

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
 Data File : BG057516.D
 Acq On : 23 May 2023 12:34
 Operator : CG/JU
 Sample : 02870-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP20

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: BG057516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.388	309	315	323	rBB	13109	20174	1.51%	0.297%
2	5.876	391	398	409	rBV	208331	357021	26.75%	5.260%
3	7.009	586	591	596	rBB2	10940	15658	1.17%	0.231%
4	7.497	666	674	685	rBV	269370	469018	35.14%	6.911%
5	8.355	813	820	831	rVB	70154	117039	8.77%	1.724%
6	9.535	1013	1021	1031	rVB	139765	253072	18.96%	3.729%
7	11.192	1295	1303	1310	rBV	89809	160499	12.03%	2.365%
8	13.595	1705	1712	1720	rBV	456638	695802	52.13%	10.252%
9	14.911	1927	1936	1941	rBV	253668	348923	26.14%	5.141%
10	14.969	1941	1946	1952	rVV	149712	224970	16.86%	3.315%
11	15.192	1979	1984	1988	rVB2	20445	25761	1.93%	0.380%
12	16.303	2165	2173	2181	rBV	40772	69579	5.21%	1.025%
13	16.408	2183	2191	2193	rVV2	22069	32964	2.47%	0.486%
14	16.450	2193	2198	2205	rVV	445041	676087	50.65%	9.962%
15	16.508	2205	2208	2216	rVB3	10072	15728	1.18%	0.232%
16	17.707	2406	2412	2419	rBV	213600	321667	24.10%	4.740%
17	18.547	2550	2555	2565	rBV2	27034	57793	4.33%	0.852%
18	20.274	2841	2849	2855	rBV	1025572	1334694	100.00%	19.666%
19	21.231	3008	3012	3017	rVB	27857	35409	2.65%	0.522%
20	21.413	3037	3043	3050	rVB	563917	747833	56.03%	11.019%
21	21.572	3065	3070	3081	rBV3	28923	63147	4.73%	0.930%
22	22.013	3139	3145	3154	rVB	210960	368978	27.65%	5.437%
23	23.534	3399	3404	3409	rVB4	7437	13403	1.00%	0.197%
24	25.514	3731	3741	3751	rVB2	117854	361677	27.10%	5.329%

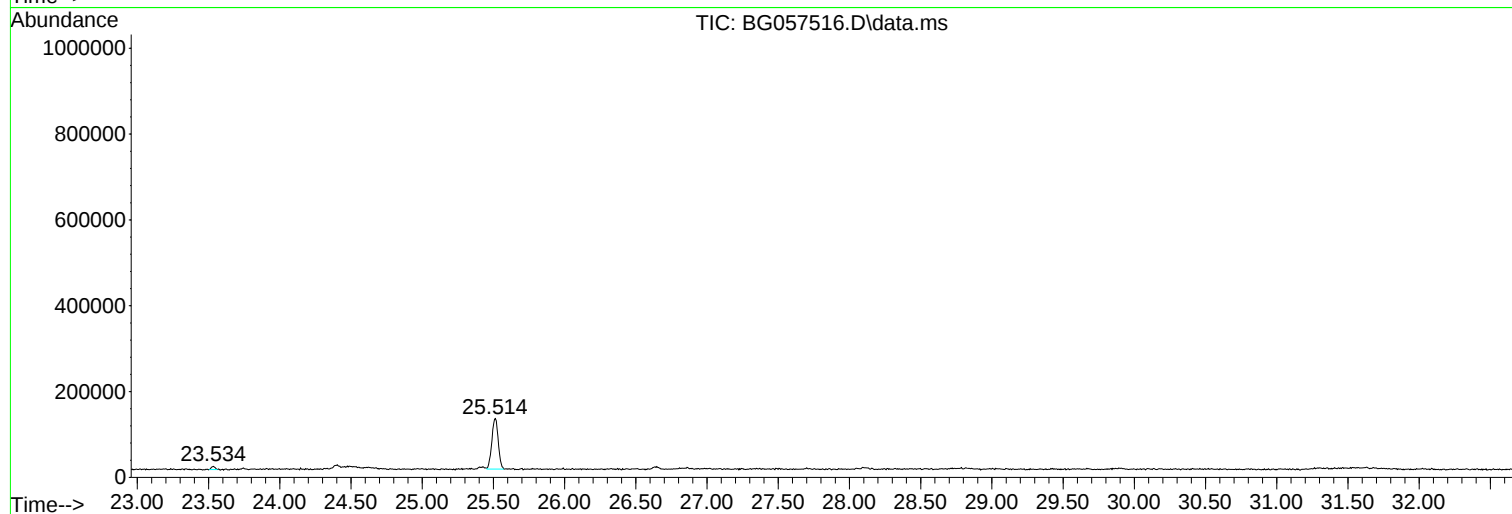
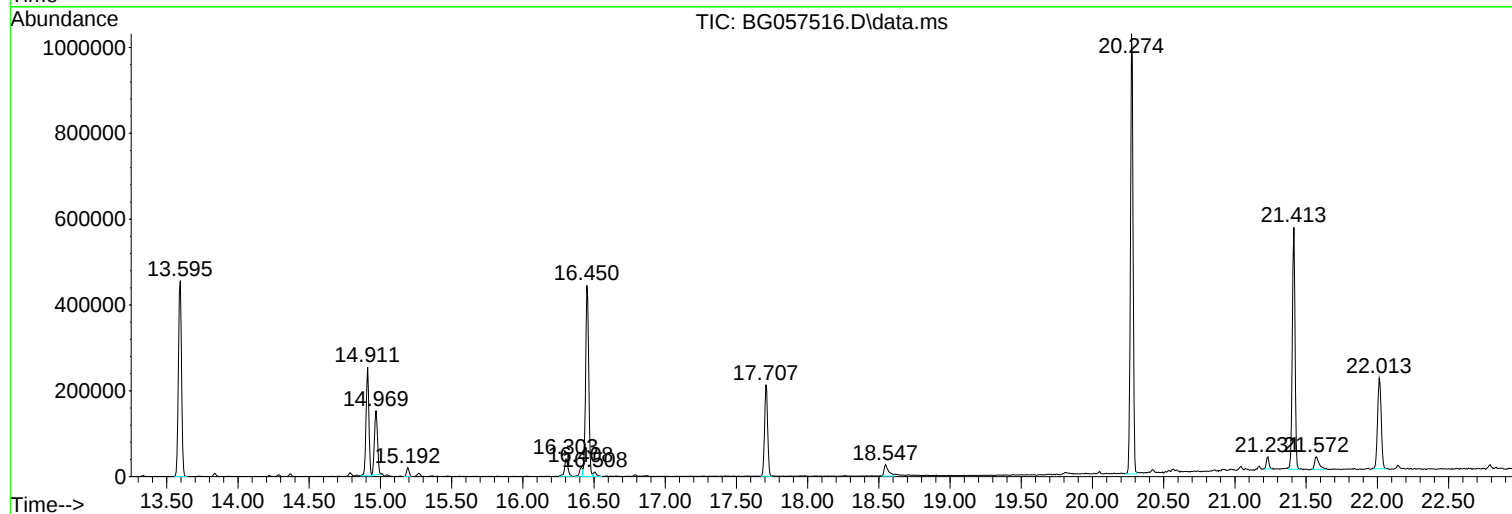
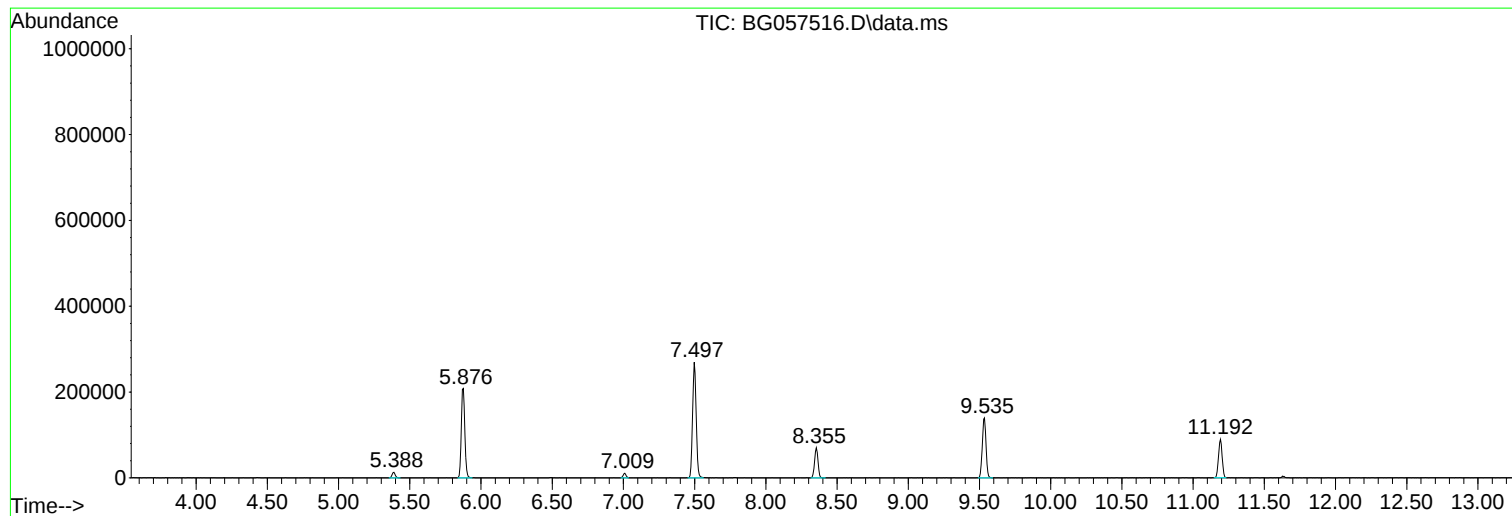
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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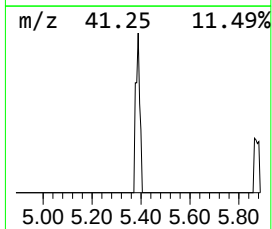
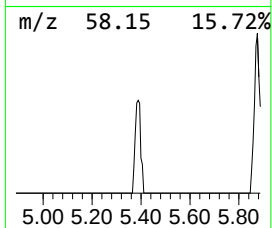
