

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
 Data File : BG057484.D
 Acq On : 20 May 2023 2:27
 Operator : CG/JU
 Sample : 02826-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-3-051723

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_G\Methods\8270-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057484.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	307	314	322	rBV	65287	104707	9.99%	1.747%
2	5.873	391	397	410	rBB	274010	460785	43.97%	7.687%
3	7.500	667	674	687	rBV	298950	523476	49.95%	8.732%
4	8.358	812	820	827	rBB	88069	146329	13.96%	2.441%
5	9.533	1013	1020	1031	rBV	176894	325966	31.10%	5.438%
6	11.195	1294	1303	1310	rBV	113786	205548	19.61%	3.429%
7	13.592	1705	1711	1722	rVB	518136	809920	77.29%	13.511%
8	14.967	1940	1945	1952	rVB	179195	277391	26.47%	4.627%
9	16.306	2168	2173	2178	rVB	28551	39370	3.76%	0.657%
10	16.453	2191	2198	2207	rBV	369390	566381	54.05%	9.448%
11	16.629	2221	2228	2234	rBV5	3915	11969	1.14%	0.200%
12	17.710	2405	2412	2416	rBV	223150	334468	31.92%	5.579%
13	17.751	2416	2419	2425	rVB	41145	57039	5.44%	0.951%
14	18.550	2550	2555	2564	rBV4	51049	105207	10.04%	1.755%
15	18.621	2564	2567	2572	rVB2	12787	19628	1.87%	0.327%
16	18.773	2587	2593	2597	rBV3	12739	26399	2.52%	0.440%
17	18.967	2621	2626	2630	rBV7	4722	10825	1.03%	0.181%
18	19.061	2638	2642	2646	rBV6	8650	12968	1.24%	0.216%
19	19.120	2648	2652	2657	rVB7	9534	17060	1.63%	0.285%
20	19.284	2676	2680	2687	rBV10	9278	17523	1.67%	0.292%
21	19.355	2687	2692	2697	rBV6	8295	17593	1.68%	0.293%
22	19.443	2704	2707	2709	rBV3	18274	21961	2.10%	0.366%
23	19.472	2709	2712	2716	rVB	14697	22135	2.11%	0.369%
24	19.743	2753	2758	2762	rBV	77022	111550	10.64%	1.861%
25	20.101	2815	2819	2824	rVB	82577	119590	11.41%	1.995%
26	20.277	2844	2849	2854	rVB	863904	1047956	100.00%	17.481%
