

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
 Data File : BG046710.D
 Acq On : 25 Sep 2020 20:30
 Operator : CG/JU
 Sample : L4132-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHRT-20413

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-BG092220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.203	12	19	28	rBV2	115880	334510	7.59%	1.307%
2	3.291	28	34	39	rVB2	45513	82512	1.87%	0.323%
3	5.224	357	363	369	rBV2	43612	70315	1.60%	0.275%
4	5.682	434	441	451	rBV	1160181	1898532	43.10%	7.421%
5	6.816	626	634	640	rVB2	41271	70690	1.60%	0.276%
6	7.268	703	711	724	rBV	1205172	2112746	47.96%	8.258%
7	7.568	755	762	769	rBV	44237	76683	1.74%	0.300%
8	7.703	779	785	792	rBV	67340	111424	2.53%	0.436%
9	8.120	849	856	864	rBV	317169	554534	12.59%	2.167%
10	9.284	1045	1054	1062	rBV	791303	1417212	32.17%	5.539%
11	10.935	1328	1335	1345	rBV	425946	762408	17.31%	2.980%
12	13.373	1742	1750	1759	rVB	2012081	3095821	70.28%	12.100%
13	14.078	1865	1870	1877	rVB3	70952	107000	2.43%	0.418%
14	14.190	1883	1889	1894	rBV	249654	357987	8.13%	1.399%
15	14.742	1976	1983	1990	rBV	652894	1026304	23.30%	4.011%
16	15.741	2144	2153	2158	rBV5	34070	63280	1.44%	0.247%
17	16.223	2228	2235	2248	rBV	1566021	2327346	52.84%	9.097%
18	17.486	2444	2450	2455	rBV	781485	1177214	26.73%	4.601%
19	17.527	2455	2457	2465	rVB	50070	65904	1.50%	0.258%
20	18.373	2594	2601	2610	rBV2	338502	543848	12.35%	2.126%
21	18.667	2647	2651	2656	rBV5	49251	69811	1.58%	0.273%
22	19.296	2755	2758	2763	rBV5	33786	48374	1.10%	0.189%
23	19.531	2794	2798	2804	rVB	136251	198868	4.51%	0.777%
24	19.642	2812	2817	2821	rBV4	116384	182735	4.15%	0.714%
25	19.889	2856	2859	2866	rVB	99228	162243	3.68%	0.634%
26	20.095	2888	2894	2899	rBV	3403442	4404907	100.00%	17.217%
27	20.341	2933	2936	2939	rBV4	54431	75302	1.71%	0.294%
28	20.406	2945	2947	2953	rVB4	74842	94456	2.14%	0.369%
29	20.717	2997	3000	3004	rBV5	39398	51125	1.16%	0.200%
30	20.858	3017	3024	3029	rBV9	129894	278235	6.32%	1.088%
31	21.246	3086	3090	3099	rVB5	184683	265221	6.02%	1.037%
32	21.411	3114	3118	3128	rVB	435804	640737	14.55%	2.504%
33	21.687	3163	3165	3170	rVB5	55083	77276	1.75%	0.302%
34	21.763	3171	3178	3184	rBV2	762855	1352622	30.71%	5.287%
35	25.048	3728	3737	3748	rVB3	425446	1202001	27.29%	4.698%
36	26.446	3970	3975	3985	rVB8	76874	224237	5.09%	0.876%

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ClientSampleId :
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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-BG092220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