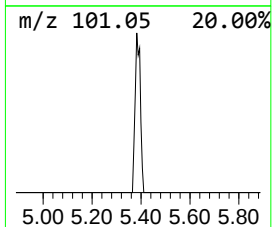
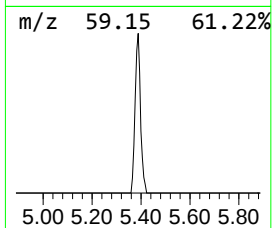
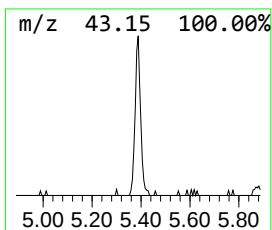
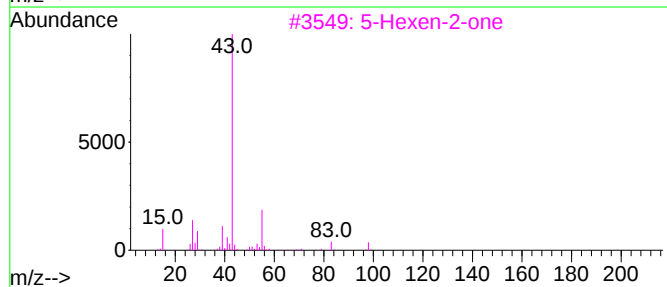
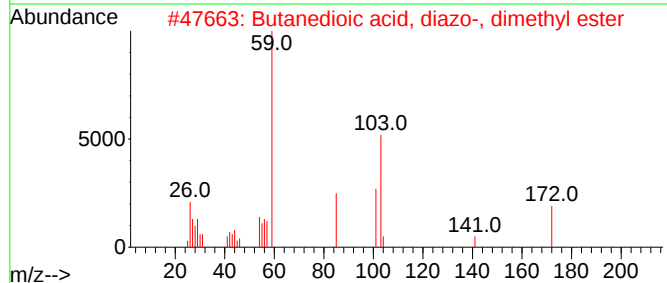
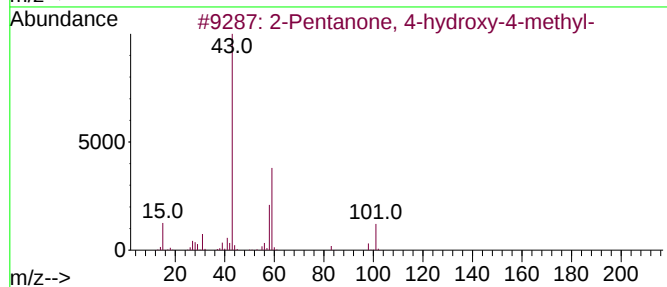
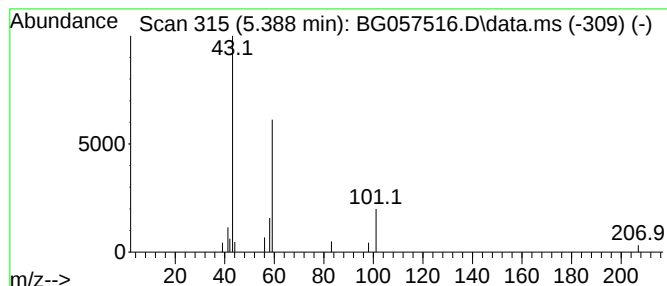
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.388	3.45 ng	20174	1,4-Dichlorobenzene-d4	8.355

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Butanedioic acid, diazo-, dimeth...	172	C6H8N2O4	055514-36-8	28
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9
5		Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	9



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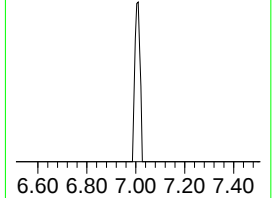
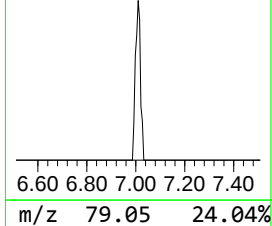
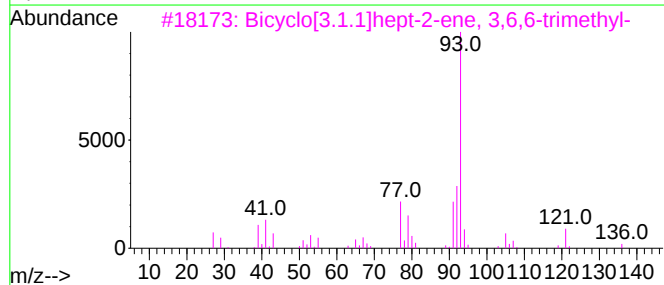
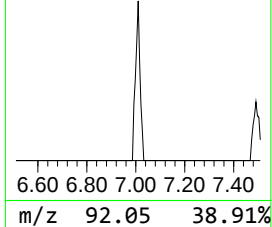
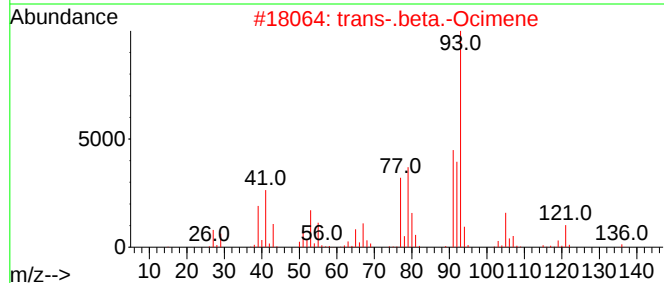
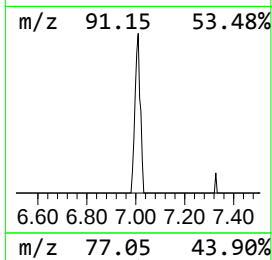
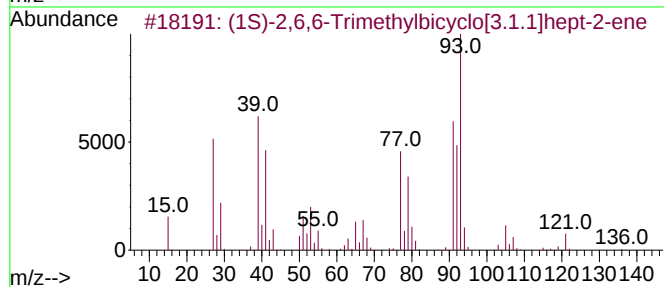
