

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
 Data File : BG057474.D
 Acq On : 19 May 2023 19:33
 Operator : CG/JU
 Sample : 02848-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP5

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: BG057474.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	308	314	321	rBB	14258	22054	2.10%	0.409%
2	5.872	391	397	407	rBV	228198	372499	35.50%	6.908%
3	7.493	666	673	685	rBV	239477	422400	40.25%	7.834%
4	8.357	812	820	826	rBV	60840	102004	9.72%	1.892%
5	9.532	1013	1020	1029	rBV	143522	256960	24.49%	4.766%
6	11.188	1294	1302	1312	rBV	76908	137845	13.14%	2.556%
7	13.591	1704	1711	1719	rBV	431973	655540	62.47%	12.158%
8	14.913	1930	1936	1940	rBV2	35784	52467	5.00%	0.973%
9	14.966	1940	1945	1951	rBV2	141319	219457	20.91%	4.070%
10	15.195	1979	1984	1988	rVB2	11729	15012	1.43%	0.278%
11	15.265	1990	1996	2002	rBV4	7912	12433	1.18%	0.231%
12	16.305	2164	2173	2180	rBV	36734	63777	6.08%	1.183%
13	16.411	2180	2191	2192	rBV3	14317	19506	1.86%	0.362%
14	16.452	2192	2198	2204	rVB	359988	545812	52.01%	10.123%
15	17.709	2405	2412	2418	rBV	199983	298437	28.44%	5.535%
