

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
 Data File : BG055970.D
 Acq On : 14 Dec 2022 22:11
 Operator : CG/JU
 Sample : N6023-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WASTE

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055970.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.408	15	20	25	rBV	16972	24824	5.00%	1.086%
2	5.417	357	362	368	rBB	10819	16024	3.23%	0.701%
3	5.887	436	442	449	rBB	84446	131647	26.54%	5.759%
4	7.497	709	716	723	rBB	90139	150920	30.42%	6.602%
5	8.372	859	865	871	rBB	27256	42085	8.48%	1.841%
6	9.542	1057	1064	1071	rBB	54574	93170	18.78%	4.076%
7	11.204	1340	1347	1354	rBV	34836	58225	11.74%	2.547%
8	13.607	1749	1756	1763	rBB	202455	296016	59.67%	12.950%
9	14.976	1983	1989	1996	rVB	61301	93250	18.80%	4.079%
10	16.316	2211	2217	2222	rBV	42373	63805	12.86%	2.791%
11	16.451	2234	2240	2249	rBV	202828	309279	62.34%	13.530%
12	16.645	2271	2273	2275	rBV3	4721	5518	1.11%	0.241%
13	16.674	2275	2278	2282	rVB4	6177	8788	1.77%	0.384%
14	16.774	2291	2295	2298	rBV2	9448	13628	2.75%	0.596%
15	16.827	2302	2304	2308	rVV4	9146	13373	2.70%	0.585%
16	16.892	2310	2315	2319	rVV6	6608	12756	2.57%	0.558%
17	16.939	2319	2323	2328	rVV8	4340	7771	1.57%	0.340%