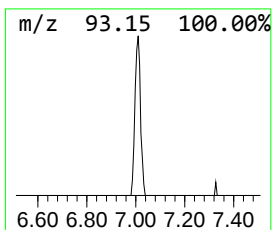
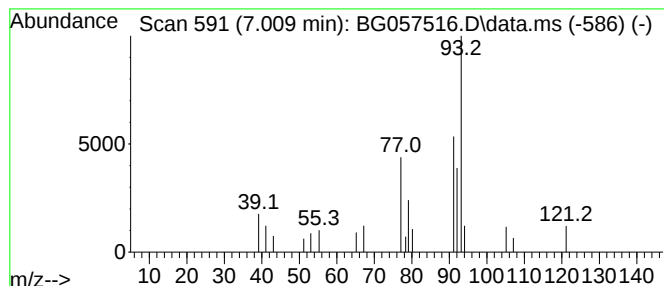
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
7.009	2.68 ng	15658	1,4-Dichlorobenzene-d4		8.355

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	83	
2	trans-.beta.-Ocimene	136	C10H16	003779-61-1	78	
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	72	
4	3,5-Methanocyclopentapyrazole, 3,4,5-trimethyl-	164	C10H16N2	087143-58-6	59	
5	1,4-Methano-1H-Cyclopropa[d]pyridine	136	C8H12N2	109746-10-3	50	



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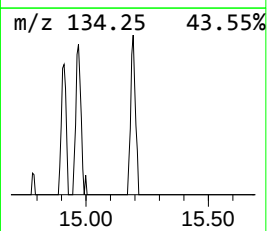
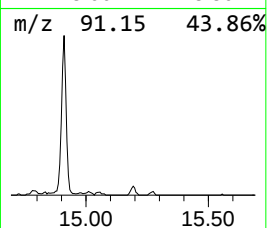
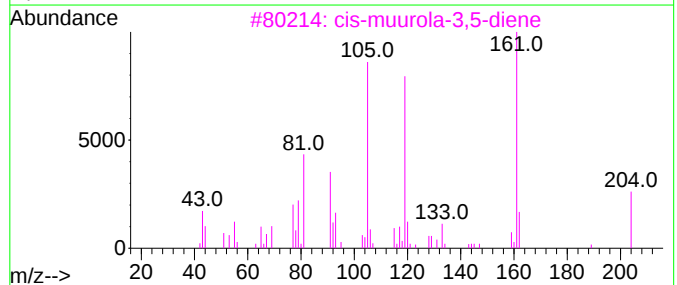
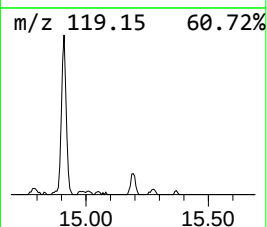
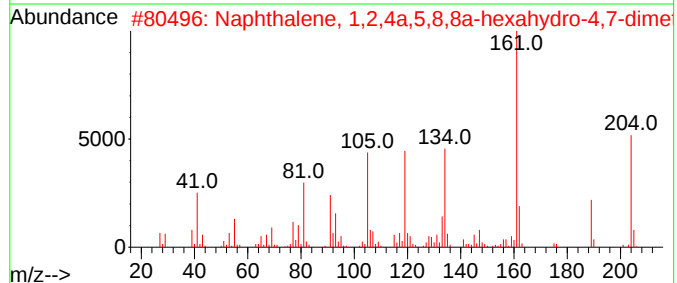
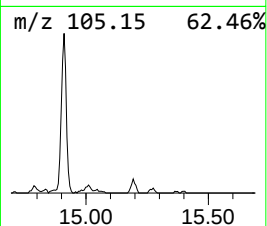
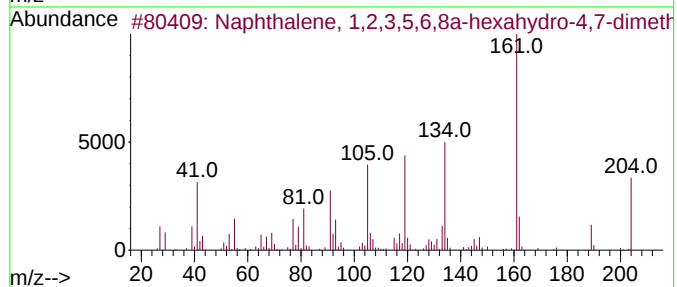
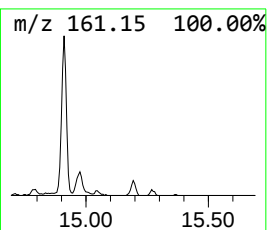
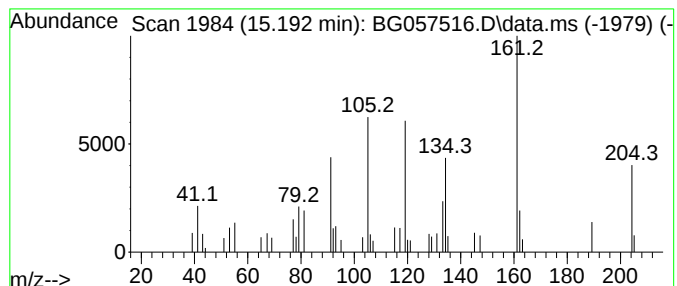