27	20.541	2891	2894	2897	rBV3	22641	33048	3.15%	0.551%
28	21.041	2976	2979	2983	rVB	33234	38194	3.64%	0.637%
29	21.575	3066	3070	3075	rBV2	49562	73602	7.02%	1.228%
30	22.016	3138	3145	3150	rBV2	194705	371159	35.42%	6.191%
31	22.151	3165	3168	3175	rVB2	40954	64916	6.19%	1.083%

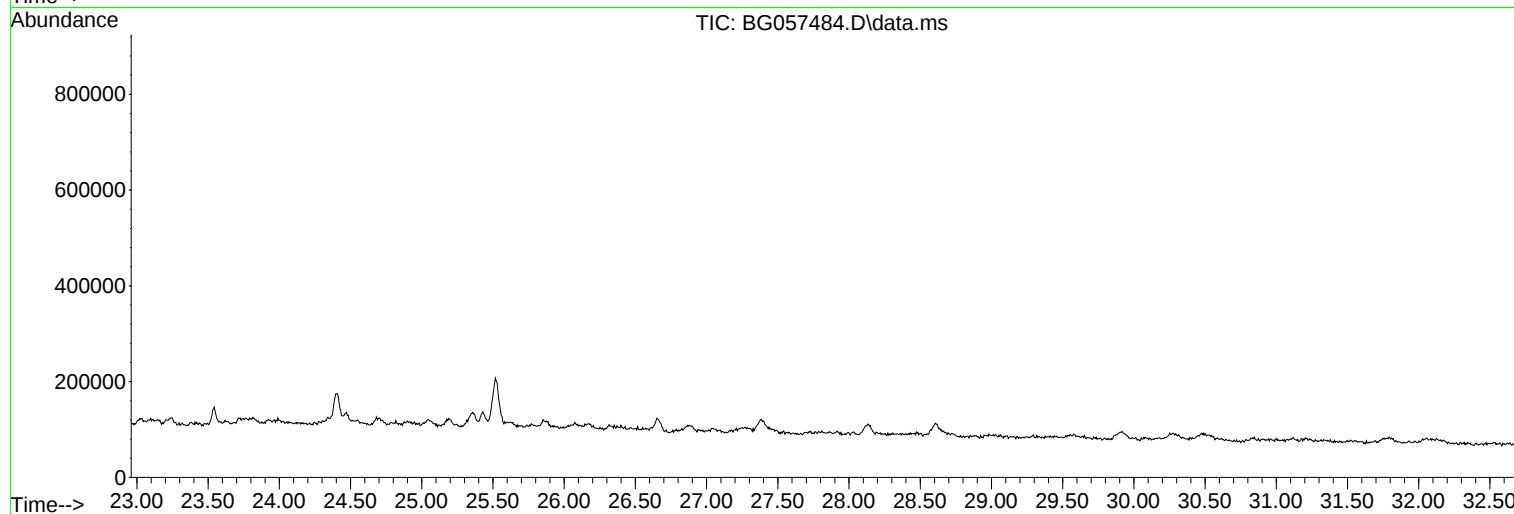
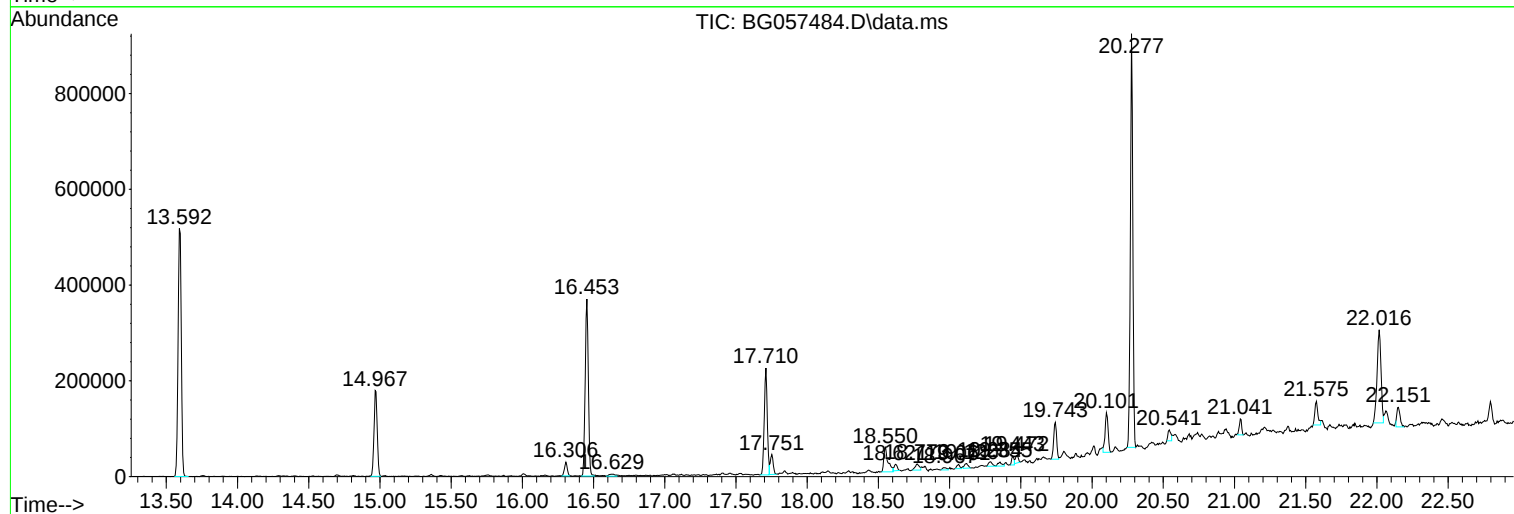
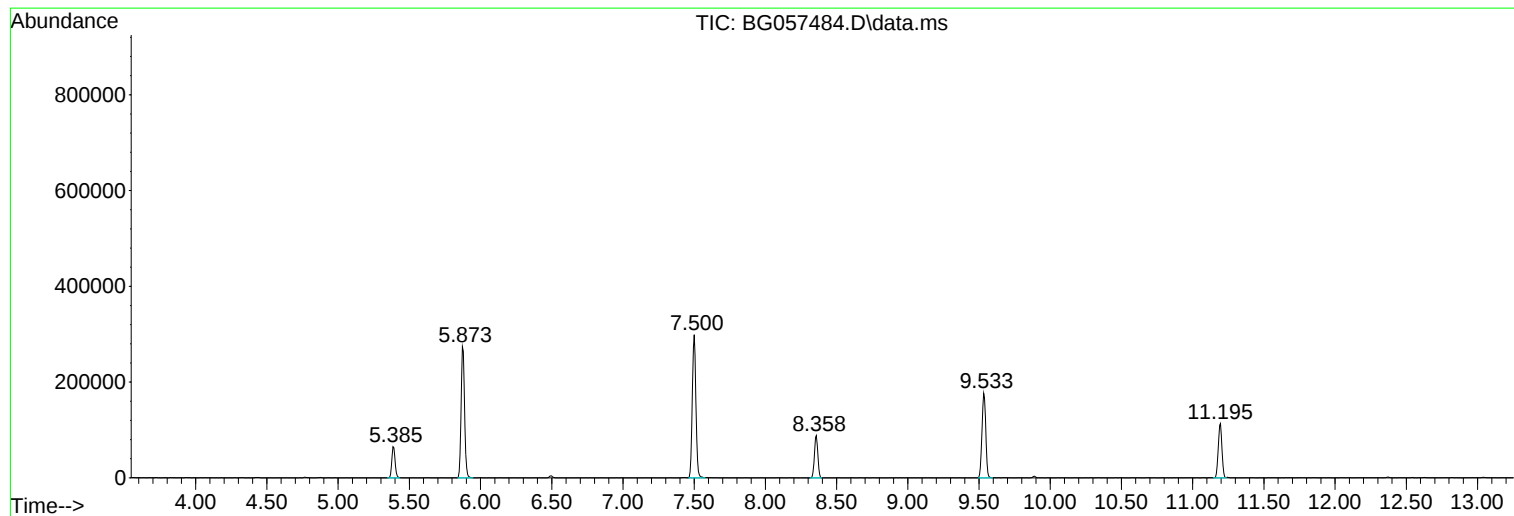
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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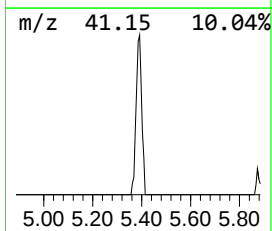
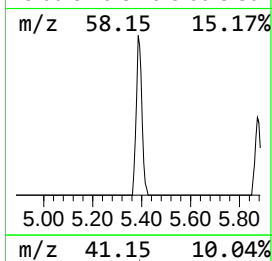
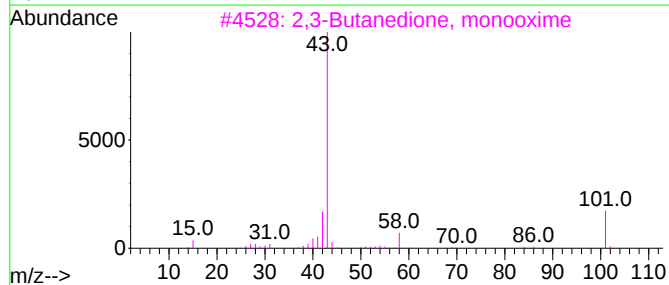
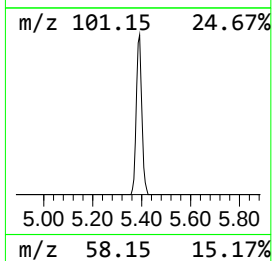
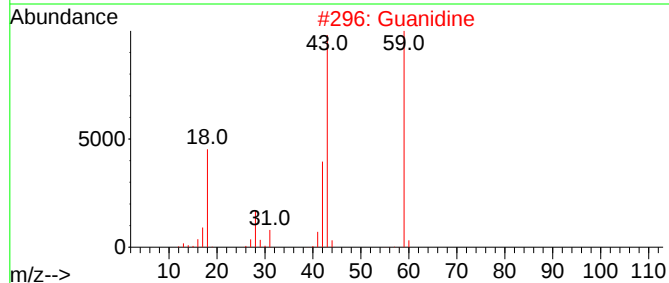
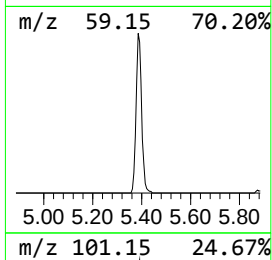
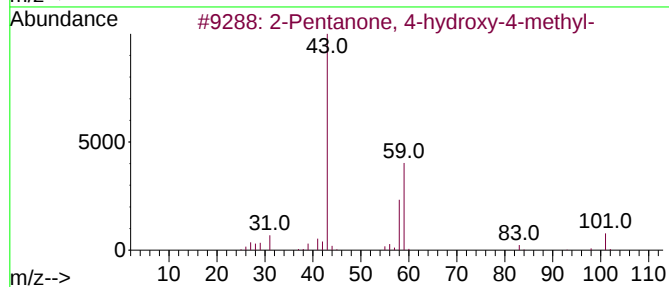
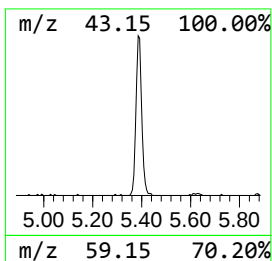
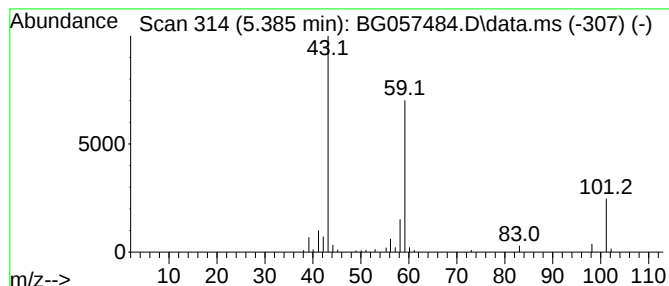
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	14.31 ng	104707	1,4-Dichlorobenzene-d4	8.358