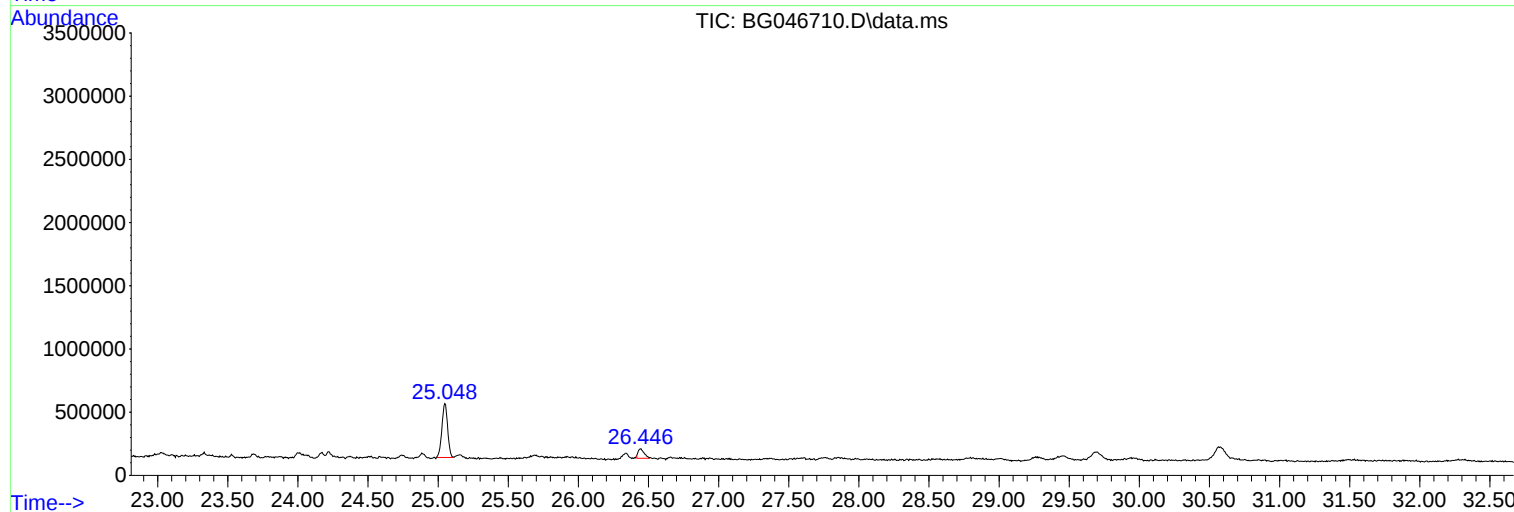
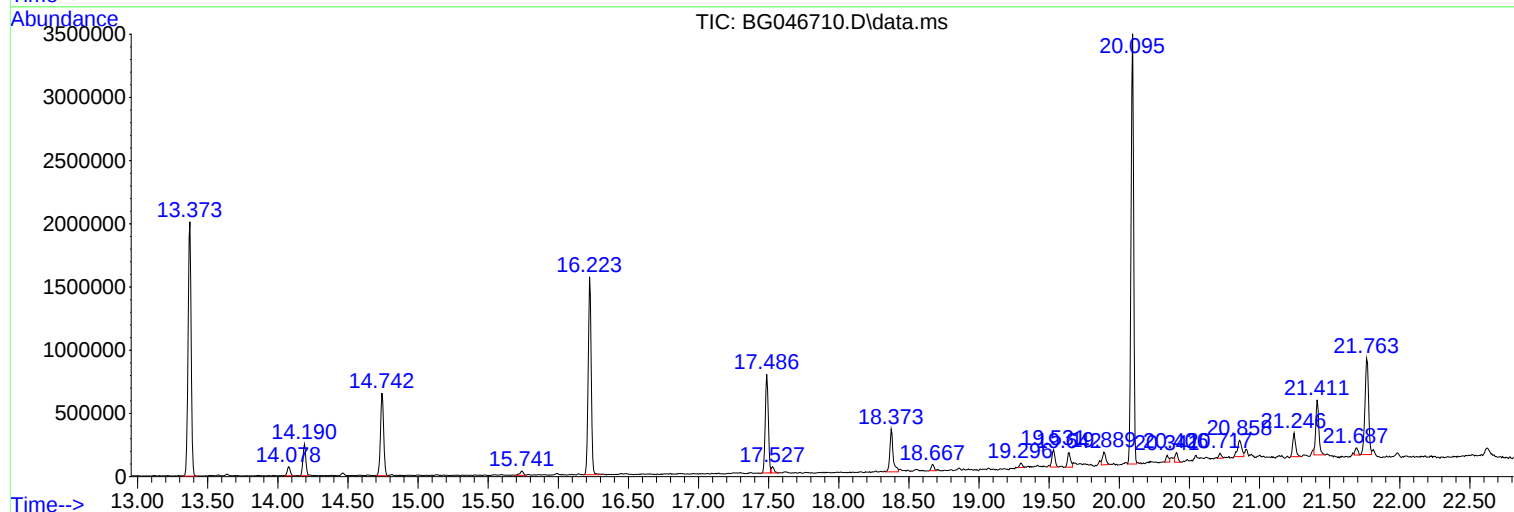
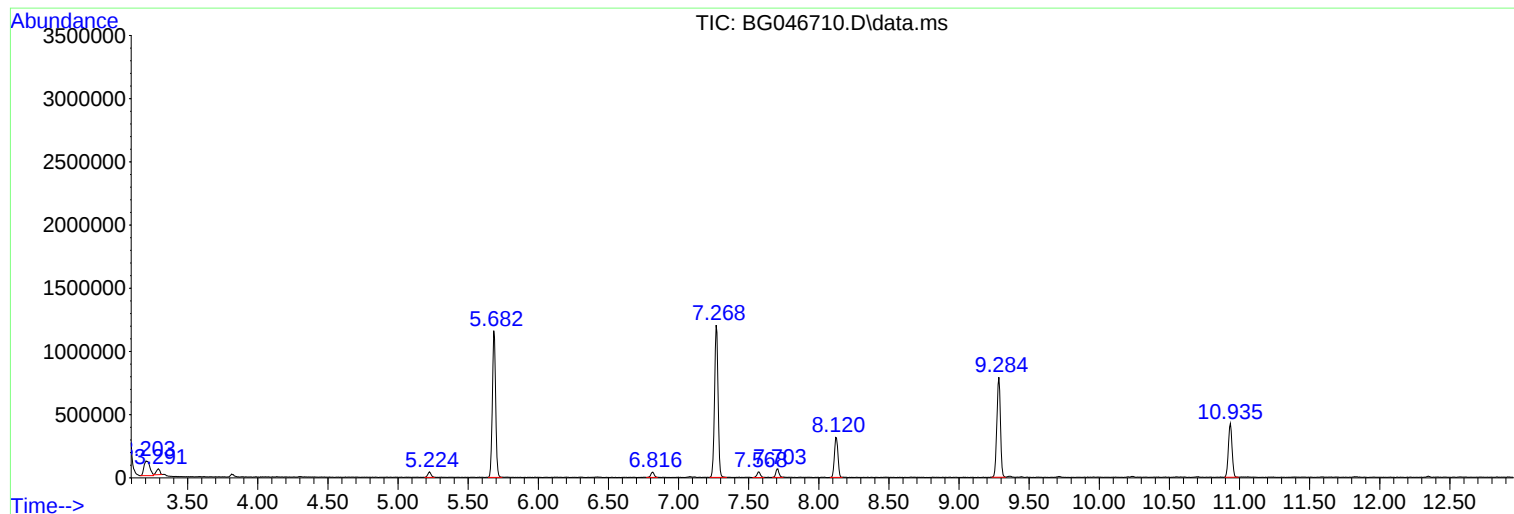
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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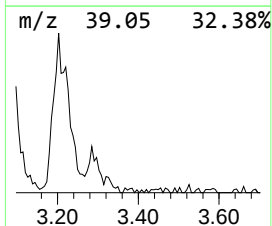
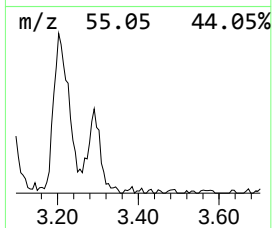
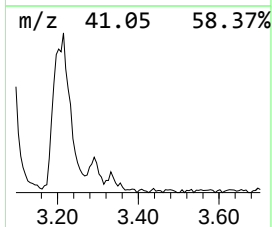
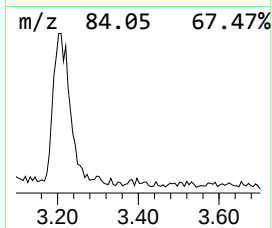