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Peak Number 4 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.193	2.29 ng	25761	Acenaphthene-d10	14.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	97
2			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	90
3			cis-muuroala-3,5-diene	204	C15H24	1000365-95-4	89
4			1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	89
5			(1S,4aR,8aS)-1-Isopropyl-7-methy...	204	C15H24	006980-46-7	81



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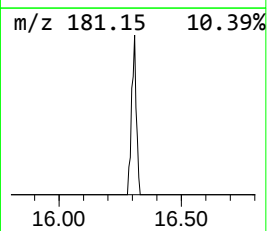
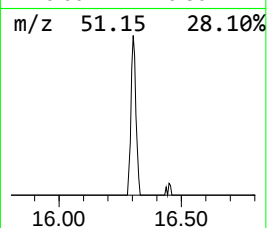
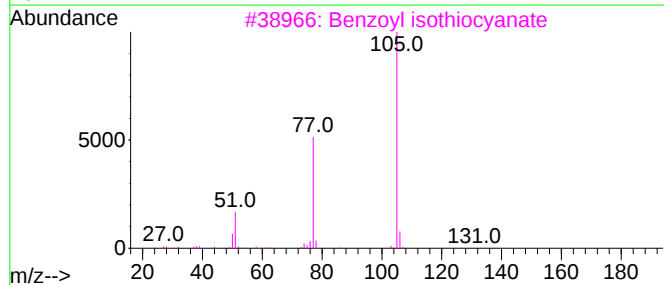
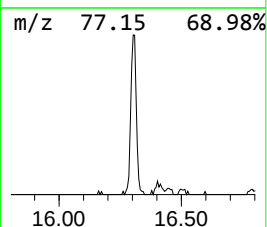
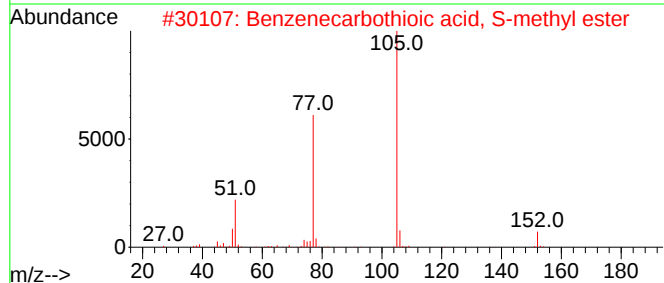
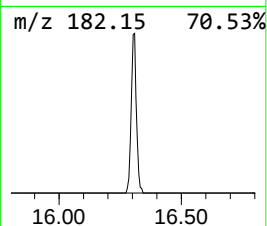
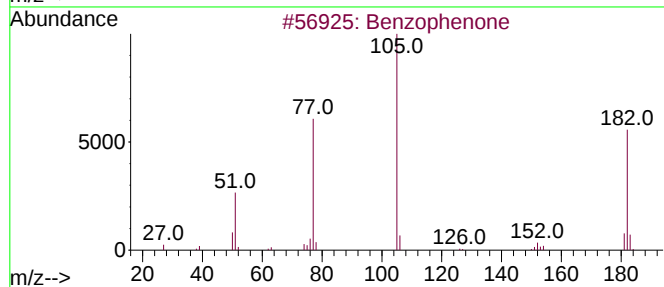
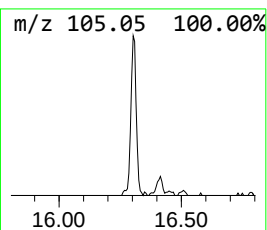
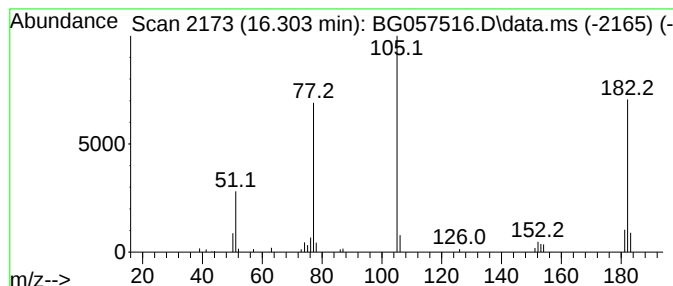
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.303	6.19 ng	69579	Acenaphthene-d10	14.969

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	46