16	18.549	2550	2555	2563	rBV2	36340	62854	5.99%	1.166%
17	19.800	2764	2768	2774	rBV5	8994	15691	1.50%	0.291%
18	20.118	2818	2822	2827	rBV8	6761	10567	1.01%	0.196%
19	20.276	2844	2849	2862	rVB	834957	1049434	100.00%	19.463%
20	21.234	3008	3012	3016	rVB4	10667	14840	1.41%	0.275%
21	21.410	3036	3042	3047	rBV	159984	220934	21.05%	4.097%
22	21.574	3065	3070	3084	rBV7	19809	57633	5.49%	1.069%
23	22.015	3138	3145	3151	rBV	189627	329200	31.37%	6.105%
24	22.796	3273	3278	3283	rBV7	6469	11360	1.08%	0.211%
25	23.536	3401	3404	3409	rVB5	8079	11311	1.08%	0.210%
26	24.394	3545	3550	3558	rBV2	16972	35605	3.39%	0.660%
27	25.428	3719	3726	3729	rBV8	8953	20037	1.91%	0.372%
28	25.510	3730	3740	3750	rVB	107349	316850	30.19%	5.876%
29	26.644	3926	3933	3944	rVB5	13762	39431	3.76%	0.731%

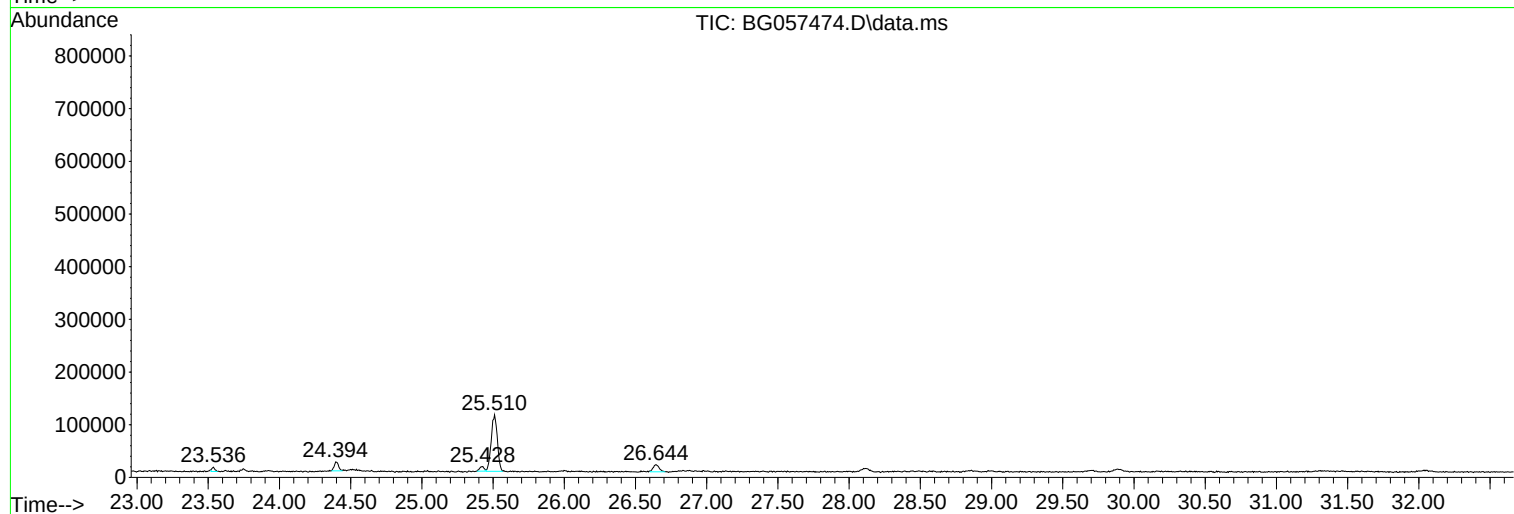
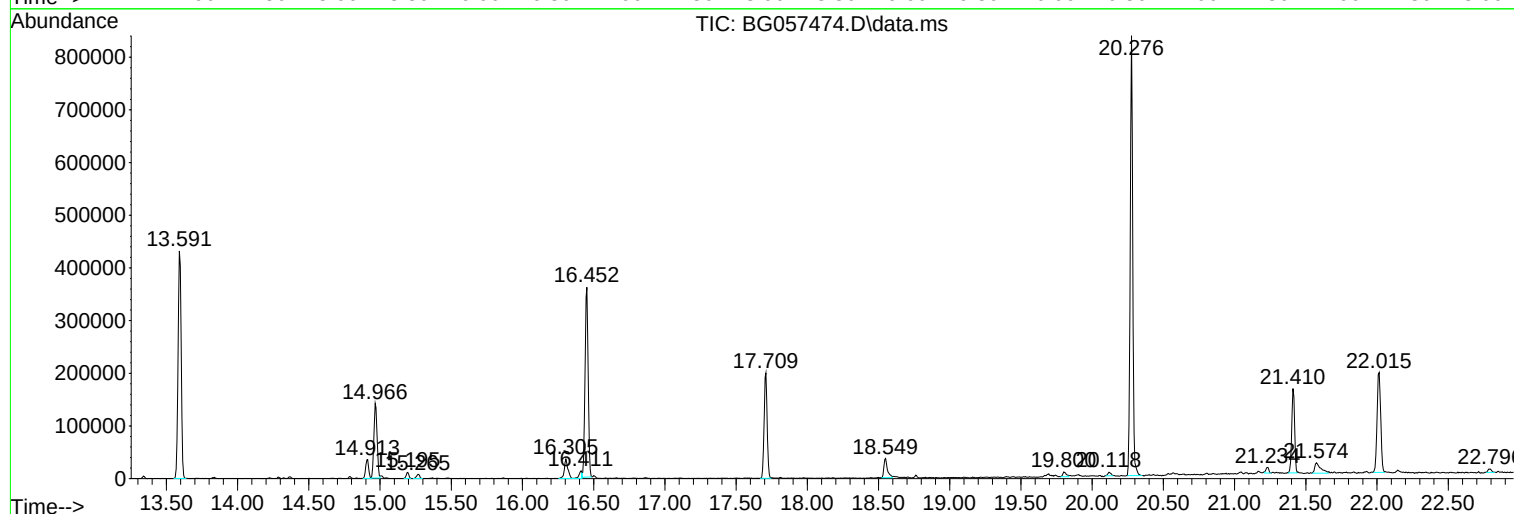
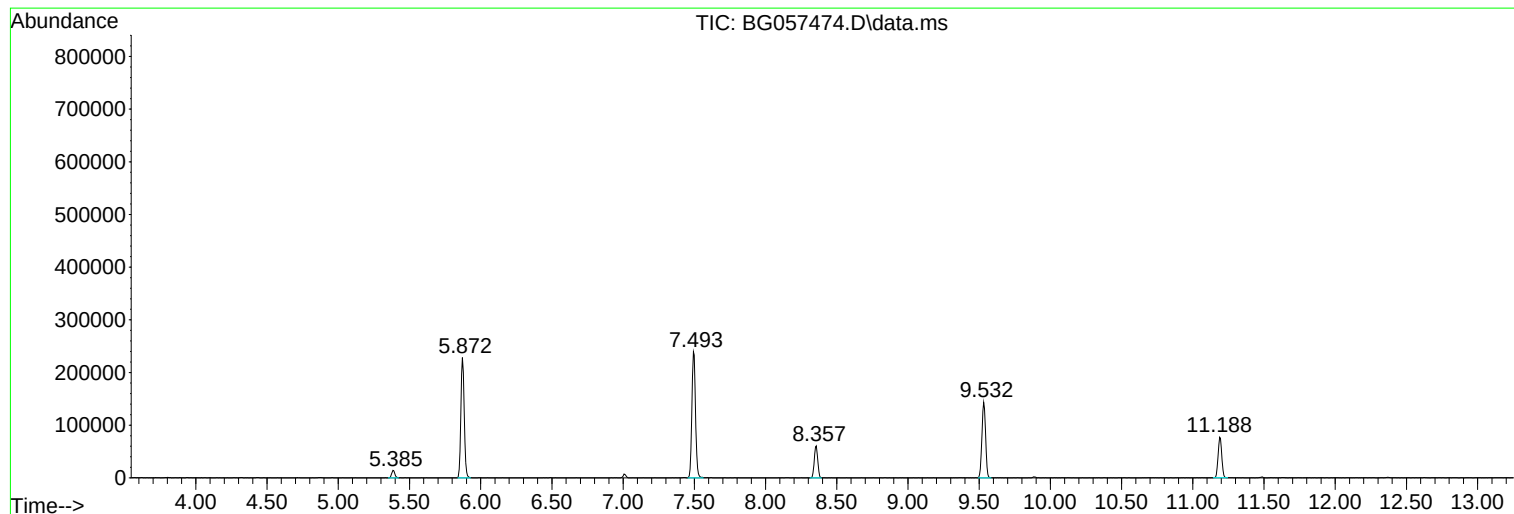
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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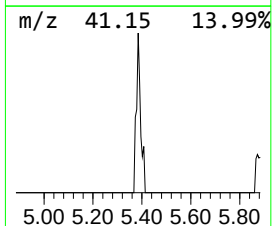
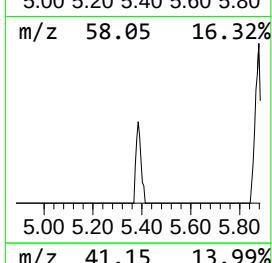
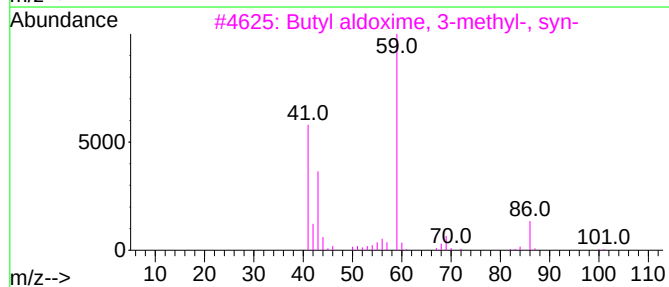