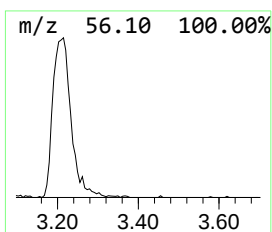
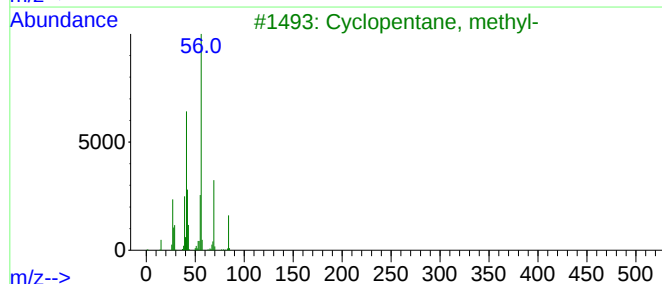
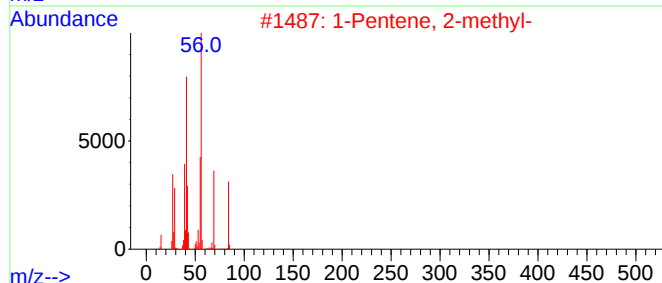
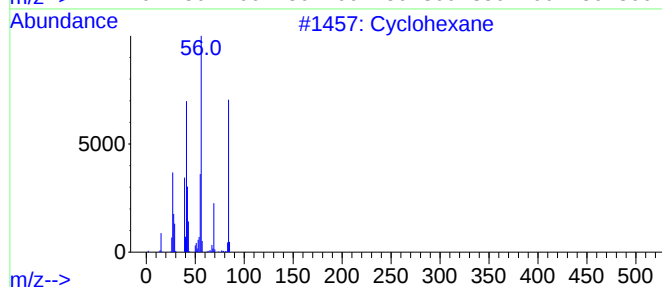
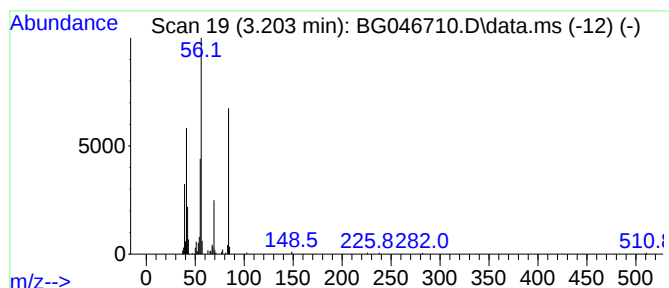
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclohexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.203	12.06 ng	334510	1,4-Dichlorobenzene-d4	8.120

