3	9.898	770679	20.0
Tridecanoic acid	11.916	4.6	ng	155003	4	11.392	669883	20.0
Cyclohexadecane	13.898	6.1	ng	198701	5	14.051	651247	20.0