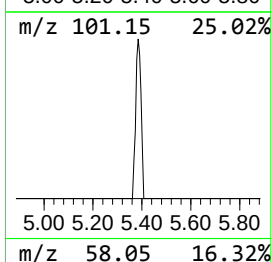
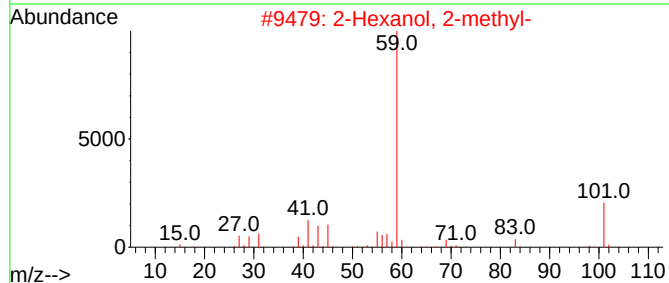
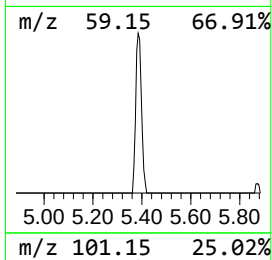
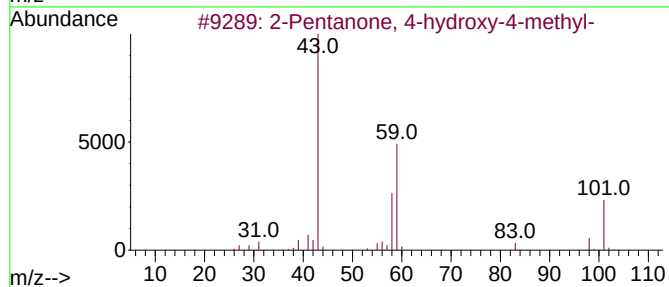
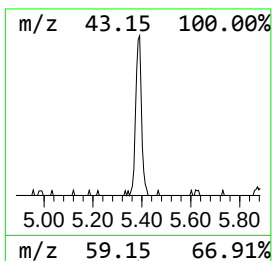
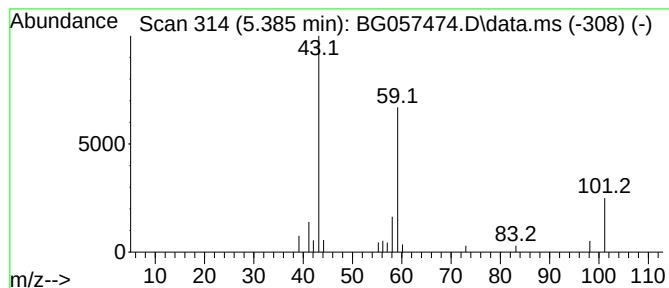
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	4.32 ng	22054	1,4-Dichlorobenzene-d4	8.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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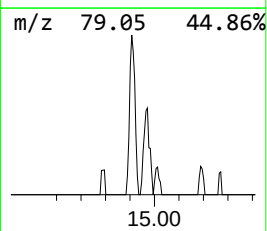
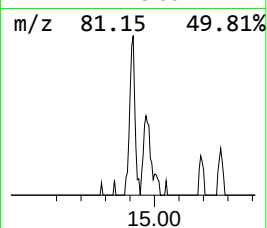
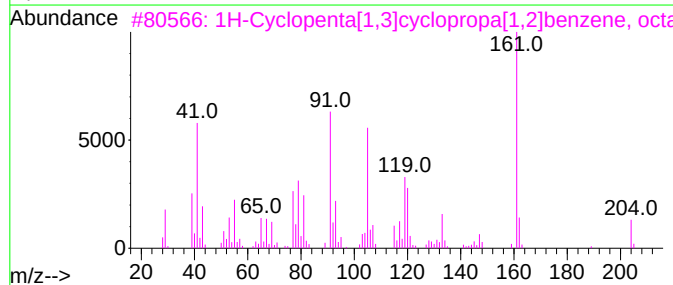
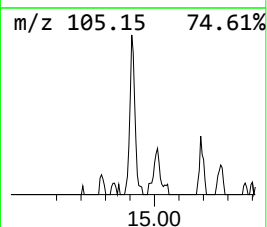
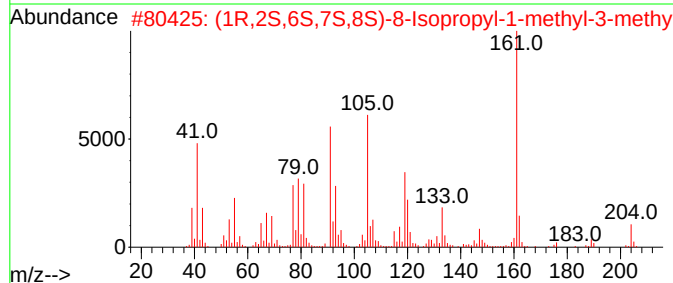
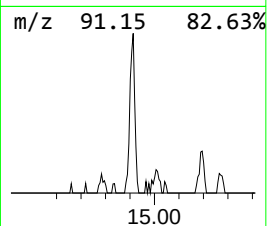
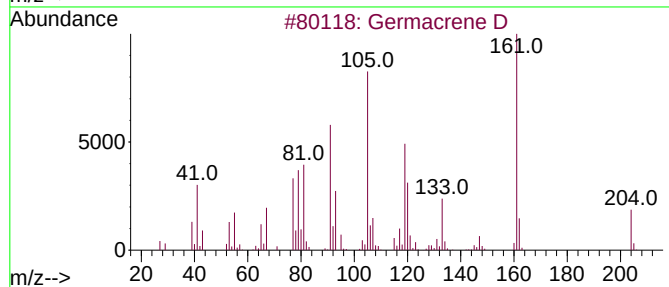
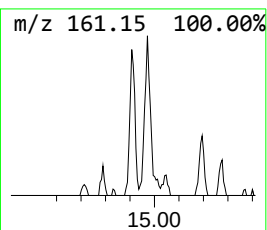
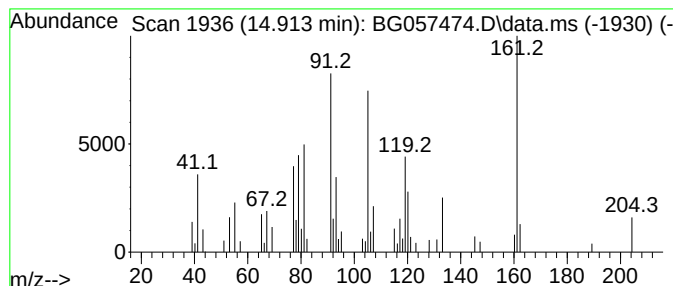
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Germacrene D Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.913	4.78 ng	52467	Acenaphthene-d10	14.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germacrene D	204	C15H24	023986-74-5	96
2			(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	94