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	43
5			Vinyl benzoate	148	C9H8O2	000769-78-8	43



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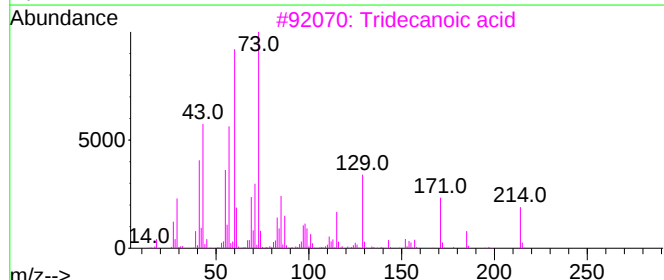
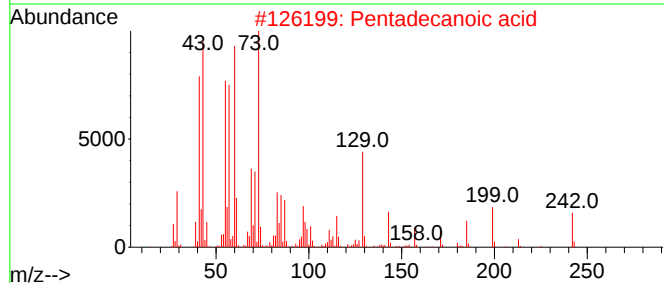
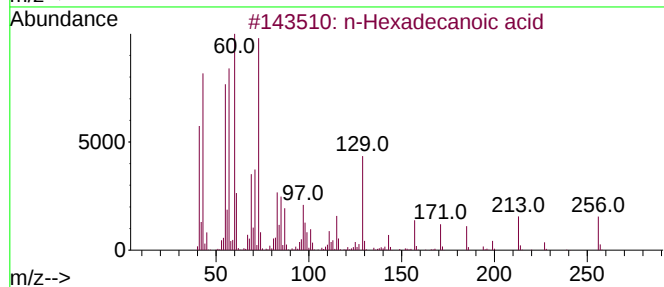
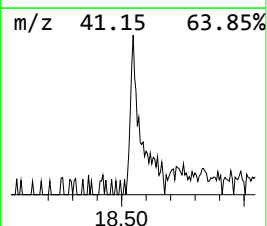
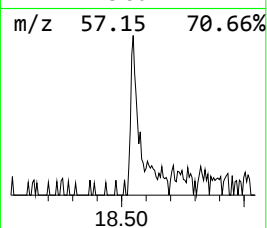
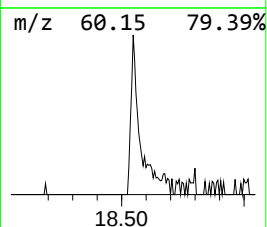
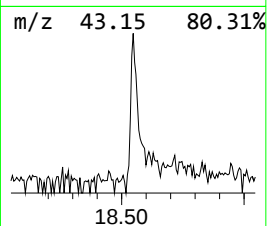
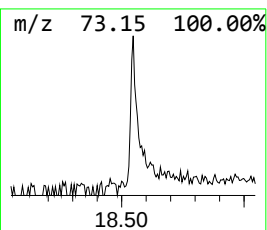
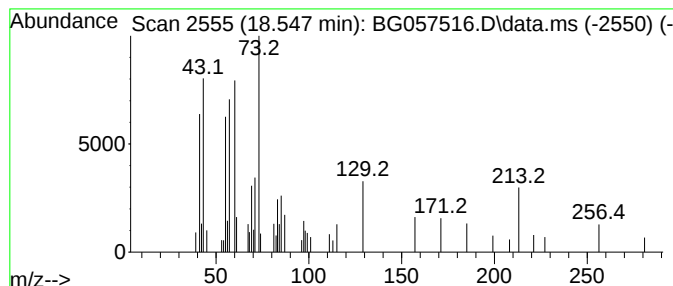
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.547	3.59 ng	57793	Phenanthrene-d10	17.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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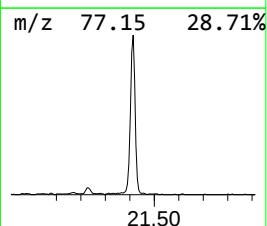
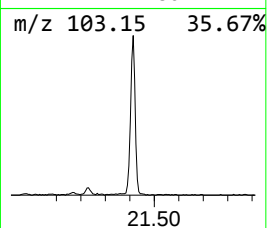
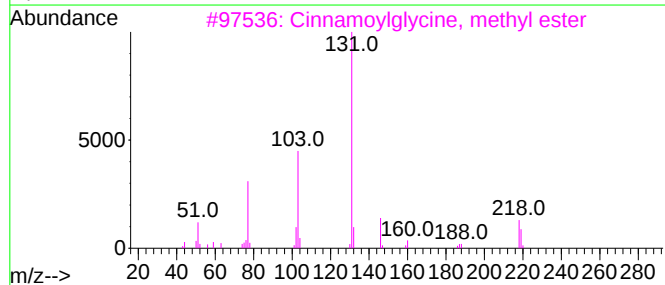
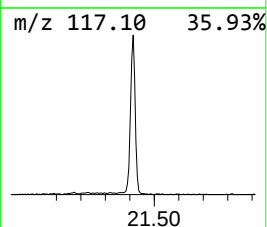
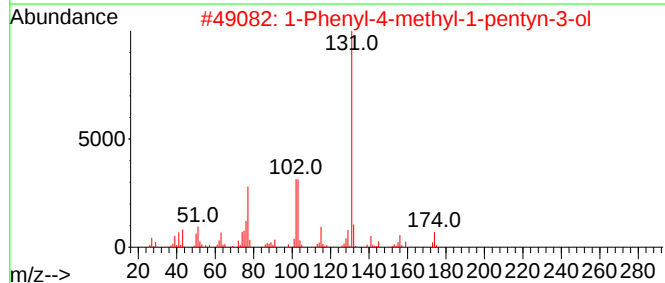
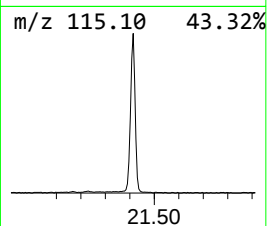