18	17.162	2357	2361	2364	rBV	10330	14038	2.83%	0.614%
19	17.233	2371	2373	2377	rBV4	6729	8737	1.76%	0.382%
20	17.444	2406	2409	2414	rBV6	8143	11617	2.34%	0.508%
21	17.714	2450	2455	2459	rBV	83404	124604	25.12%	5.451%
22	17.755	2459	2462	2471	rVB	38536	61498	12.40%	2.690%
23	18.572	2597	2601	2606	rBV6	26962	47423	9.56%	2.075%
24	19.747	2797	2801	2806	rVB	82693	115131	23.21%	5.037%
25	20.106	2860	2862	2867	rVB	55699	65577	13.22%	2.869%
26	20.294	2889	2894	2899	rVB	395786	496121	100.00%	21.704%

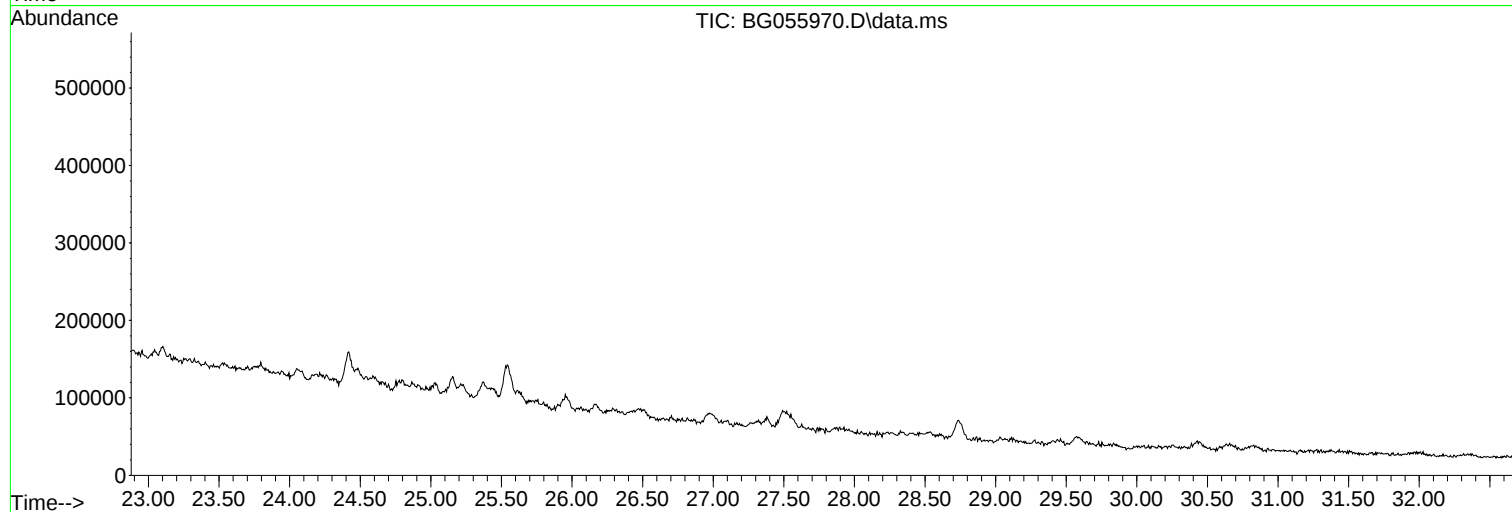
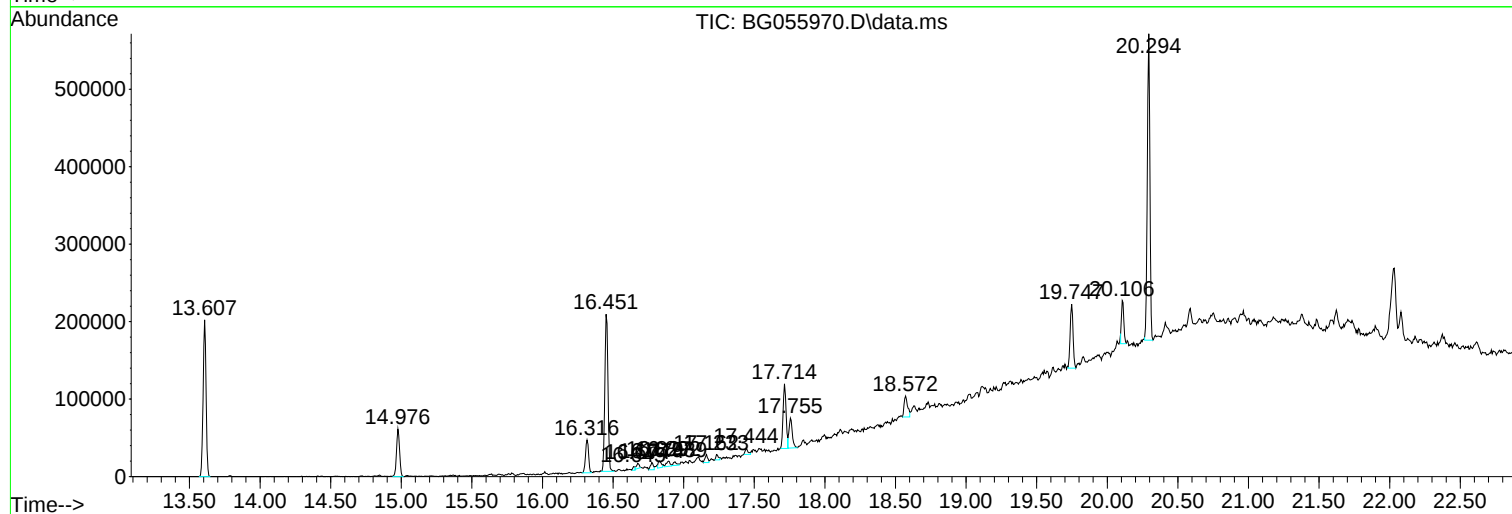
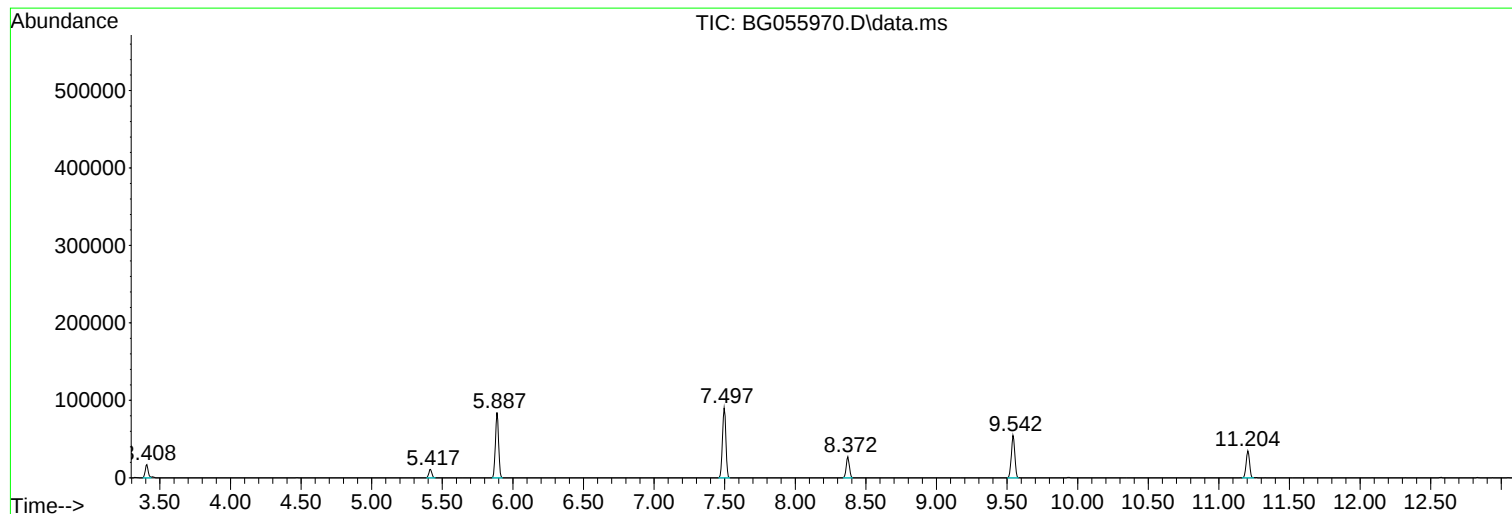
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Instrument :
BNA_G
ClientSampleId :
WASTE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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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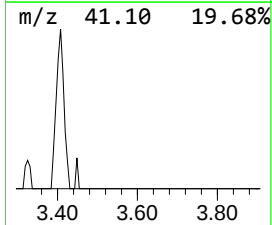
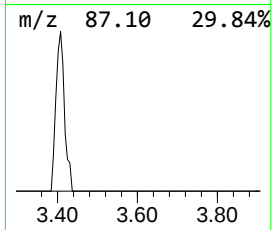
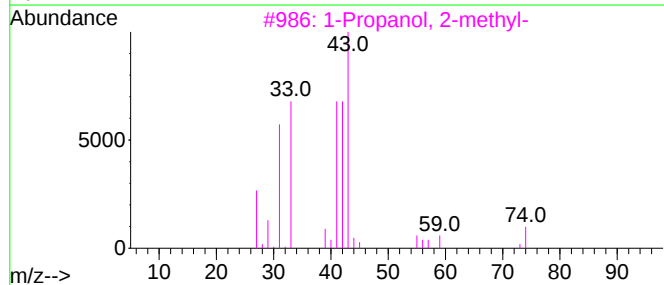
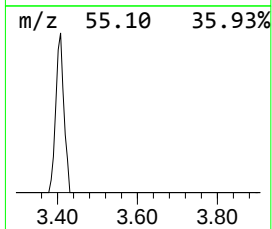
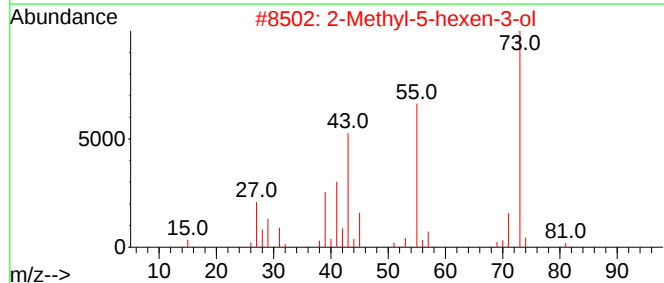
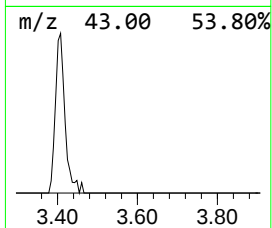
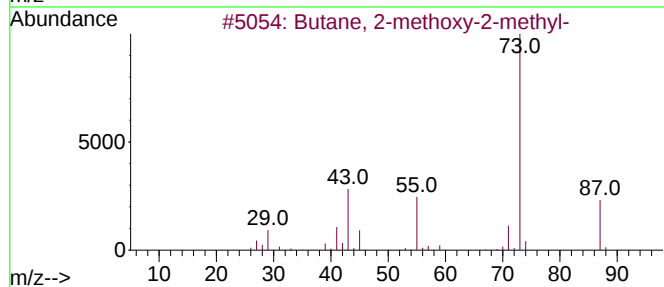