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Guanidine	59	CH5N3	000113-00-8	43		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17		



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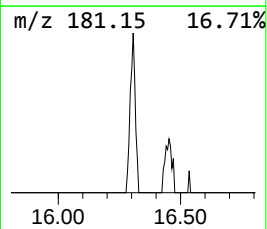
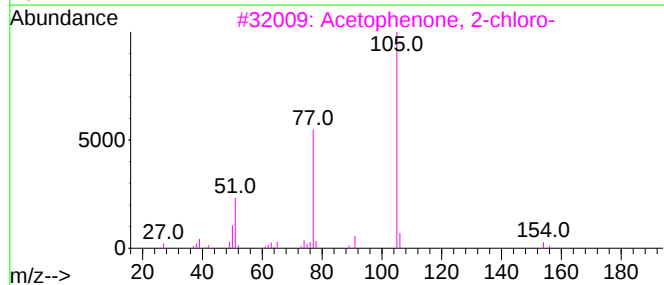
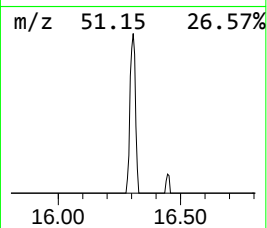
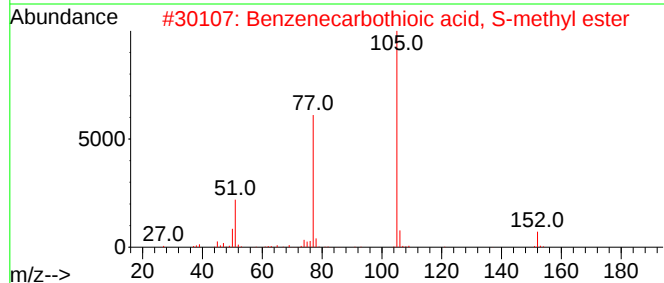
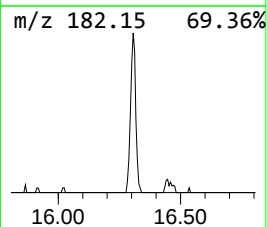
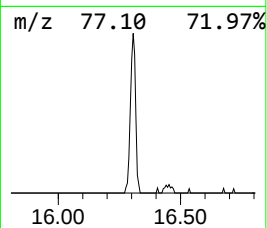
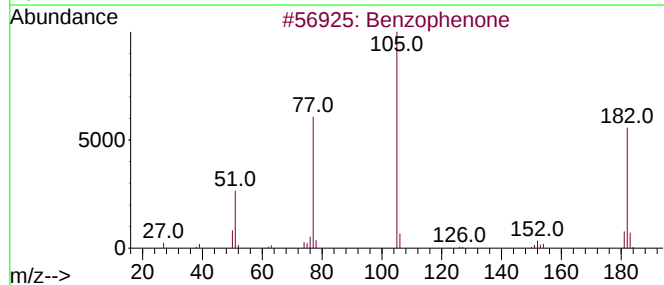
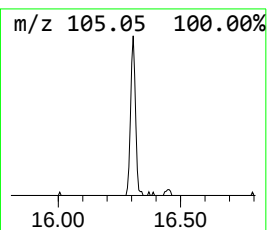
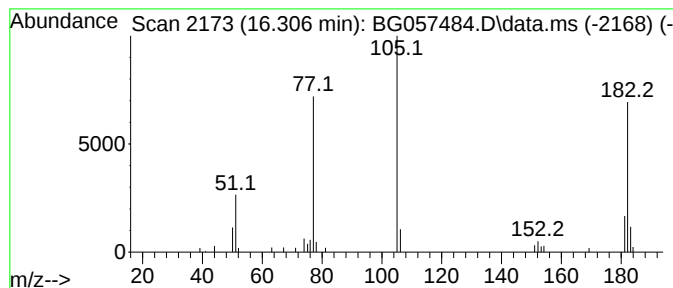
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.306	2.84 ng	39370	Acenaphthene-d10	14.967

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	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			N-cyanobenzamide	146	C8H6N2O	015150-25-1	43
5			Vinyl benzoate	148	C9H8O2	000769-78-8	43