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane	84	C6H12	000110-82-7	91
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	50
4			1-Hexene	84	C6H12	000592-41-6	50
5			2-Amino-oxazole	84	C3H4N2O	004570-45-0	47



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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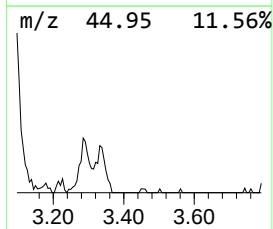
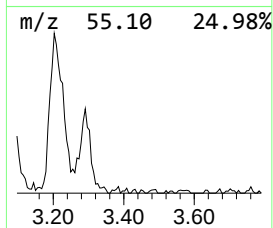
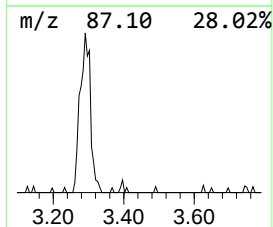
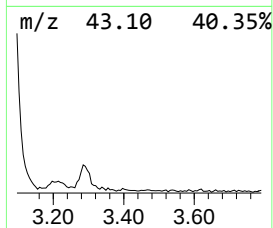
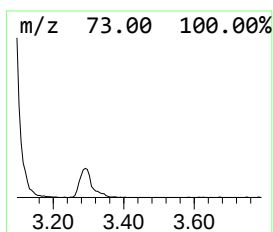
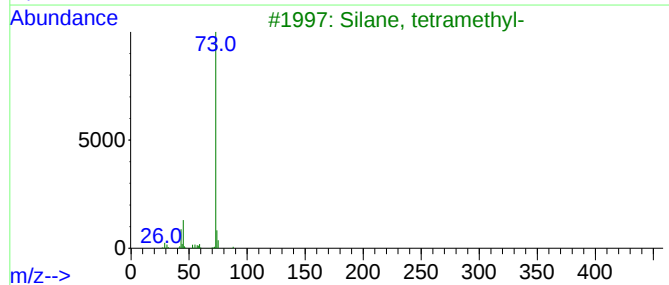
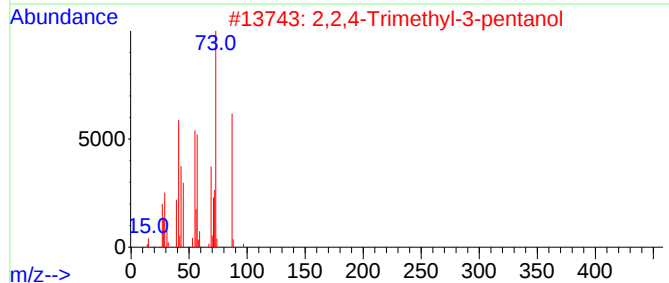
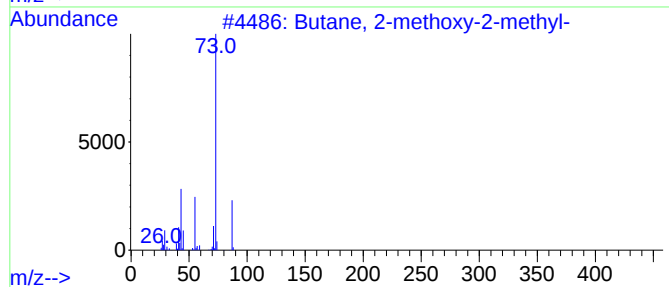
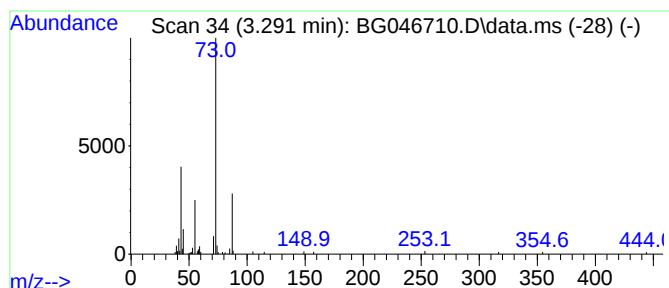
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.291 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.291	2.98 ng	82512	1,4-Dichlorobenzene-d4	8.120

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23
5			1,3-Dioxolane, 2-butyl-	130	C7H14O2	004360-76-3	12



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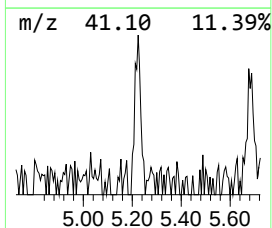
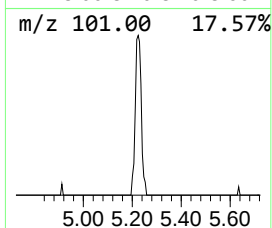
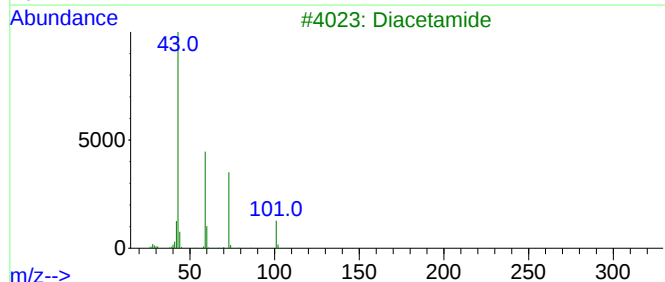
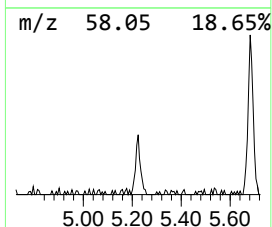
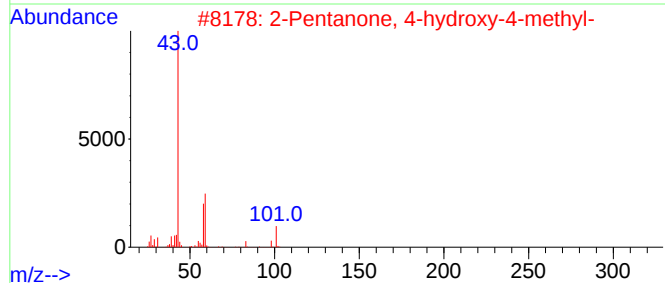
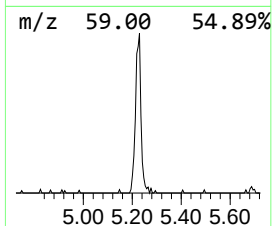
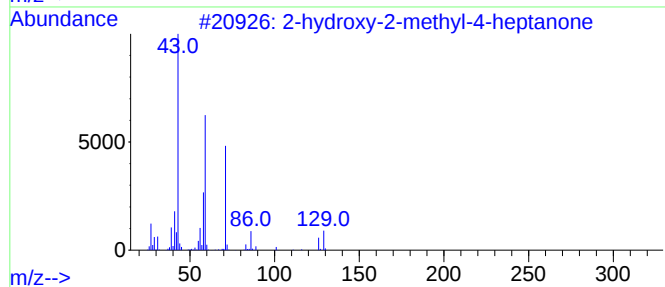
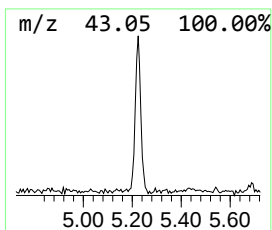
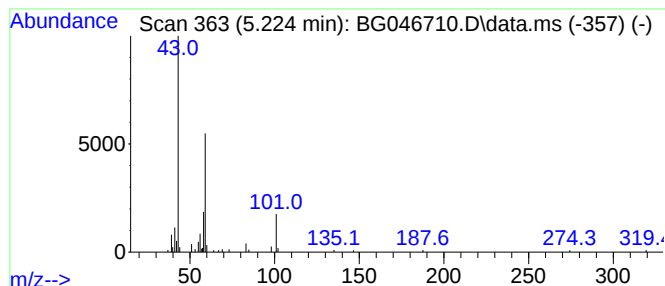
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.224 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.224	2.54 ng	70315	1,4-Dichlorobenzene-d4	8.120