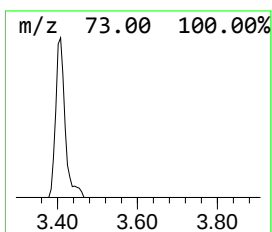
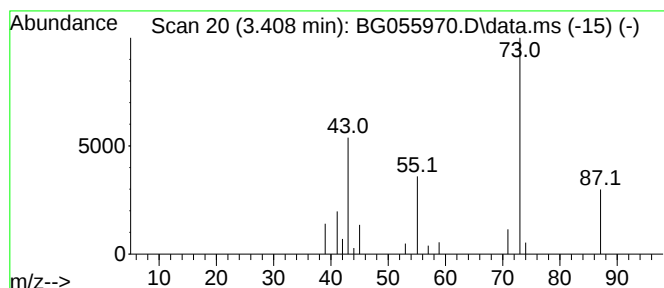
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.408	11.80 ng	24824	1,4-Dichlorobenzene-d4	8.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5			1-Hepten-4-ol	114	C7H14O	003521-91-3	9



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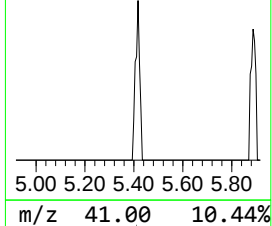
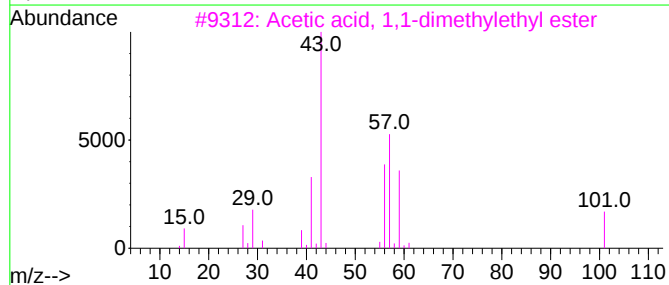
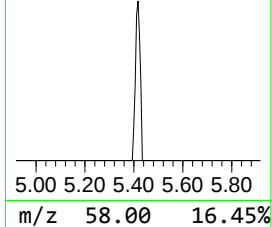
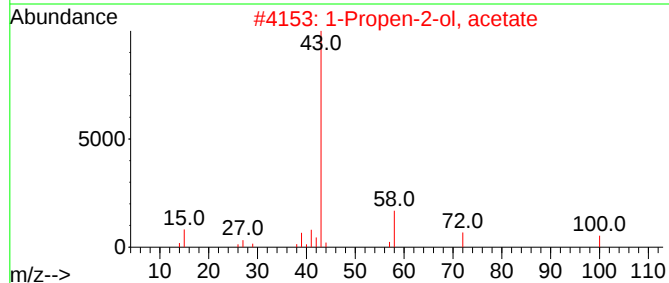
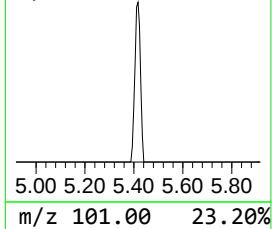
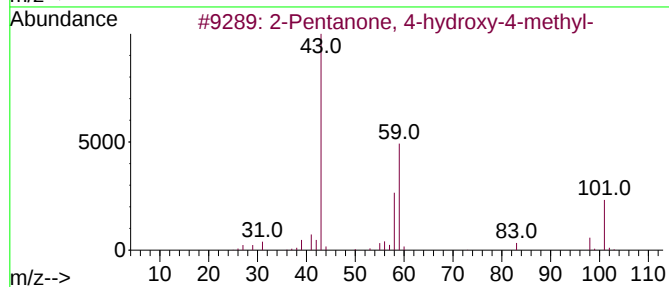
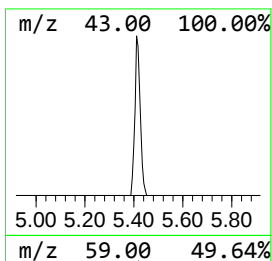
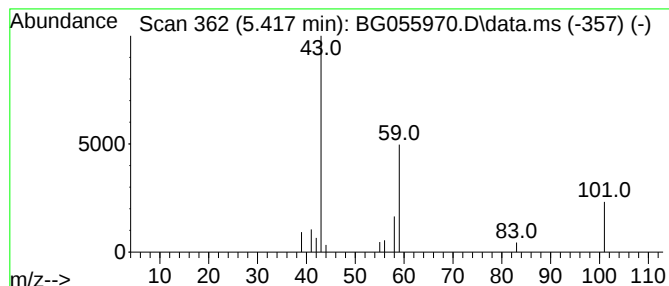
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.417	7.62 ng	16024	1,4-Dichlorobenzene-d4	8.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			Acetone	58	C3H6O	000067-64-1	7
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7



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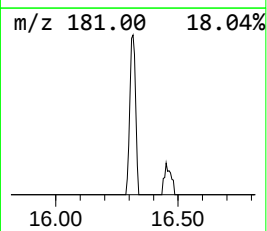
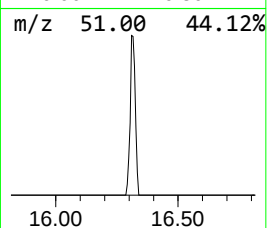
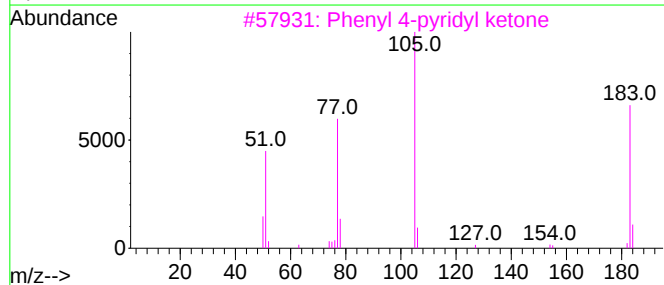
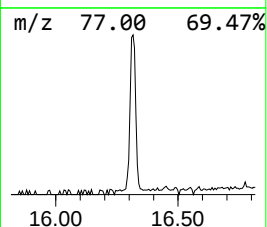
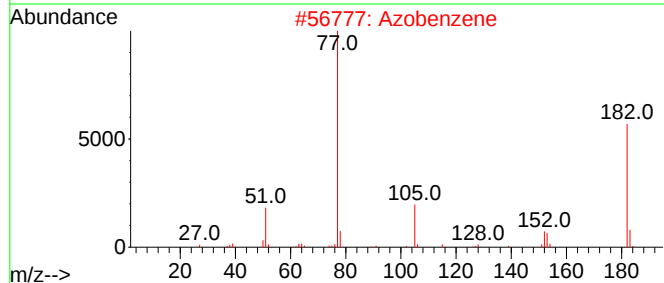
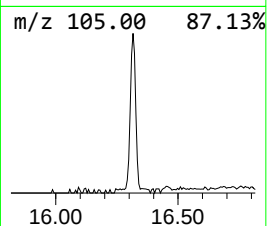
