

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
 Data File : BF134264.D
 Acq On : 13 Jul 2023 16:19
 Operator : CG\JU
 Sample : 03541-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-WWS-08

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-BF062623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134264.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	505	509	520	rVB	31975	45379	2.54%	0.335%
2	5.475	572	576	592	rBV	1792016	1668201	93.39%	12.319%
3	6.481	742	747	764	rBV	1691327	1786186	100.00%	13.191%
4	6.840	805	808	818	rBV	560608	445701	24.95%	3.291%
5	7.404	900	904	915	rBV	1143250	1017919	56.99%	7.517%
6	8.116	1022	1025	1030	rBV	620174	572922	32.08%	4.231%
7	9.198	1205	1209	1212	rBV	1862030	1572313	88.03%	11.611%
8	9.875	1321	1324	1328	rBV	730231	629694	35.25%	4.650%
9	10.592	1443	1446	1454	rBV	178942	155866	8.73%	1.151%
10	10.669	1455	1459	1473	rVV	1494636	1402960	78.55%	10.361%
11	11.375	1575	1579	1586	rBV	767536	681829	38.17%	5.035%
12	11.904	1665	1669	1677	rBV2	192037	236419	13.24%	1.746%
13	12.692	1800	1803	1810	rBV	104670	123151	6.89%	0.909%
14	12.969	1846	1850	1853	rBV	1849271	1559934	87.33%	11.520%
15	13.545	1943	1948	1950	rBV3	23354	24859	1.39%	0.184%
16	13.874	2001	2004	2006	rBV2	33864	38769	2.17%	0.286%
17	14.033	2027	2031	2038	rVB	673486	602556	33.73%	4.450%
18	14.192	2055	2058	2061	rBV	34165	33726	1.89%	0.249%
19	14.504	2107	2111	2115	rBV	58182	57811	3.24%	0.427%
20	14.816	2159	2164	2168	rBV	77539	92338	5.17%	0.682%
21	15.163	2219	2223	2229	rBV	74929	100175	5.61%	0.740%
22	15.539	2281	2287	2299	rBV	391690	619182	34.67%	4.573%
23	16.021	2365	2369	2374	rVB2	32841	52791	2.96%	0.390%