3			1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	93
4			cis-Muurolo-4(15),5-diene	204	C15H24	157477-72-0	78
5			.alpha.-Cubebene	204	C15H24	017699-14-8	60



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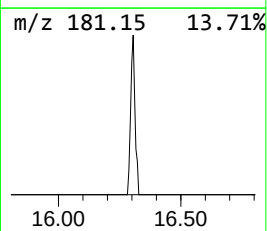
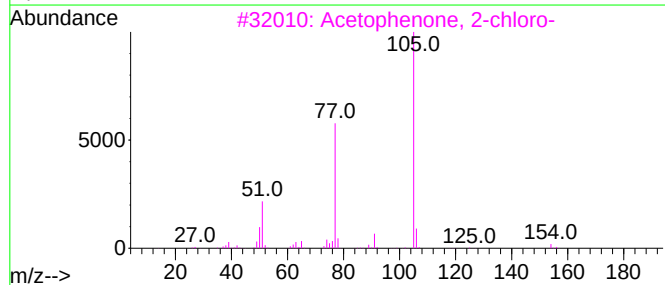
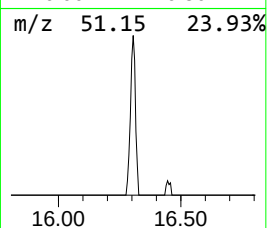
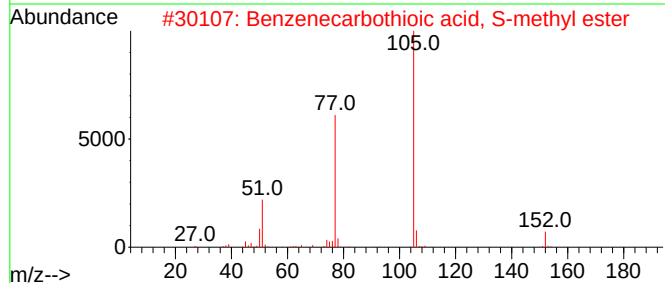
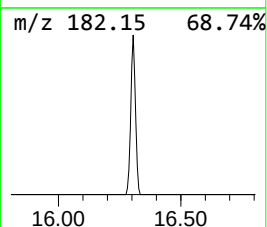
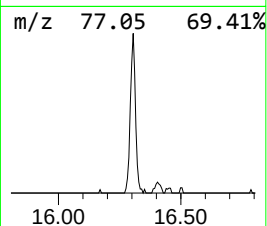
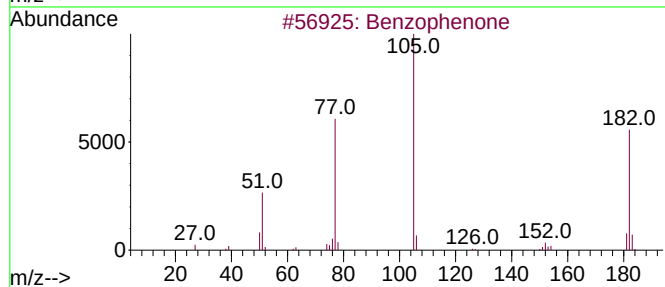
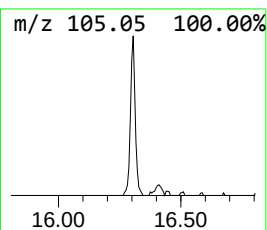
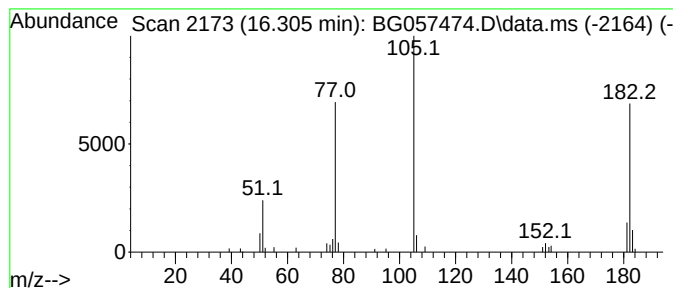
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.305	5.81 ng	63777	Acenaphthene-d10	14.966

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	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43



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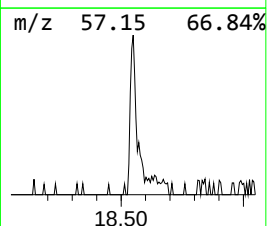
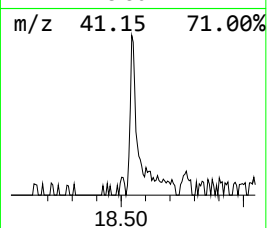
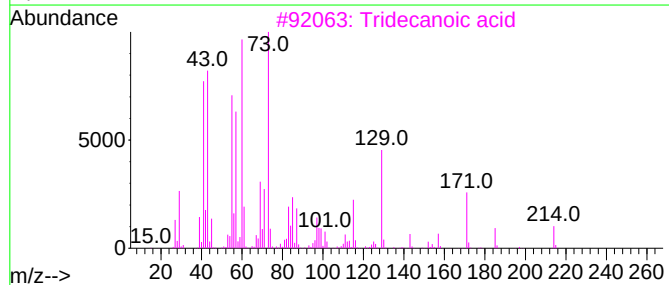
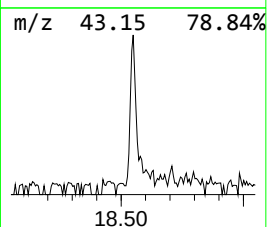
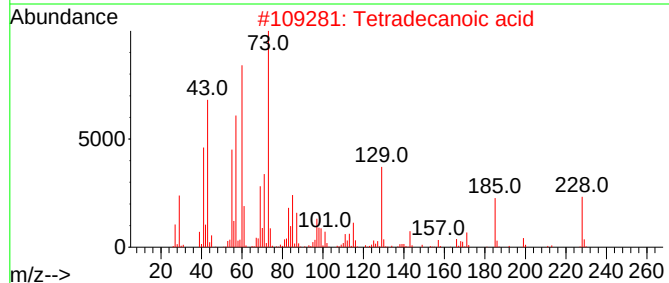
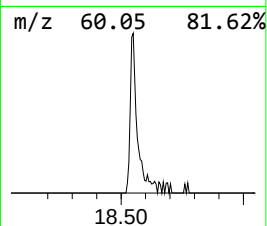
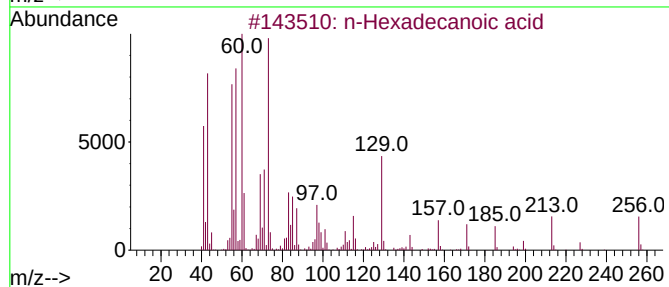