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	45
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		Diacetamide	101	C4H7NO2	000625-77-4	38
4		3-Octanol	130	C8H18O	000589-98-0	28
5		Tetraglyme	222	C10H22O5	000143-24-8	28



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-20413

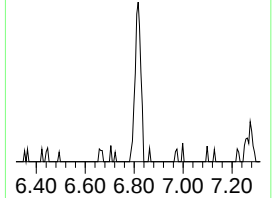
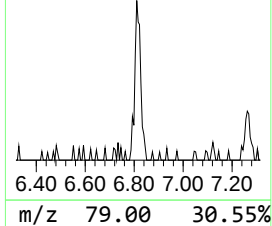
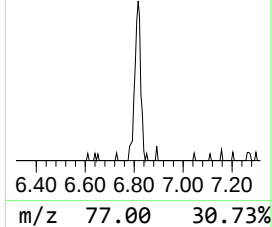
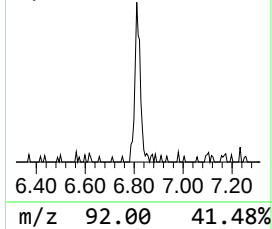
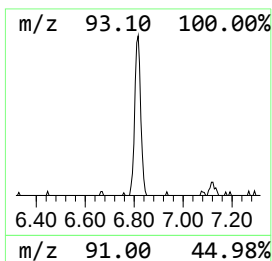
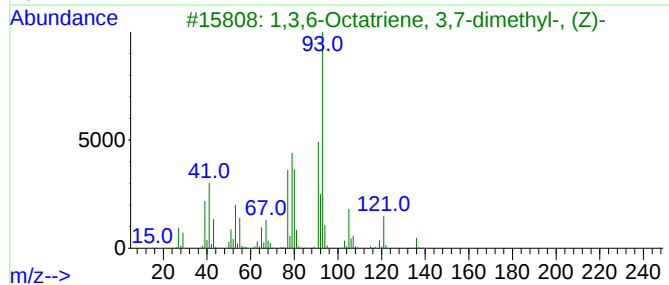
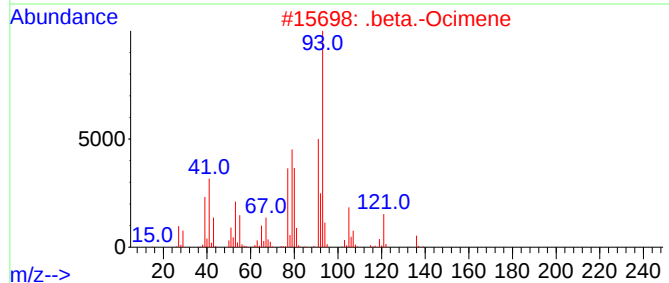
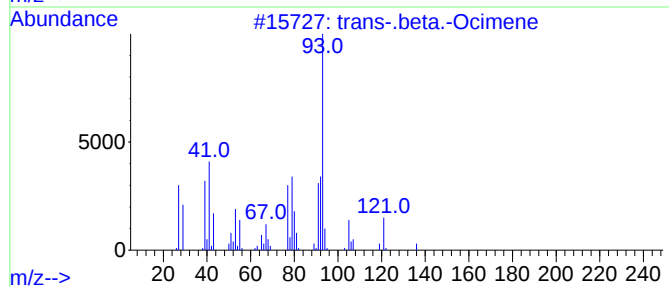
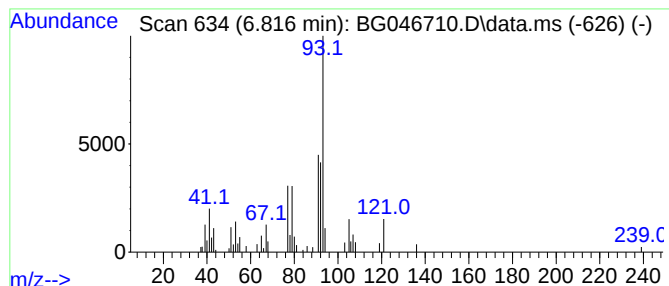
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 trans-.beta.-Ocimene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.816	2.55 ng	70690	1,4-Dichlorobenzene-d4	8.120