24	16.874	2508	2514	2517	rBV7	10493	20556	1.15%	0.152%

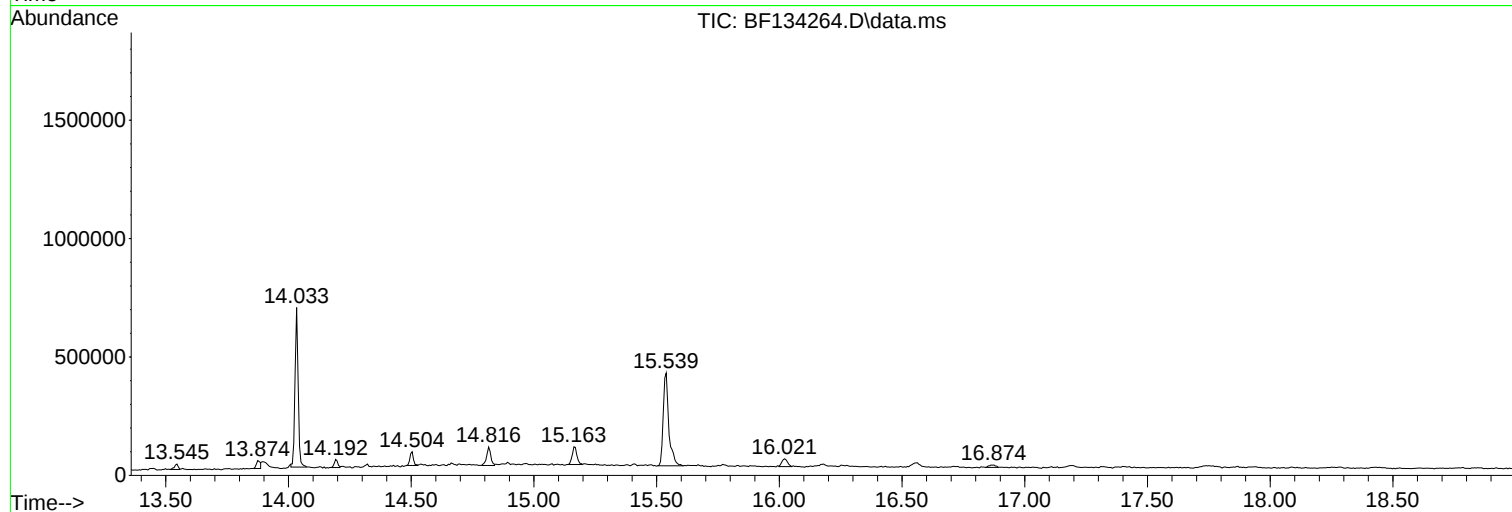
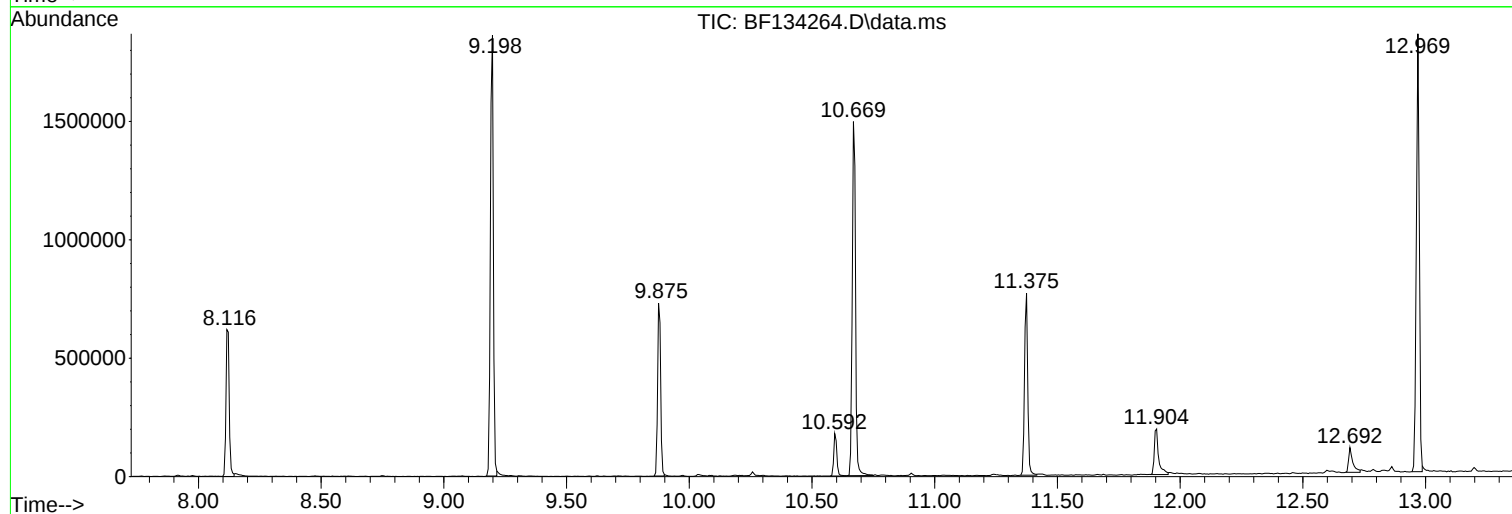
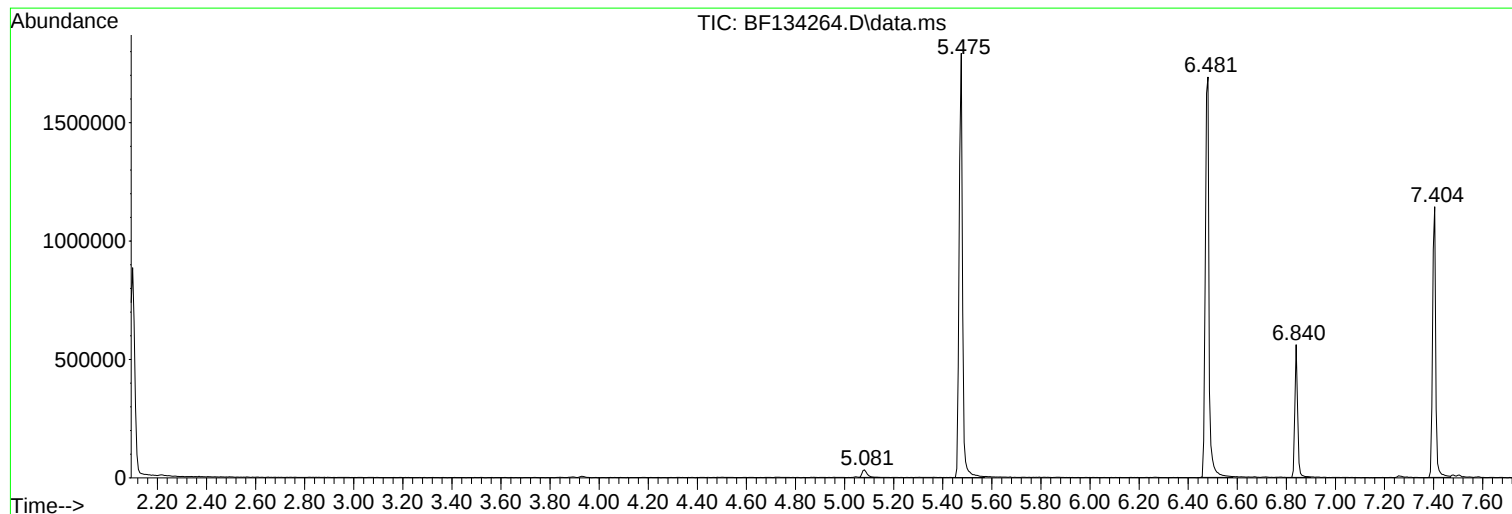
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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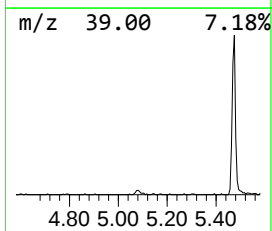
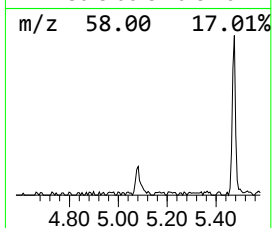
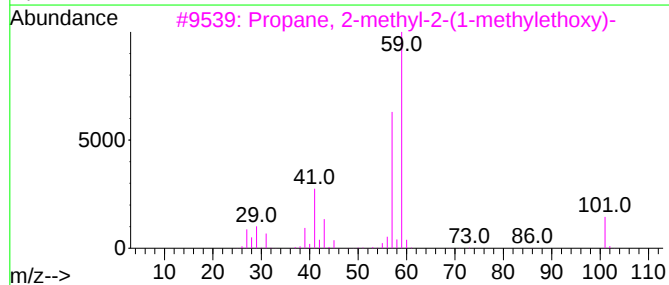
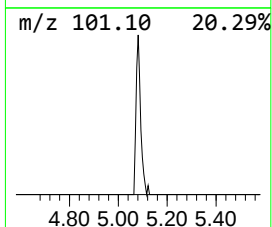
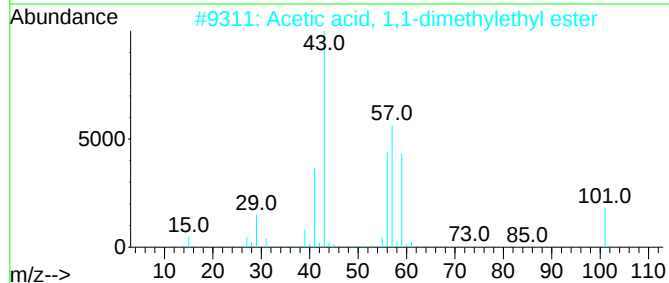
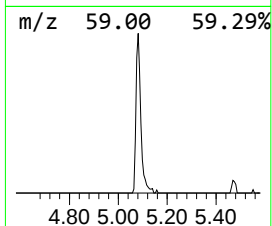
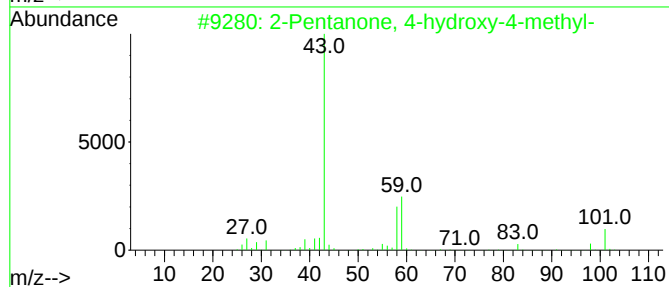
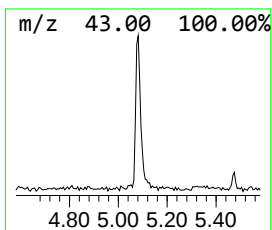
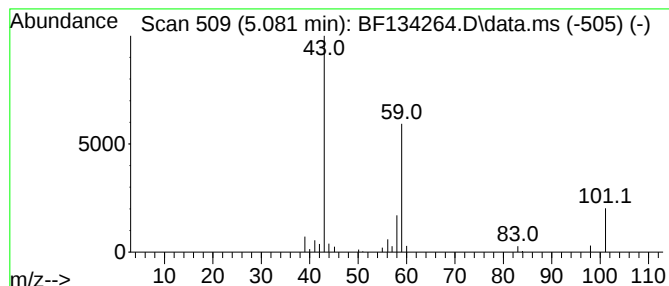
Instrument :
BNA_F
ClientSampleId :
WC-WWS-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.081	2.04 ng	45379	1,4-Dichlorobenzene-d4		6.840	