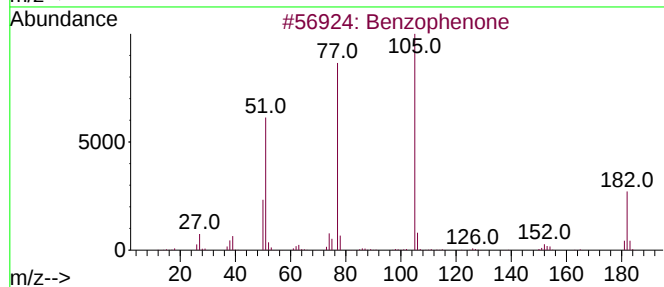
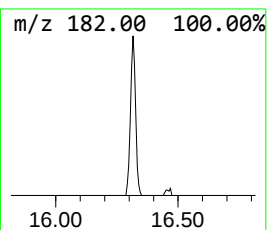
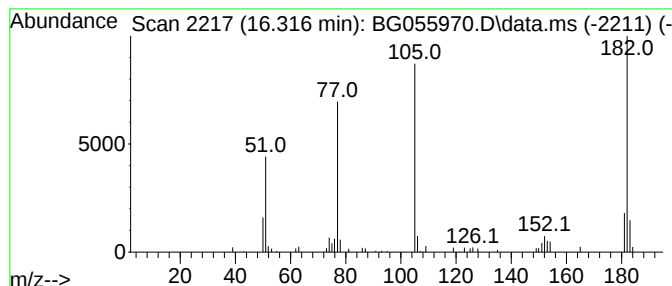
Instrument :
BNA_G
ClientSampleId :
WASTE

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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 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.316	13.68 ng	63805	Acenaphthene-d10		14.976
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	53
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
5	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	43



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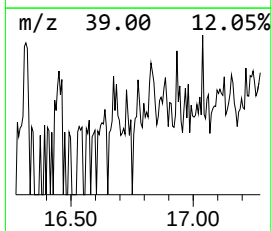
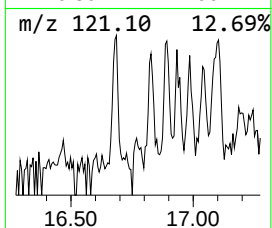
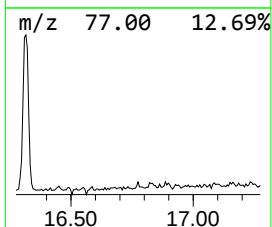
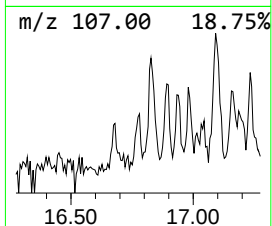
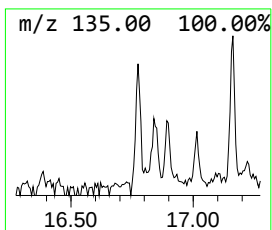
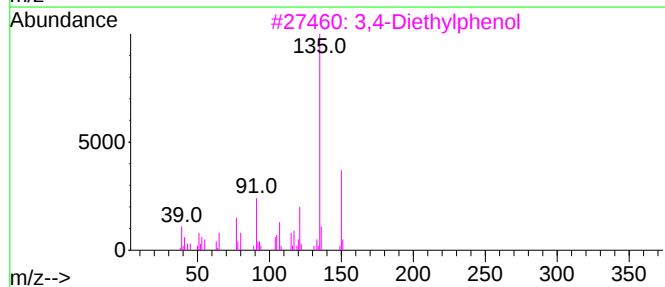
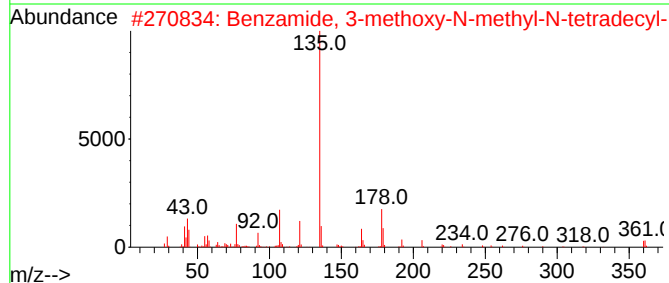
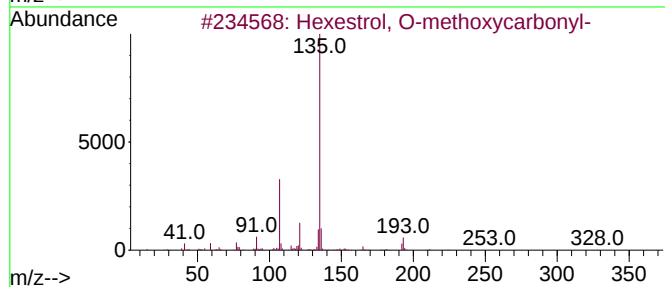
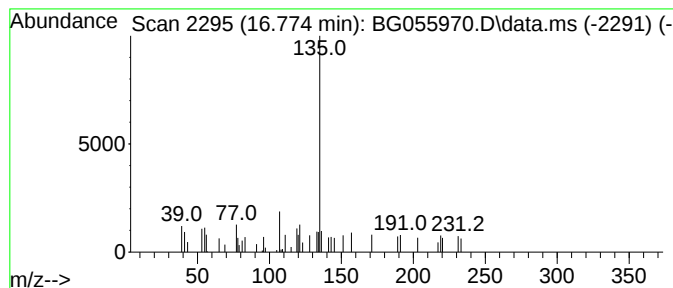
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexestrol, O-methoxycarbonyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	2.19 ng	13628	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexestrol, O-methoxycarbonyl-	328	C20H24O4	1000487-66-3	59