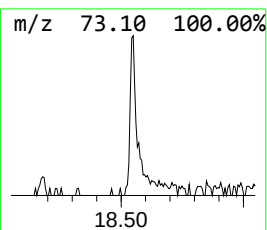
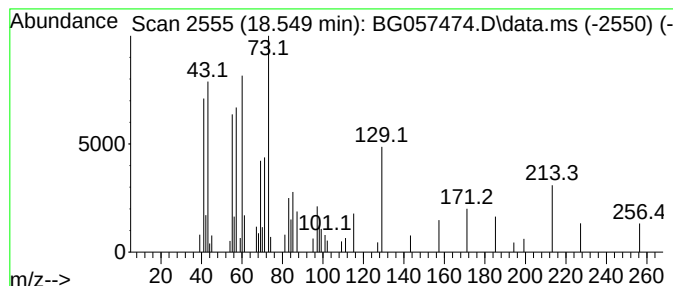
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.549	4.21 ng	62854	Phenanthrene-d10	17.709

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3		Tridecanoic acid	214	C13H26O2	000638-53-9	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		n-Decanoic acid	172	C10H20O2	000334-48-5	43



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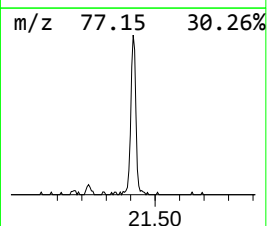
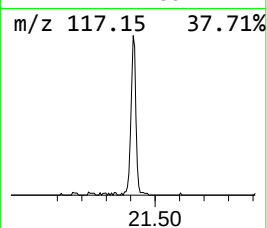
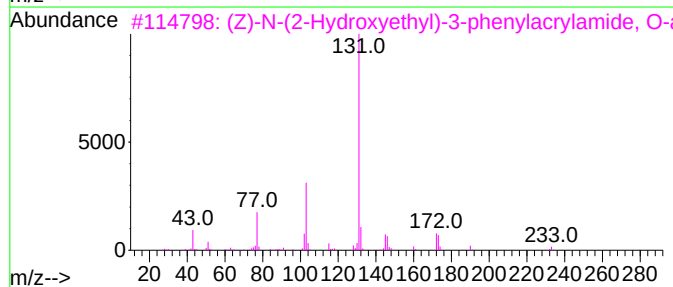
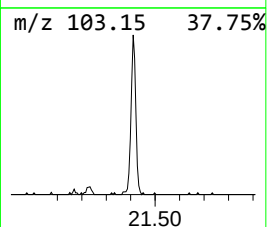
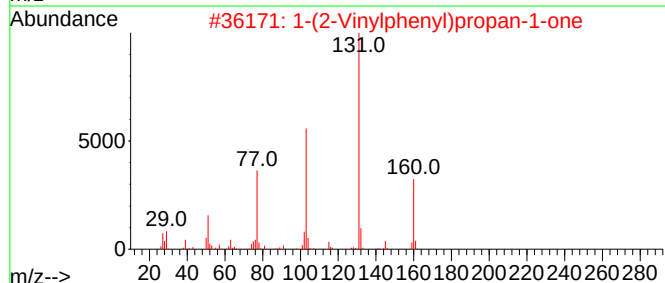
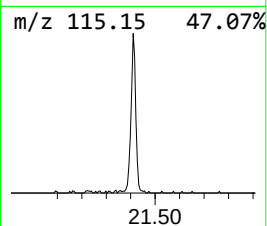
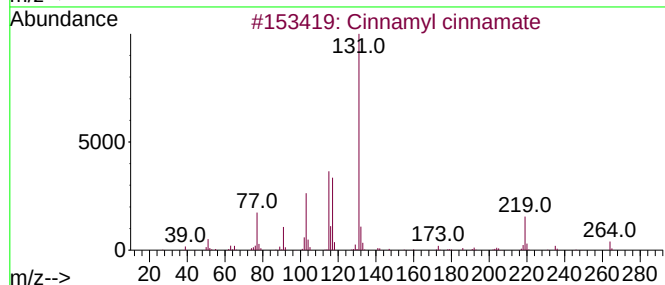
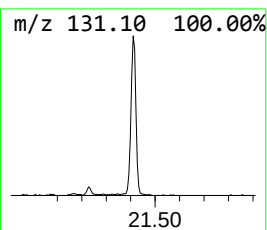
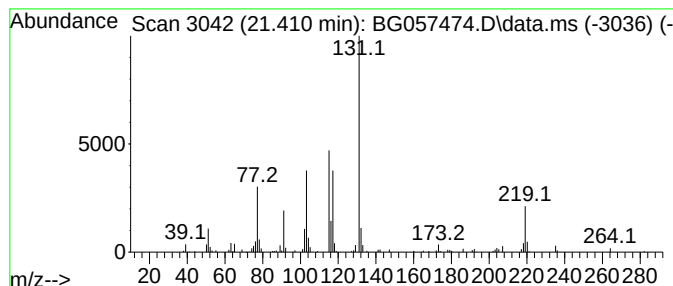
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Peak Number 5 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	13.42 ng	220934	Chrysene-d12	22.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			1-(2-Vinylphenyl)propan-1-one	160	C11H12O	052095-41-7	47
3			(Z)-N-(2-Hydroxyethyl)-3-phenyla...	233	C13H15NO3	1000512-63-0	47