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	56
3	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	33
4	3-Hexanol		102	C6H14O	000623-37-0	33
5	3-Octanol		130	C8H18O	000589-98-0	28



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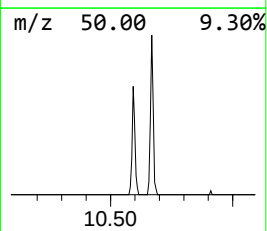
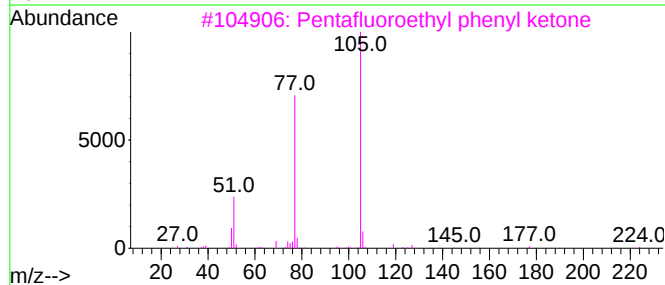
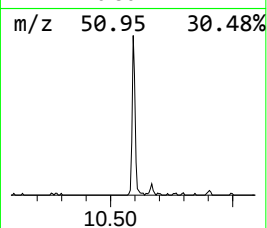
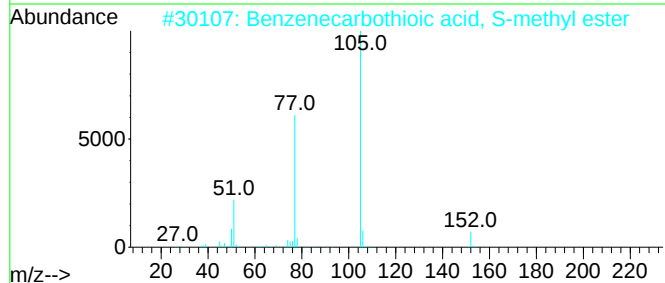
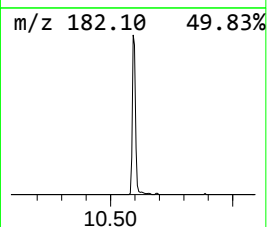
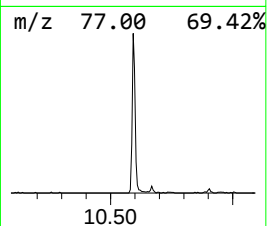
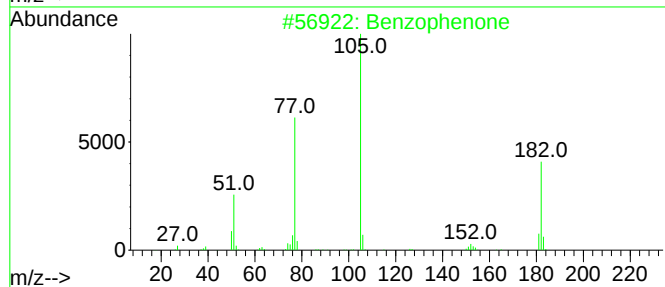
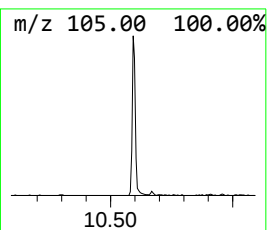
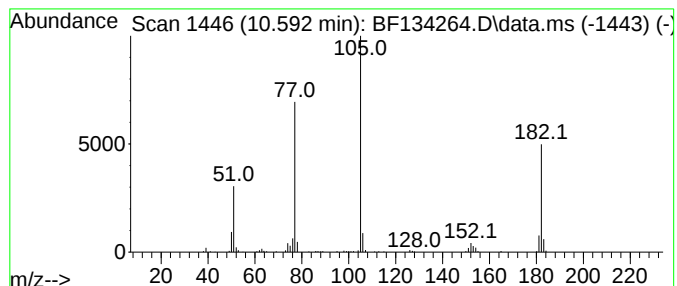
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.592	4.95 ng	155866	Acenaphthene-d10	9.875

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	52
3			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50