2			Benzamide, 3-methoxy-N-methyl-N...	361	C23H39NO2	1000449-93-4	53
3			3,4-Diethylphenol	150	C10H14O	000875-85-4	53
4			2-n-Hexyladamantane	220	C16H28	1000441-03-5	50
5			3,5-Dihydropyrrolo(3,2-d)pyrimid...	135	C6H5N3O	005655-01-6	50



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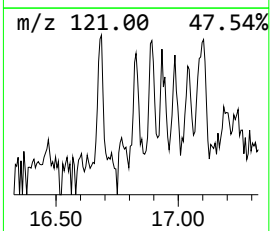
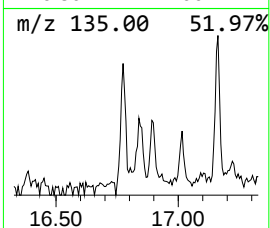
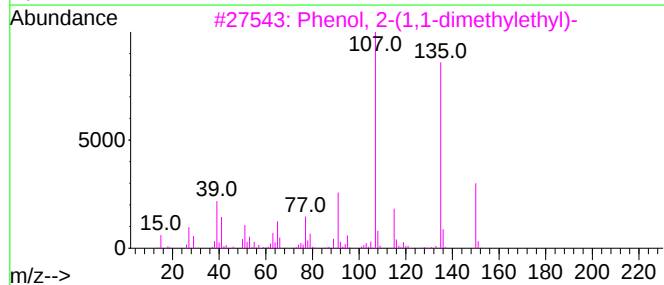
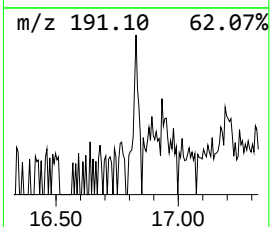
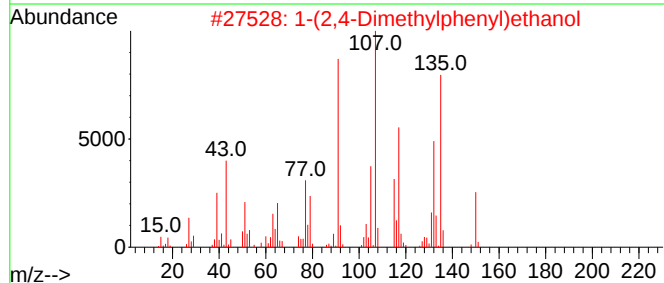
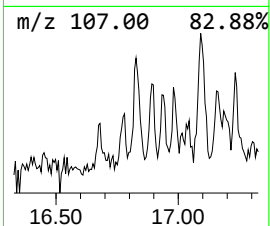
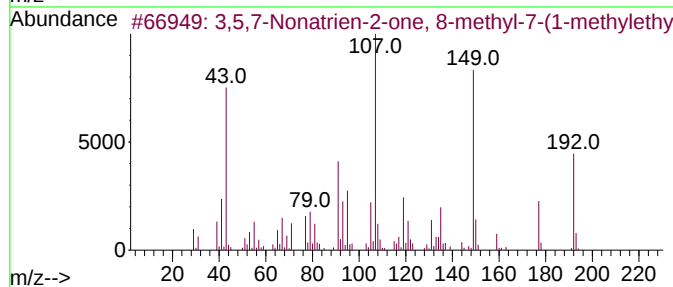
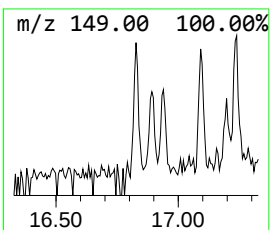
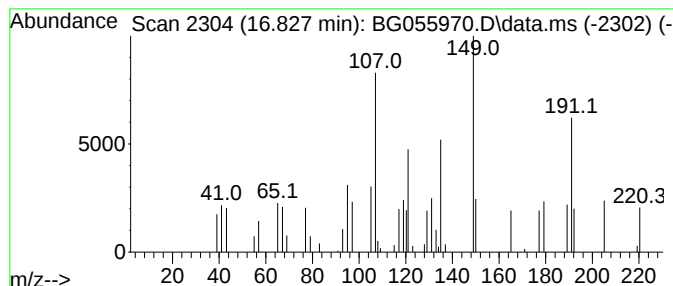
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.827 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.827	2.15 ng	13373	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5,7-Nonatrien-2-one, 8-methyl-...	192	C13H20O	070372-94-0	47
2			1-(2,4-Dimethylphenyl)ethanol	150	C10H14O	099500-87-5	14
3			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	14
4			N-(Chroman-5-yl)acetamide	191	C11H13NO2	1000306-69-8	12
5			Benzestrol	298	C20H26O2	000085-95-0	12