4			N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	47
5			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47



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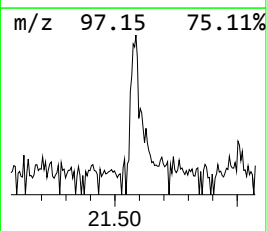
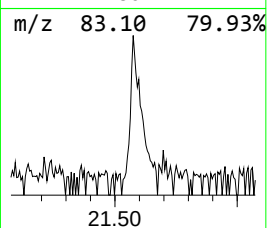
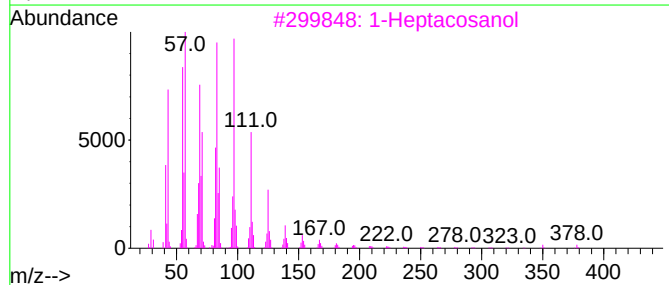
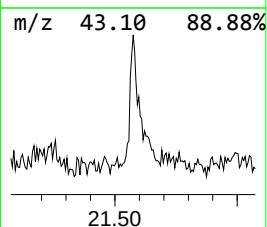
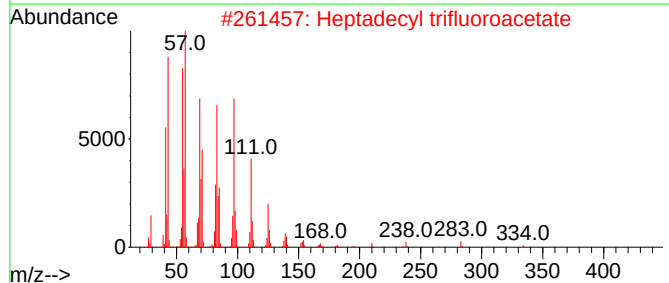
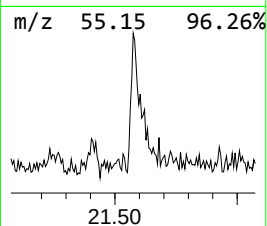
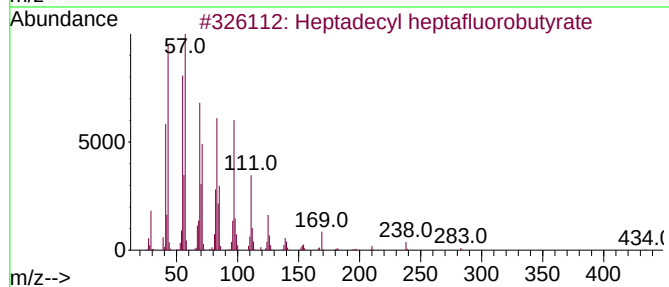
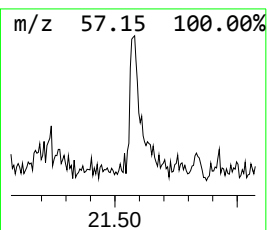
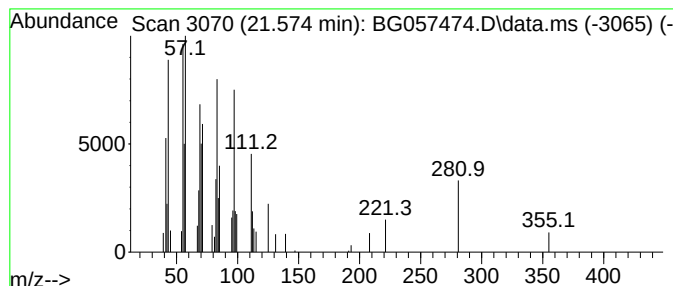
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.574	3.50 ng	57633	Chrysene-d12	22.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
3			1-Heptacosanol	396	C27H56O	002004-39-9	90
4			Pentafluoropropionic acid, hexadec...	388	C19H33F5O2	006222-07-7	90
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057474.D
Acq On : 19 May 2023 19:33
Operator : CG/JU
Sample : 02848-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP5

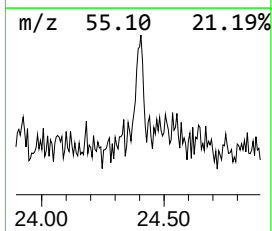
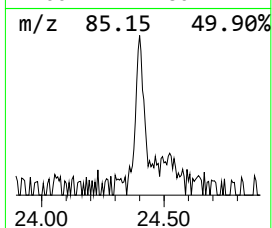
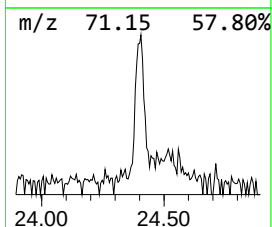