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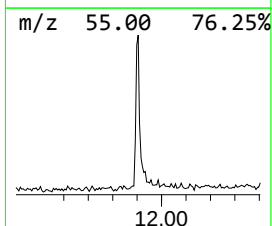
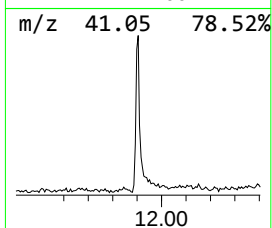
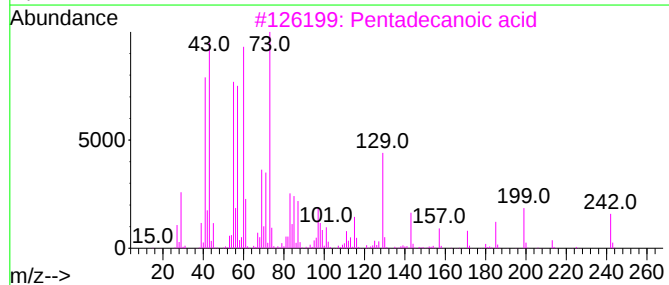
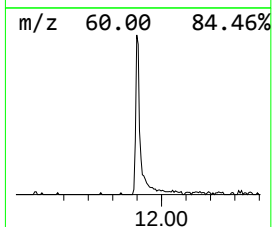
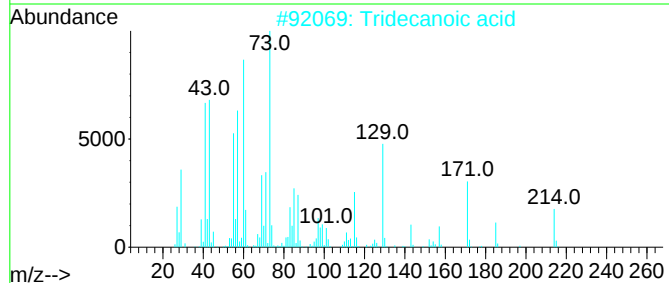
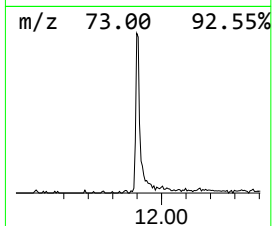
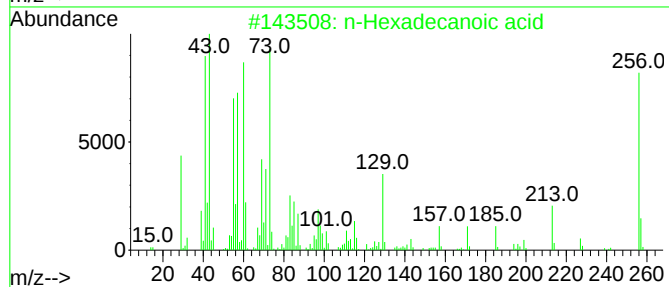
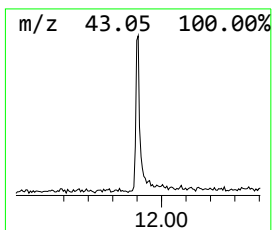
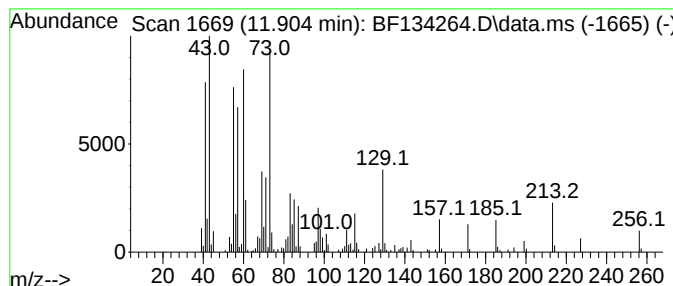
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	6.93 ng	236419	Phenanthrene-d10	11.375

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	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5			Undecanoic acid	186	C11H22O2	000112-37-8	52



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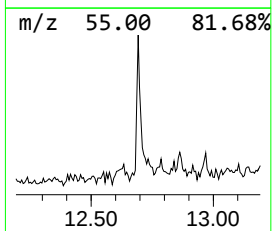
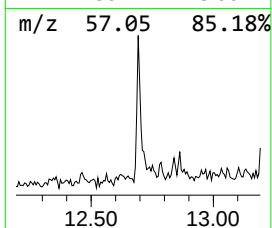
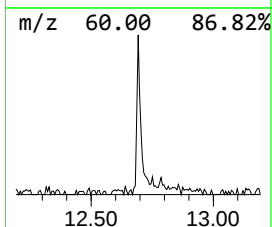