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
2			.beta.-Ocimene	136	C10H16	013877-91-3	90
3			1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	90
4			.alpha.-Pinene	136	C10H16	000080-56-8	90
5			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	86



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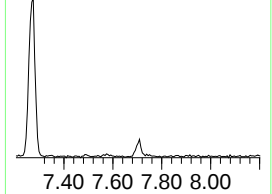
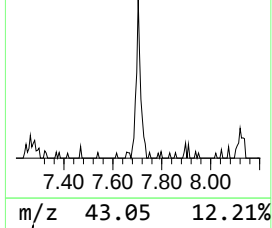
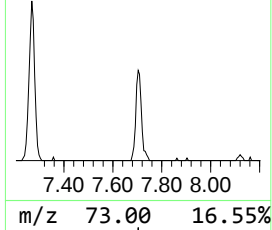
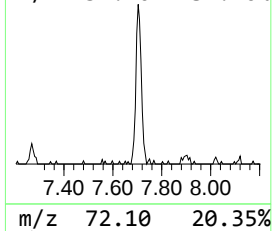
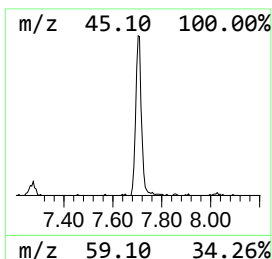
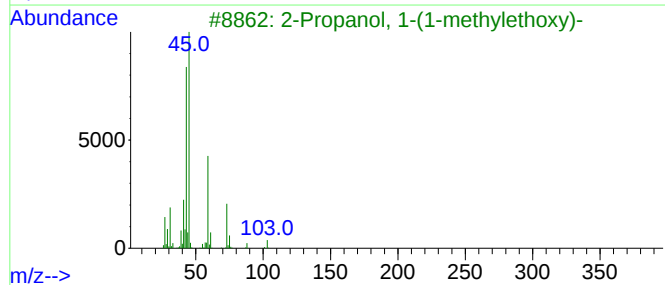
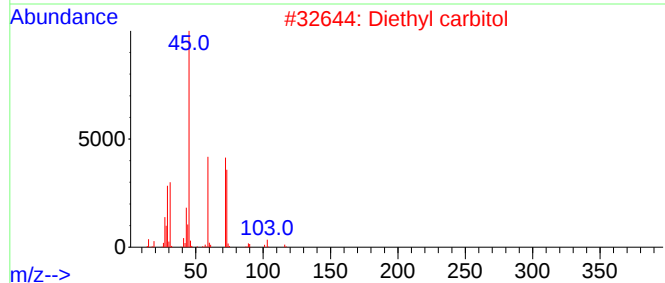
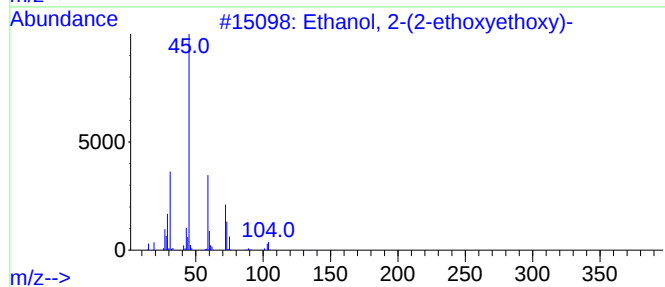
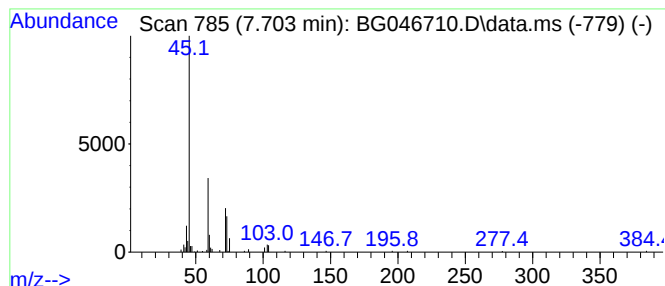
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.703	4.02 ng	111424	1,4-Dichlorobenzene-d4	8.120

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	78
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	43
5			1H-Pyrimidine-2,4-dione, 1-(2-et...	232	C9H13FN2O4	1000310-13-7	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
Operator : CG/JU
Sample : L4132-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-20413