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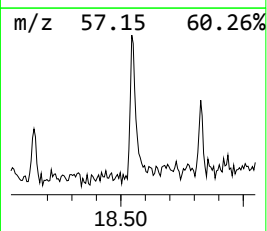
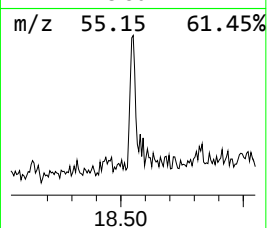
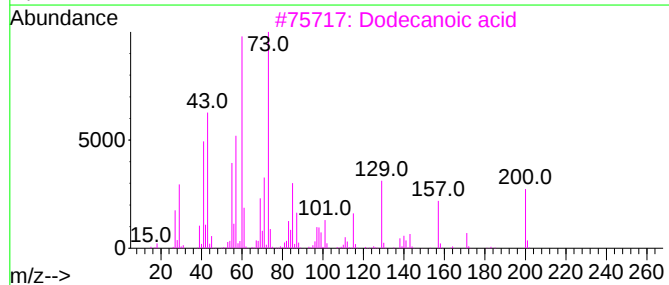
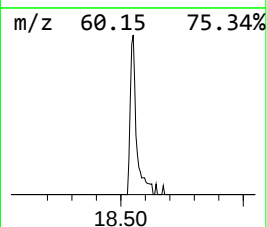
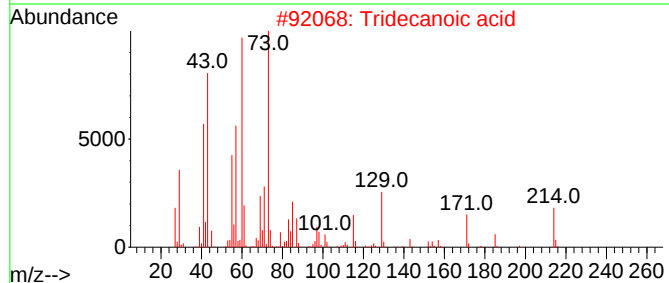
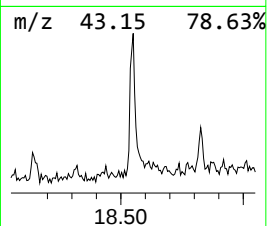
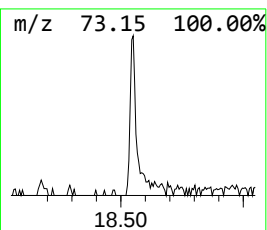
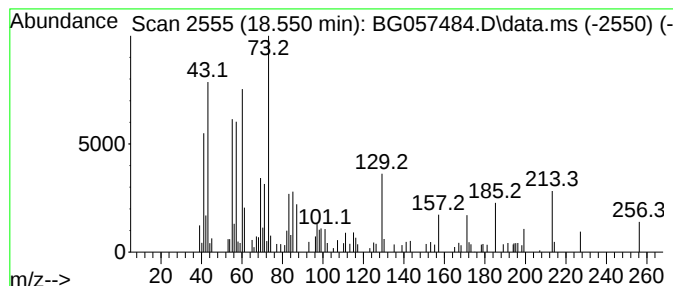
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.550	6.29 ng	105207	Phenanthrene-d10	17.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Dodecanoic acid	200	C12H24O2	000143-07-7	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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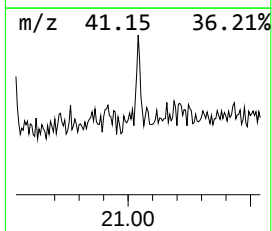
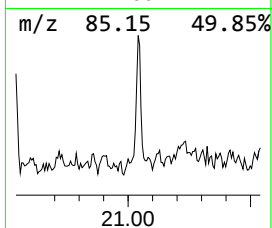
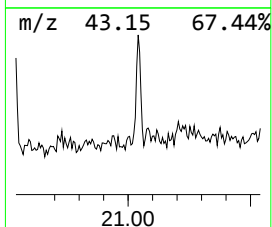
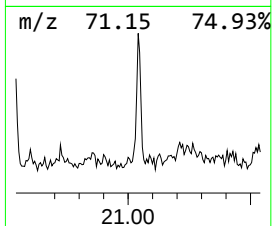
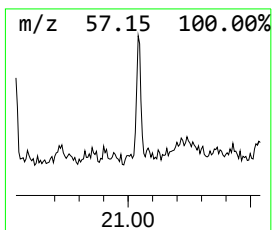
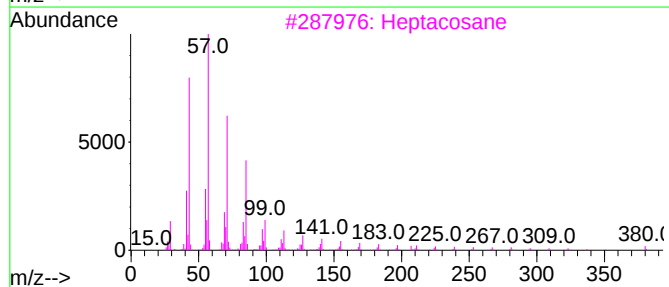