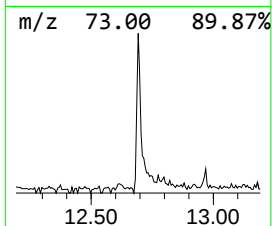
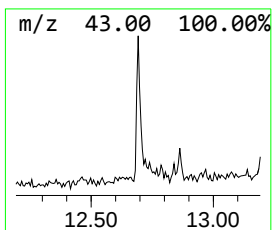
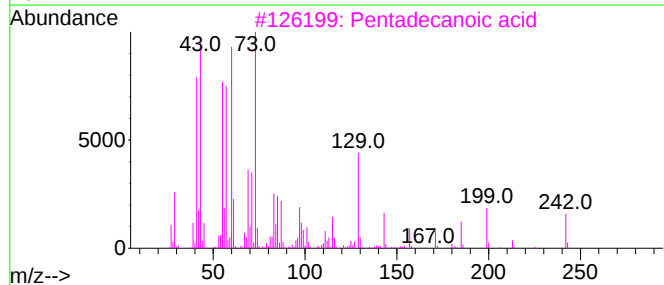
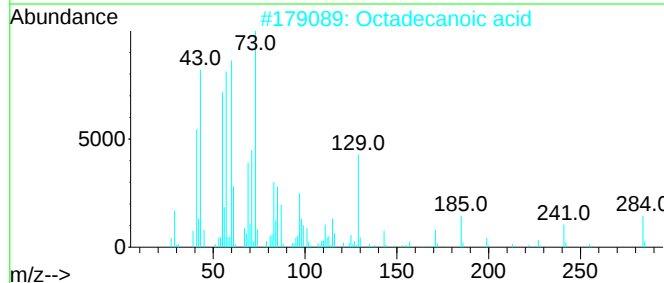
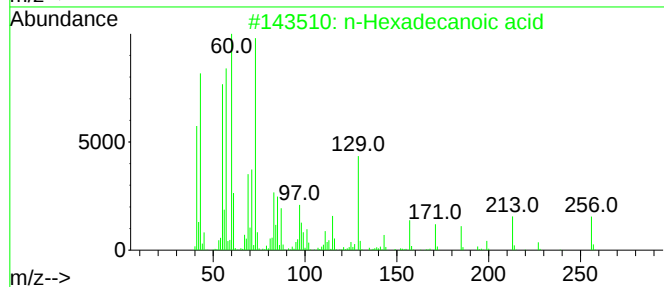
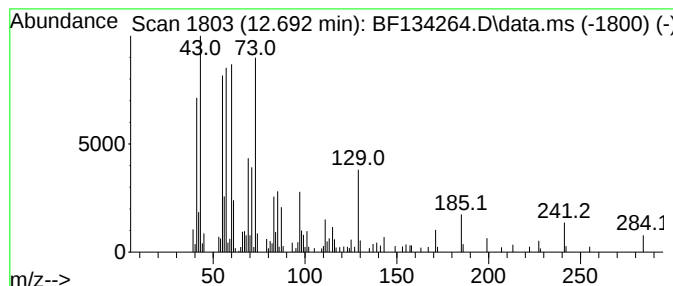
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.692	3.61 ng	123151	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Octadecanoic acid	284	C18H36O2	000057-11-4	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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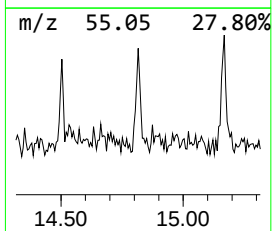
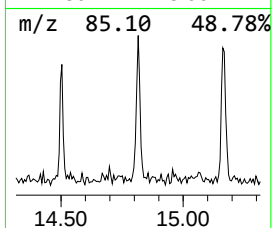
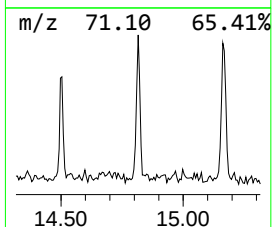
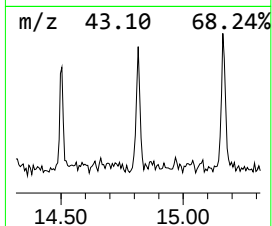
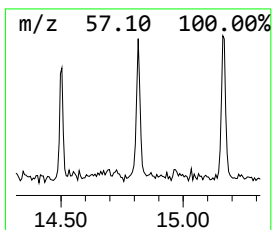
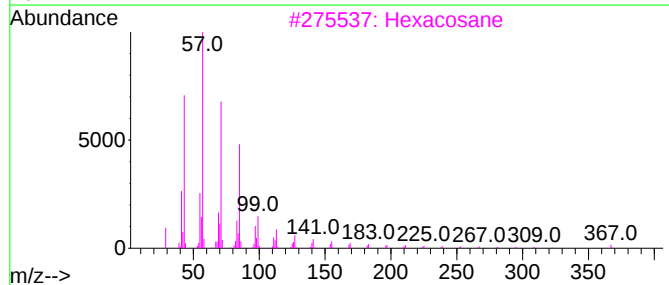
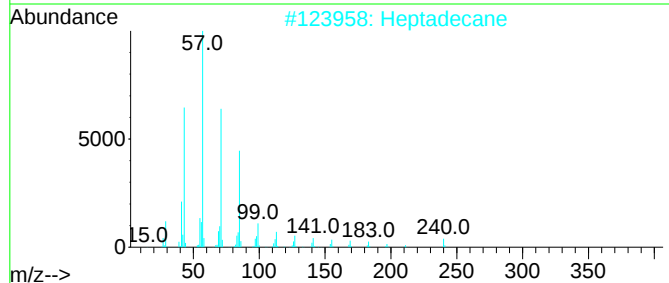