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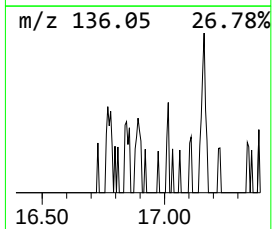
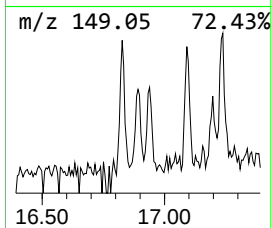
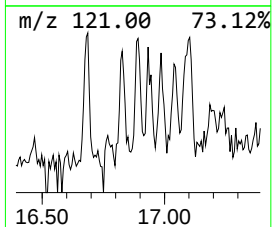
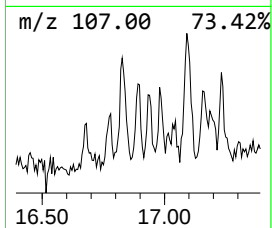
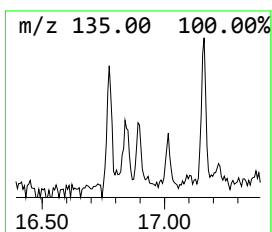
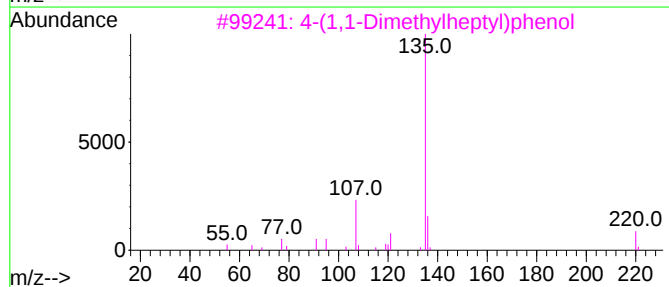
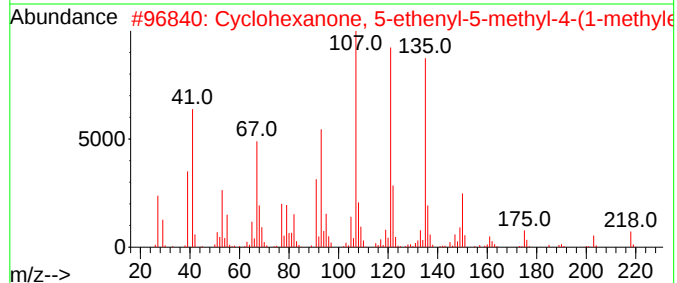
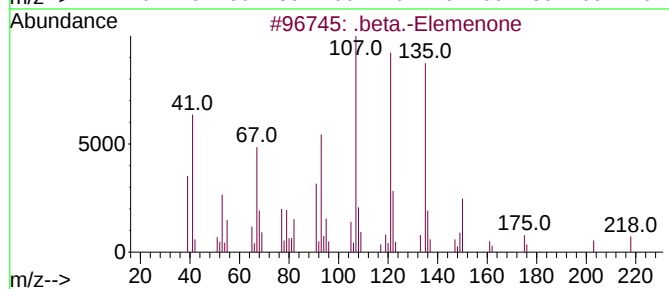
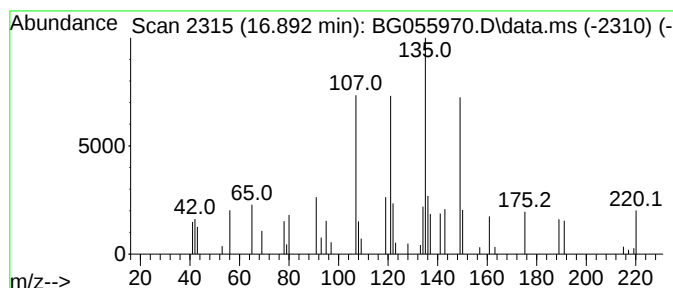
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.892 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	2.05 ng	12756	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-Elemenone	218	C15H22O	020303-60-0	43	
2	Cyclohexanone, 5-ethenyl-5-methy...	218	C15H22O	032663-57-3	43		
3	4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	38		
4	1H-Indene, 1-ethylideneoctahydro...	164	C12H20	056362-87-9	27		
5	1-[3-(2,6,6-Trimethyl-cyclohex-2...	234	C14H22N2O	1000185-64-0	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055970.D
Acq On : 14 Dec 2022 22:11
Operator : CG/JU
Sample : N6023-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

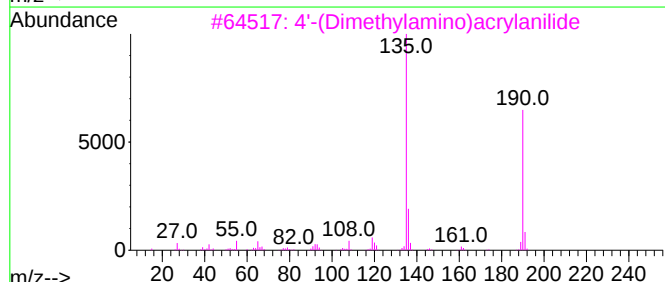
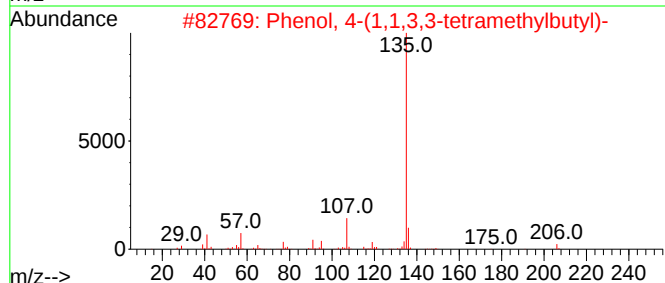