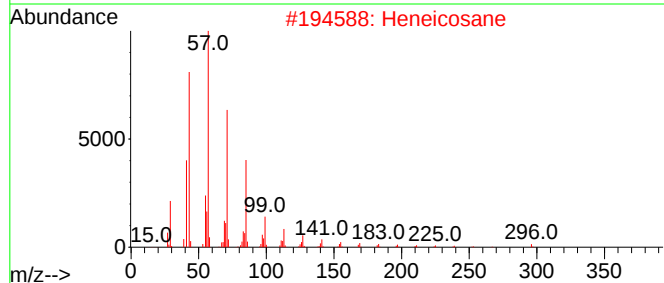
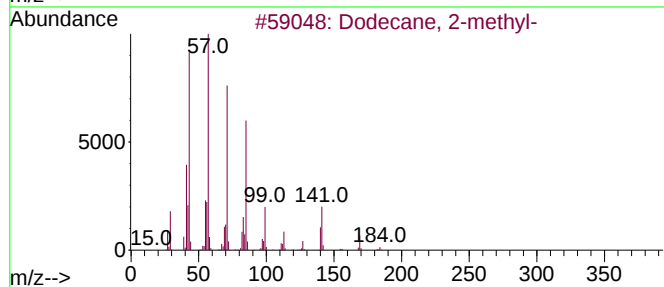
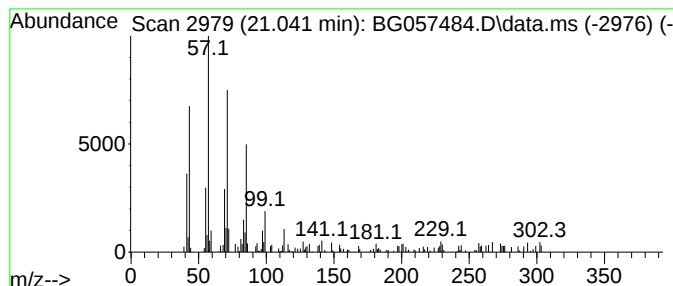
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Peak Number 4 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.041	2.06 ng	38194	Chrysene-d12	22.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
2		Heneicosane	296	C21H44	000629-94-7	80
3		Heptacosane	380	C27H56	000593-49-7	80
4		Hexacosane	366	C26H54	000630-01-3	80
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72



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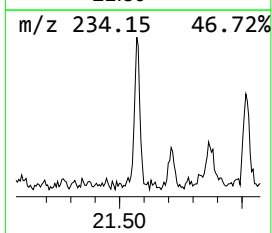
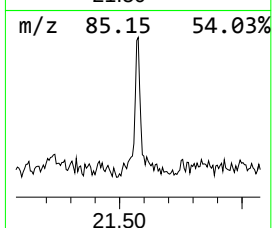
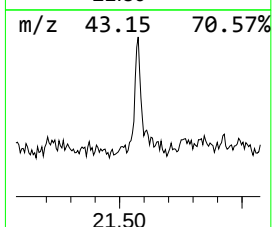
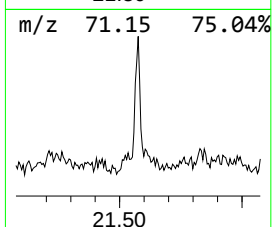
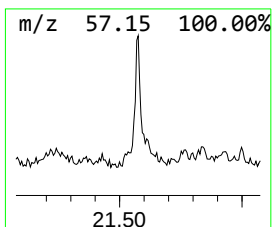
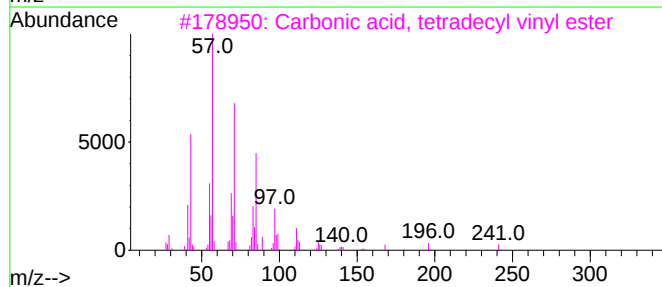
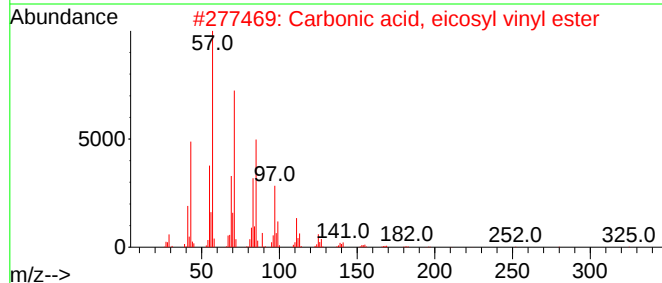
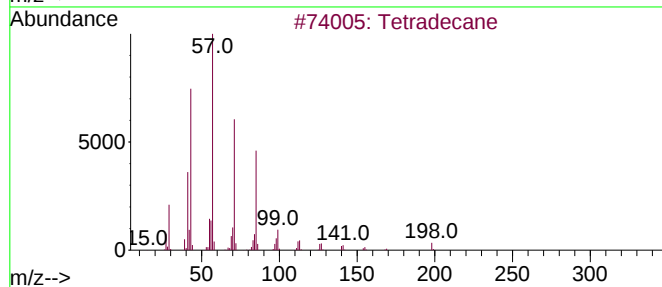
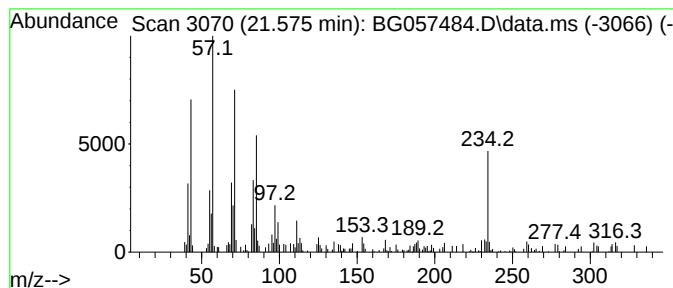