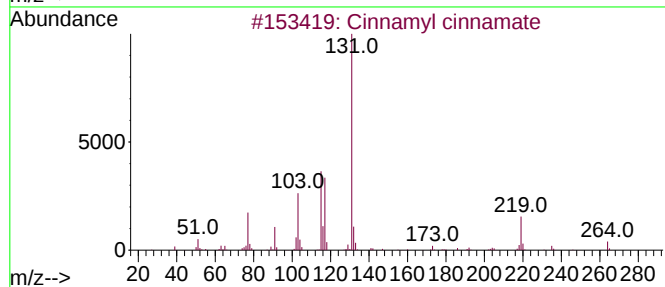
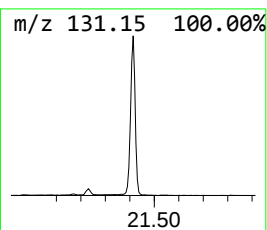
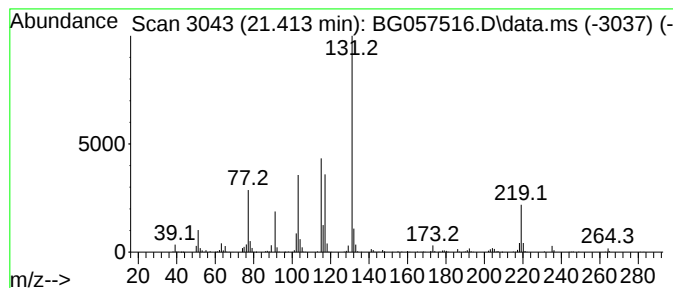
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.413	40.54 ng	747833	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			1-Phenyl-4-methyl-1-pentyn-3-ol	174	C12H14O	005923-02-4	47
3			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
4			3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	43
5			(2E)-N-(2-Fluorophenyl)-3-phenyl...	241	C15H12FNO	025893-50-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057516.D
Acq On : 23 May 2023 12:34
Operator : CG/JU
Sample : 02870-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP20

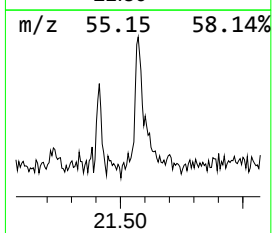
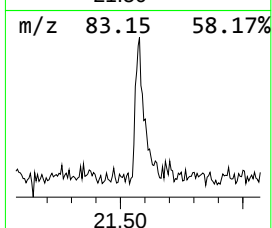
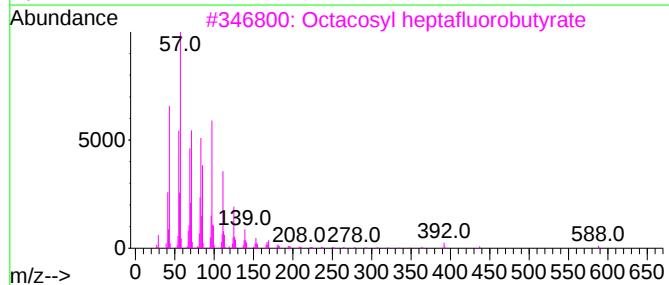
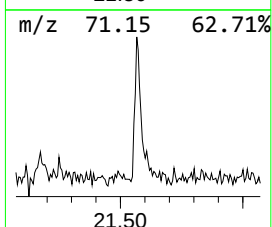
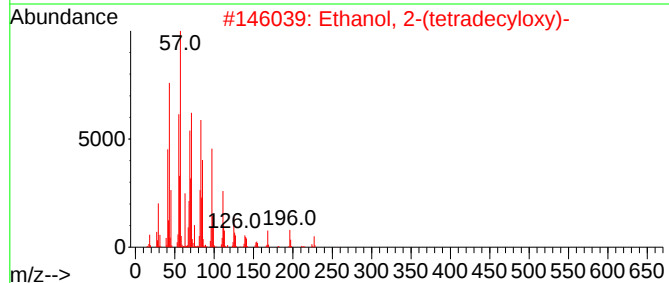
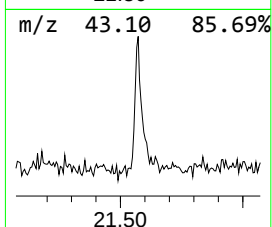
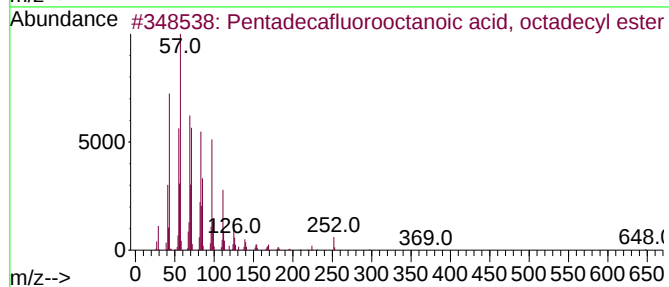