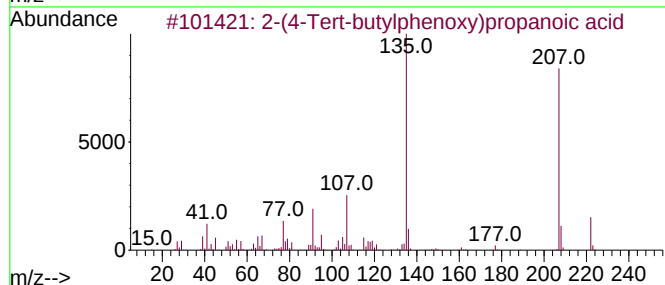
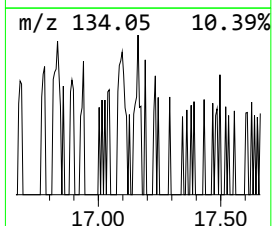
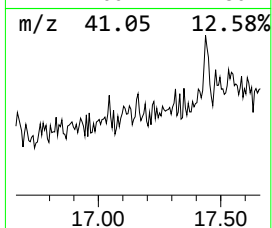
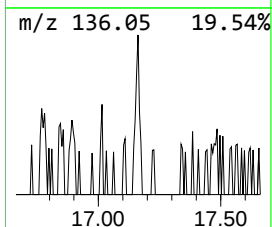
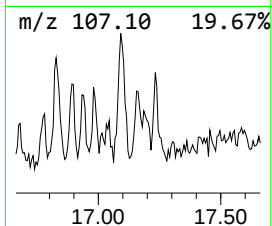
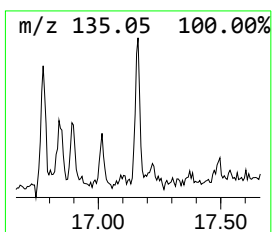
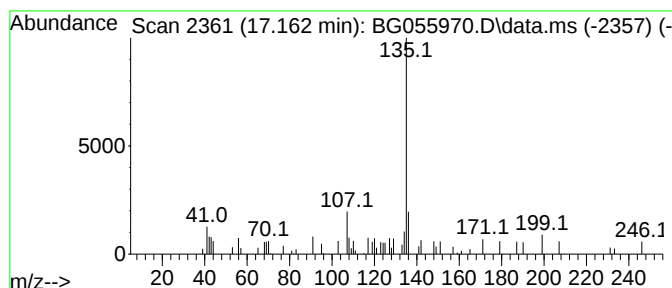
Instrument :
BNA_G
ClientSampleId :
WASTE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-(4-Tert-butylphenoxy)prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.162	2.25 ng	14038	Phenanthrene-d10	17.714	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Tert-butylphenoxy)propanoic...	222	C13H18O3	006941-12-4	53
2	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	50
3	4'-(Dimethylamino)acrylanilide	190	C11H14N2O	013304-63-7	50
4	4-tert-Butylphenol, 0-ethoxycarb...	222	C13H18O3	026177-66-2	50
5	2-(4-Tert-butylphenoxy)ethanamine	193	C12H19NO	050634-73-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055970.D
Acq On : 14 Dec 2022 22:11
Operator : CG/JU
Sample : N6023-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WASTE

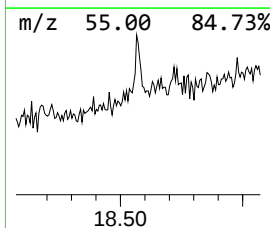
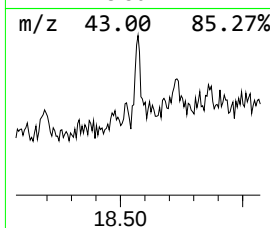
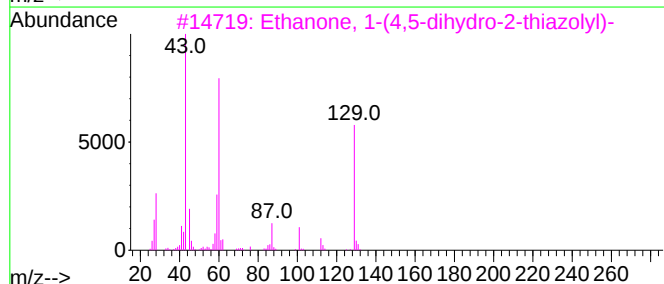
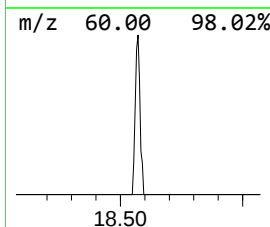