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Peak Number 5 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.575	3.97 ng	73602	Chrysene-d12	22.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	70
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	64
3			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	58
4			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	58
5			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	58



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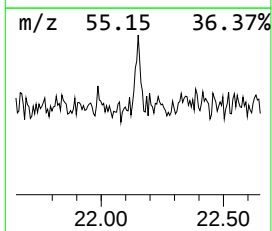
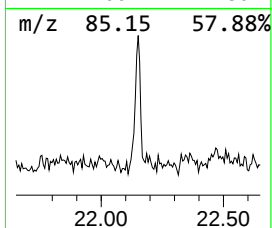
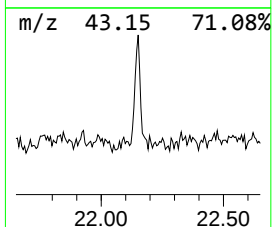
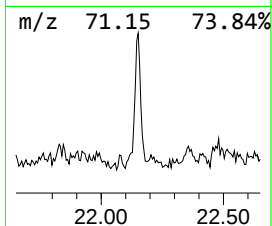
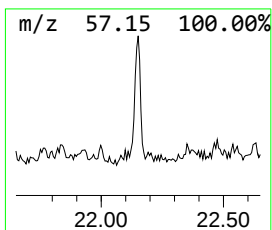
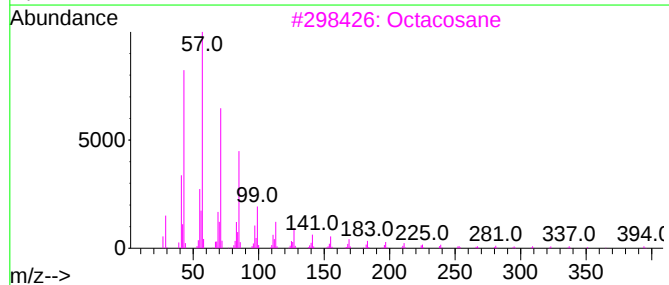
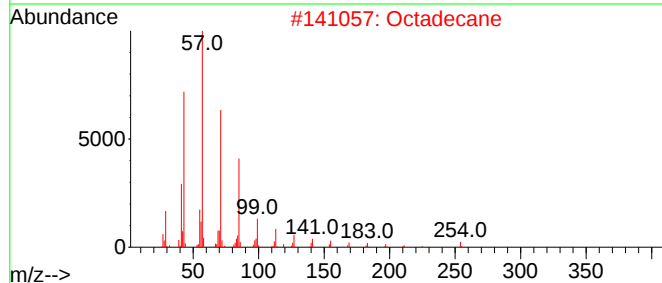
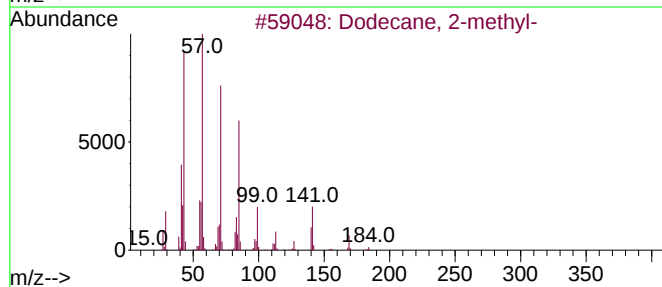
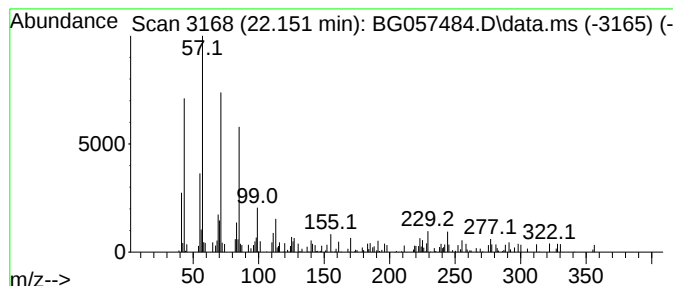
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.151	3.50 ng	64916	Chrysene-d12	22.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	76
2			Octadecane	254	C18H38	000593-45-3	68
3			Octacosane	394	C28H58	000630-02-4	64
4			Tetratriacontane	479	C34H70	014167-59-0	64
5			10-Methylnonadecane	282	C20H42	056862-62-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057484.D
Acq On : 20 May 2023 2:27
Operator : CG/JU
Sample : 02826-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-3-051723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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-...	5.385	14.3	ng	104707	1	8.358	146329	20.0
Benzophenone	16.306	2.8	ng	39370	3	14.967	277391	20.0
n-Hexadecanoic ...	18.550	6.3	ng	105207	4	17.710	334468	20.0
Dodecane, 2-met...	21.041	2.1	ng	38194	5	22.016	371159	20.0
Tetradecane	21.575	4.0	ng	73602	5	22.016	371159	20.0
Octadecane	22.151	3.5	ng	64916	5	22.016	371159	20.0