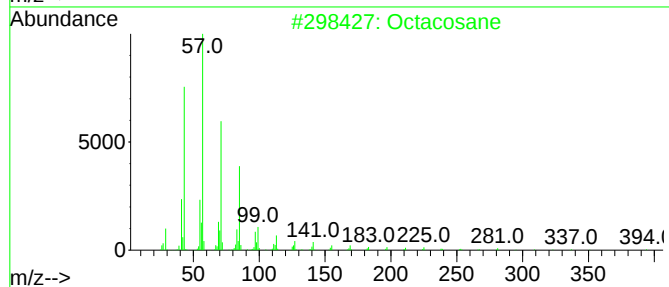
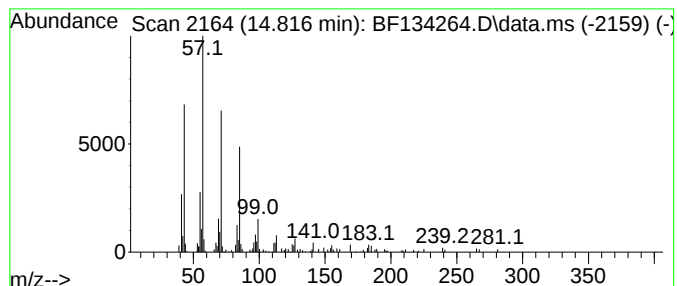
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.98 ng	92338	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heptadecane	240	C17H36	000629-78-7	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octadecane	254	C18H38	000593-45-3	87
5			Docosane	310	C22H46	000629-97-0	87



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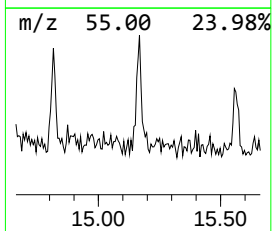
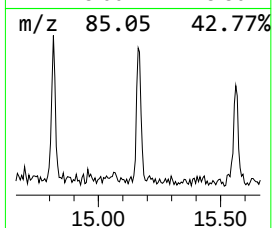
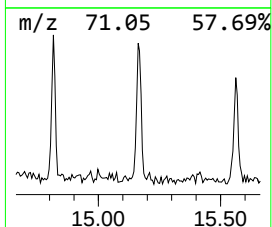
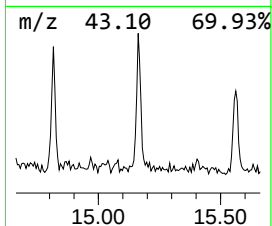
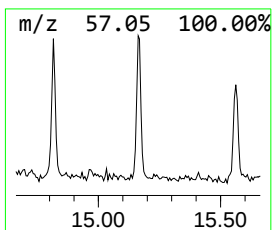
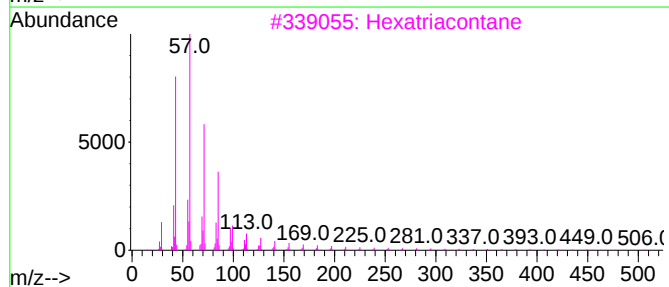
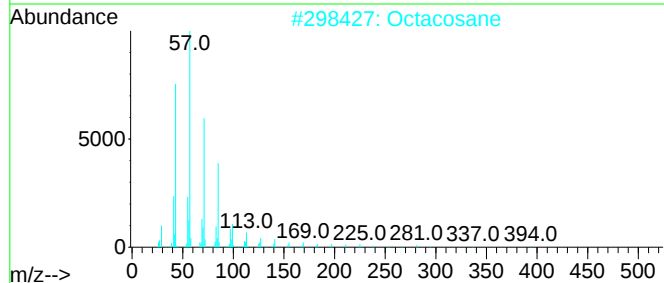
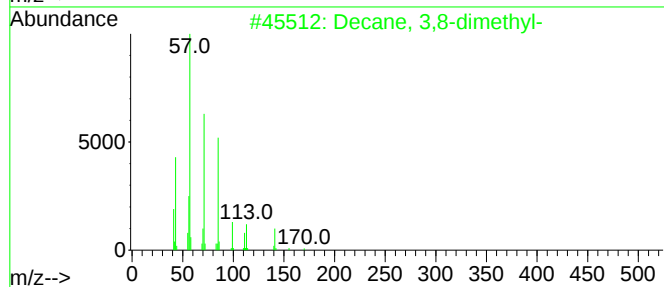
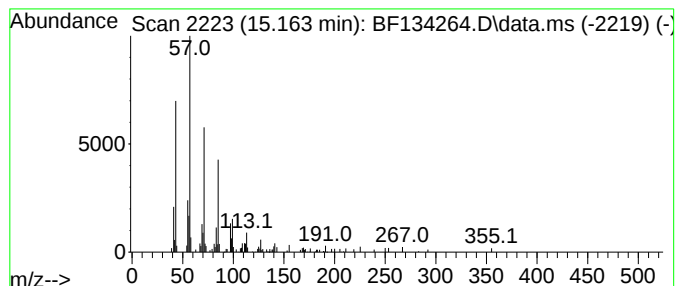
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decane, 3,8-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	3.24 ng	100175	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexatriacontane	507	C36H74	000630-06-8	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
Data File : BF134264.D
Acq On : 13 Jul 2023 16:19
Operator : CG\JU
Sample : 03541-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-WWS-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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-...	5.081	2.0	ng	45379	1	6.840	445701	20.0
Benzophenone	10.592	5.0	ng	155866	3	9.875	629694	20.0
n-Hexadecanoic ...	11.904	6.9	ng	236419	4	11.375	681829	20.0
Octadecanoic acid	12.692	3.6	ng	123151	4	11.375	681829	20.0
Octacosane	14.816	3.0	ng	92338	6	15.539	619182	20.0
Decane, 3,8-dim...	15.163	3.2	ng	100175	6	15.539	619182	20.0