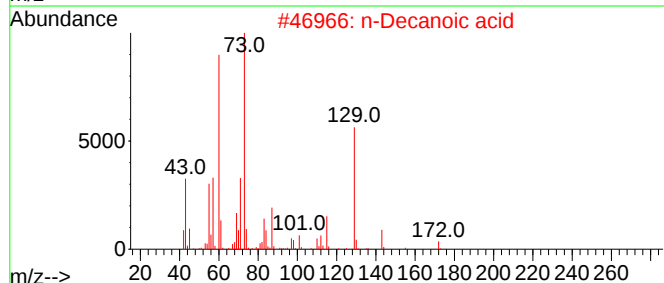
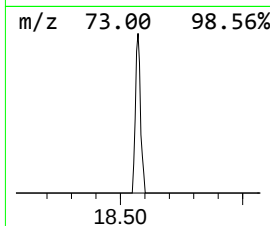
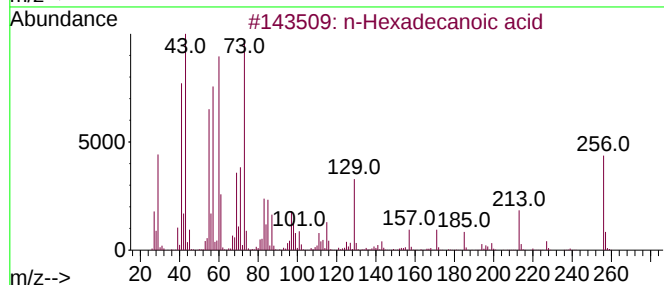
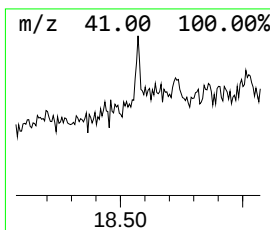
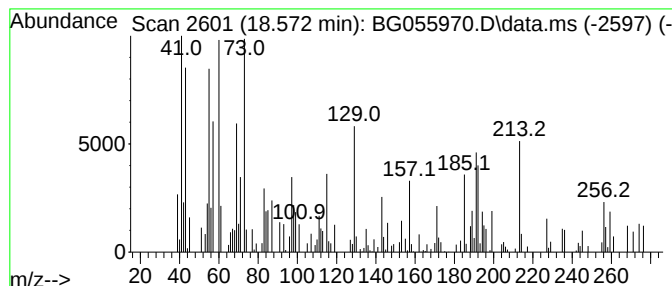
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.572	7.61 ng	47423	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2			n-Decanoic acid	172	C10H20O2	000334-48-5	42
3			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	30
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055970.D
Acq On : 14 Dec 2022 22:11
Operator : CG/JU
Sample : N6023-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WASTE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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
Butane, 2-metho...	3.408	11.8	ng	24824	1	8.372	42085	20.0
2-Pentanone, 4-...	5.417	7.6	ng	16024	1	8.372	42085	20.0
Benzophenone	16.316	13.7	ng	63805	3	14.976	93250	20.0
Hexestrol, O-me...	16.774	2.2	ng	13628	4	17.714	124604	20.0
unknown16.827	16.827	2.1	ng	13373	4	17.714	124604	20.0
unknown16.892	16.892	2.0	ng	12756	4	17.714	124604	20.0
2-(4-Tert-butyl...	17.162	2.3	ng	14038	4	17.714	124604	20.0
n-Hexadecanoic ...	18.572	7.6	ng	47423	4	17.714	124604	20.0