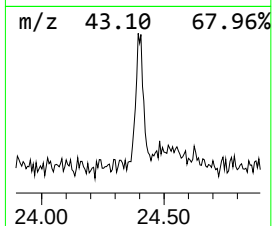
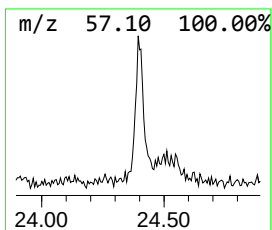
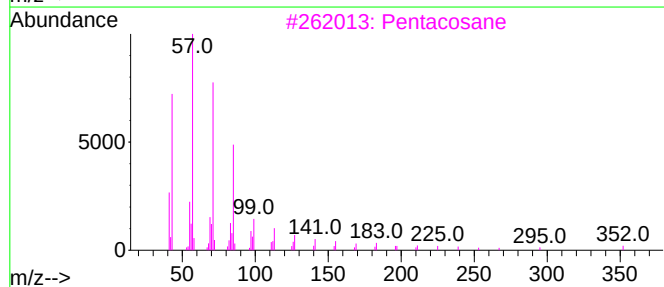
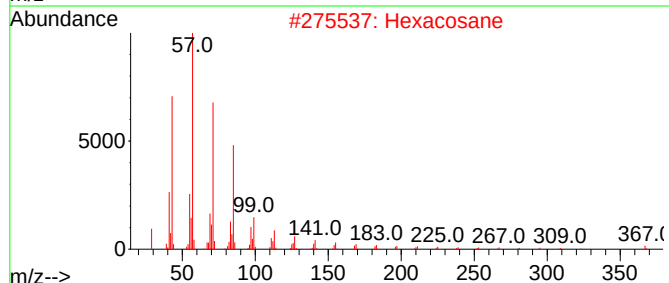
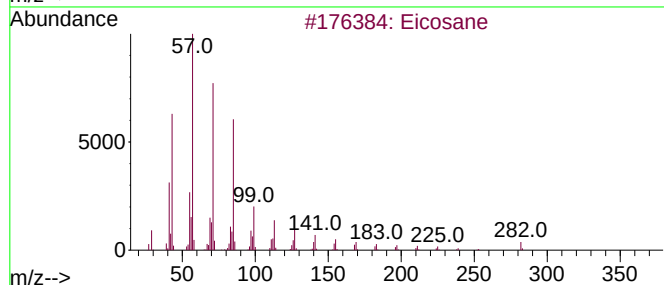
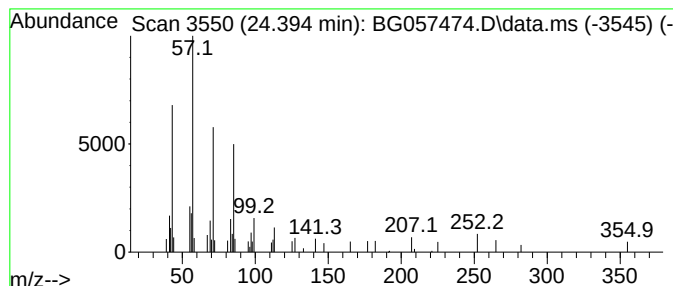
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.394	2.25 ng	35605	Perylene-d12	25.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Hexacosane	366	C26H54	000630-01-3	87
3			Pentacosane	352	C25H52	000629-99-2	83
4			Nonadecane	268	C19H40	000629-92-5	83
5			Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057474.D
Acq On : 19 May 2023 19:33
Operator : CG/JU
Sample : 02848-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

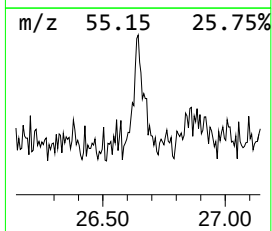
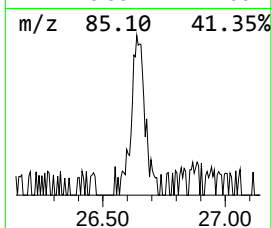
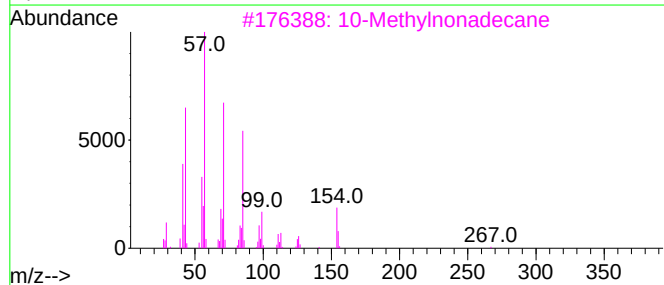
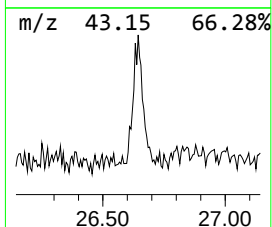
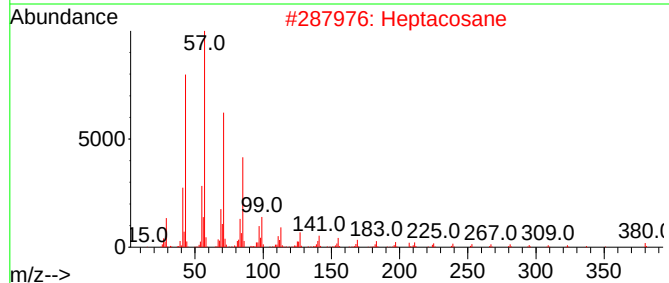
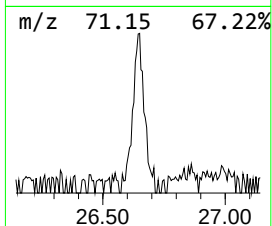
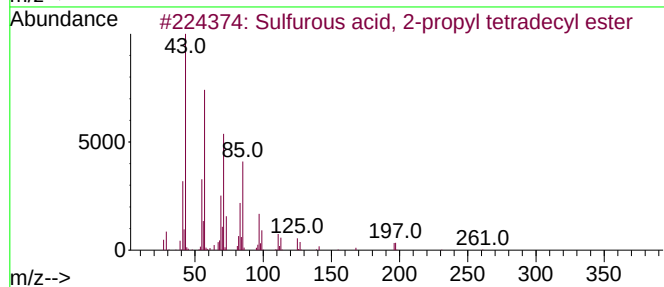
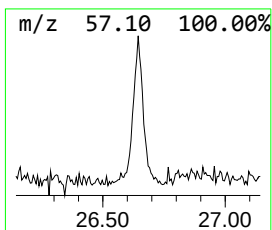
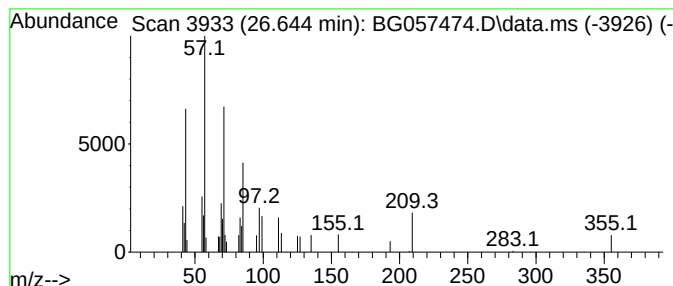
Instrument :
BNA_G
ClientSampleId :
TP5

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

Peak Number 8 Sulfurous acid, 2-propyl te... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
26.644	2.49 ng	39431	Perylene-d12		25.510	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetradec...		320	C17H36O3S	1010309-12-5	80
2	Heptacosane		380	C27H56	000593-49-7	72
3	10-Methylnonadecane		282	C20H42	056862-62-5	64
4	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	59
5	Nonadecane		268	C19H40	000629-92-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057474.D
Acq On : 19 May 2023 19:33
Operator : CG/JU
Sample : 02848-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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-...	5.385	4.3	ng	22054	1	8.351	102004	20.0
Germacrene D	14.913	4.8	ng	52467	3	14.966	219457	20.0
Benzophenone	16.305	5.8	ng	63777	3	14.966	219457	20.0
n-Hexadecanoic ...	18.549	4.2	ng	62854	4	17.709	298437	20.0
Cinnamyl cinnamate	21.410	13.4	ng	220934	5	22.015	329200	20.0
Heptadecyl hept...	21.574	3.5	ng	57633	5	22.015	329200	20.0
Eicosane	24.394	2.3	ng	35605	6	25.510	316850	20.0
Sulfurous acid,...	26.644	2.5	ng	39431	6	25.510	316850	20.0