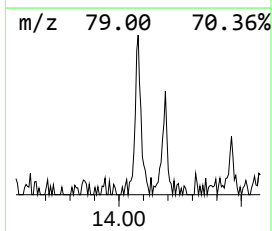
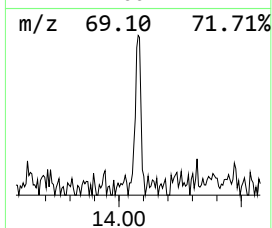
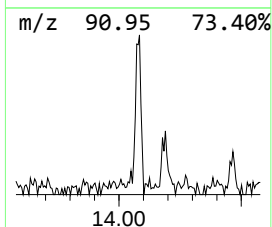
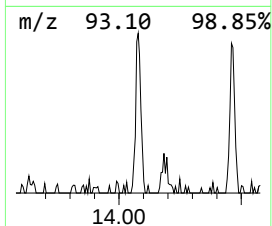
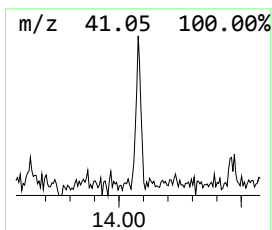
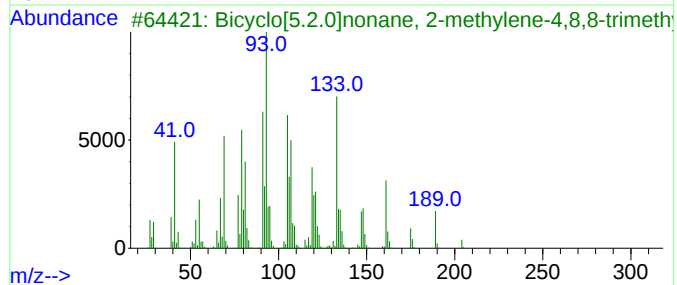
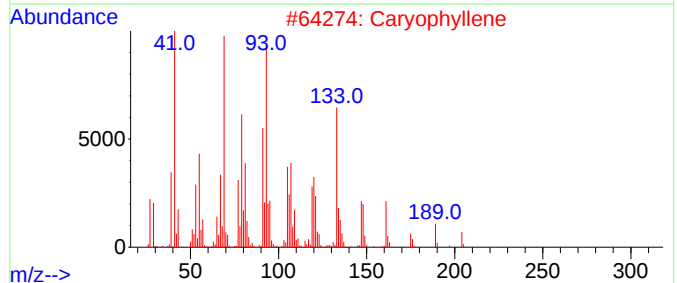
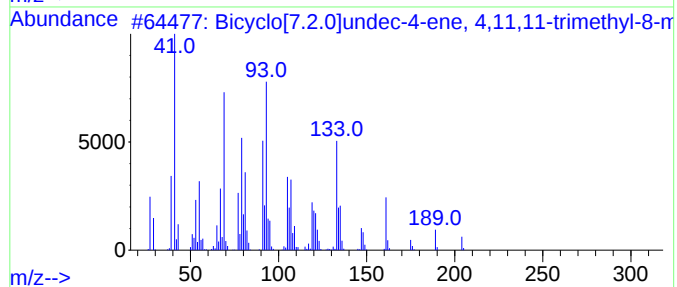
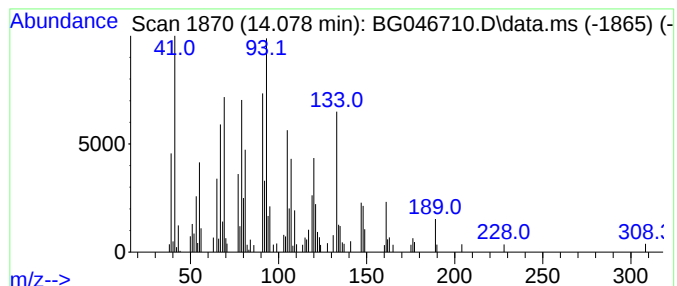
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bicyclo[7.2.0]undec-4-ene, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.078	2.09 ng	107000	Acenaphthene-d10	14.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	89
2			Caryophyllene	204	C15H24	000087-44-5	87
3			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	83
4			Alloaromadendrene	204	C15H24	025246-27-9	55
5			11,11-Dimethyl-spiro[2,9]dodeca-...	190	C14H22	1000062-28-4	51