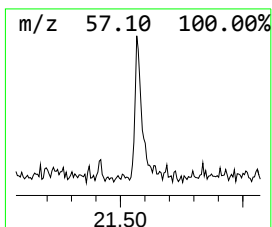
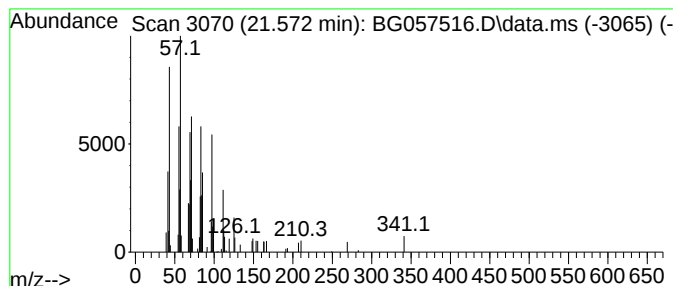
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	3.42 ng	63147	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	87
4			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87
5			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057516.D
Acq On : 23 May 2023 12:34
Operator : CG/JU
Sample : 02870-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP20

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-...	5.388	3.5	ng	20174	1	8.355	117039	20.0
(1S)-2,6,6-Trim...	7.009	2.7	ng	15658	1	8.355	117039	20.0
(1R,2S,6S,7S,8S...	14.911	31.0	ng	348923	3	14.969	224970	20.0
Naphthalene, 1,...	15.193	2.3	ng	25761	3	14.969	224970	20.0
Benzophenone	16.303	6.2	ng	69579	3	14.969	224970	20.0
n-Hexadecanoic ...	18.547	3.6	ng	57793	4	17.707	321667	20.0
Cinnamyl cinnamate	21.413	40.5	ng	747833	5	22.013	368978	20.0
Pentadecafluoro...	21.572	3.4	ng	63147	5	22.013	368978	20.0