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
Operator : CG/JU
Sample : L4132-04
Misc :
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ClientSampleId :
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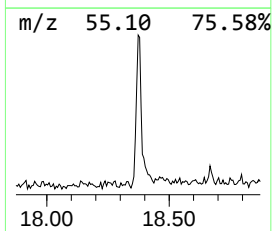
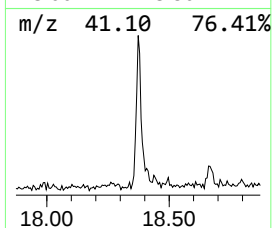
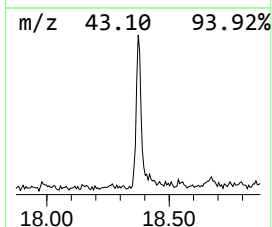
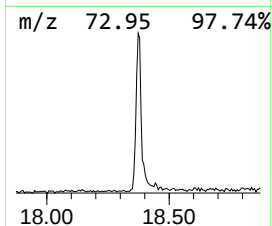
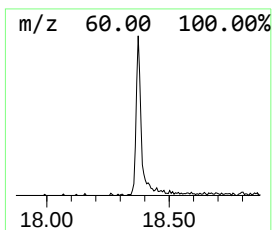
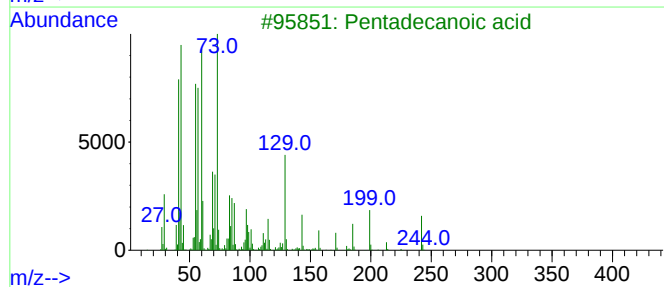
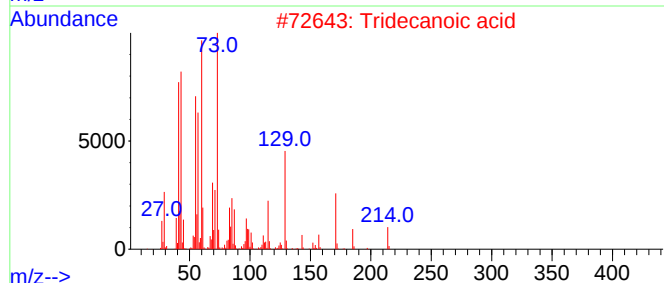
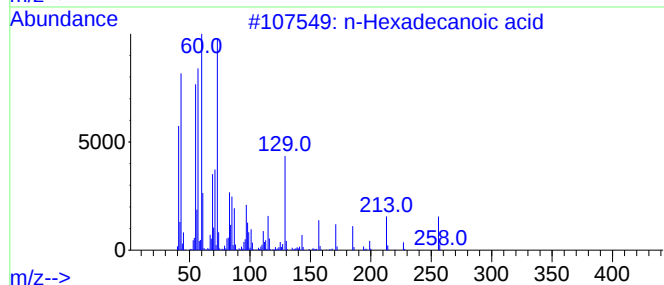
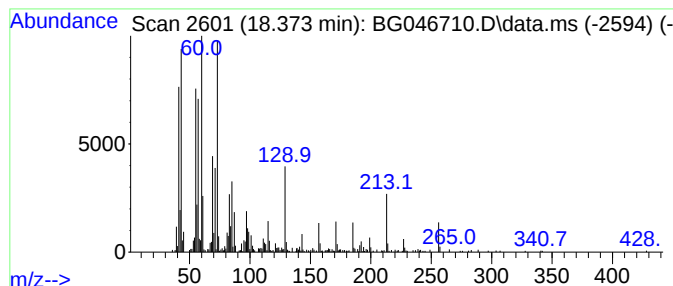
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	9.24 ng	543848	Phenanthrene-d10	17.486

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
Operator : CG/JU
Sample : L4132-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-20413

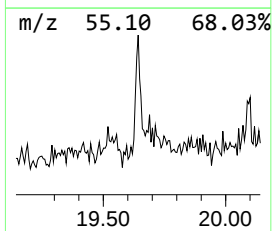
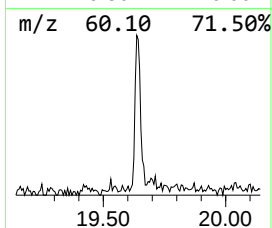
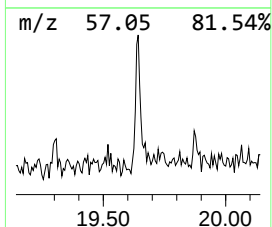
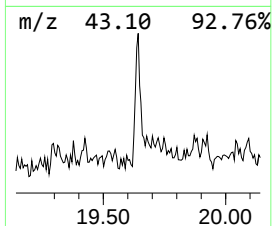
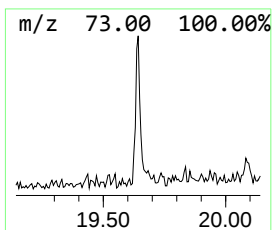
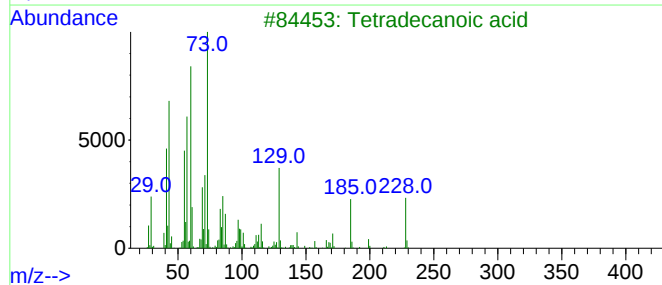
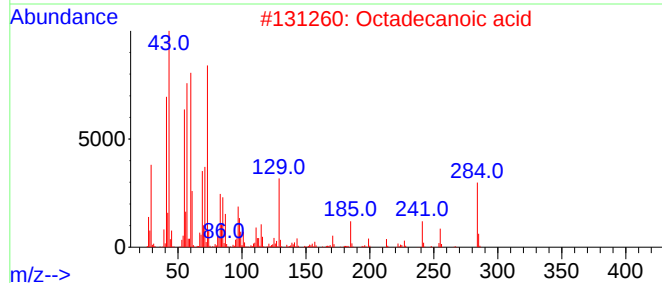
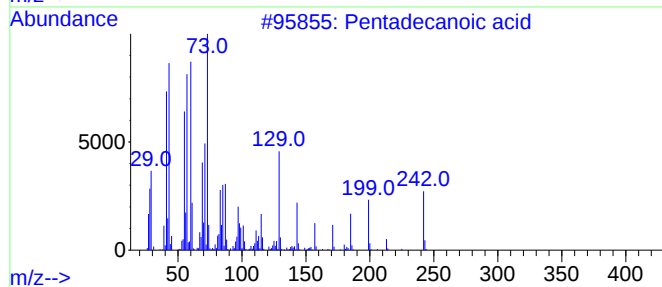
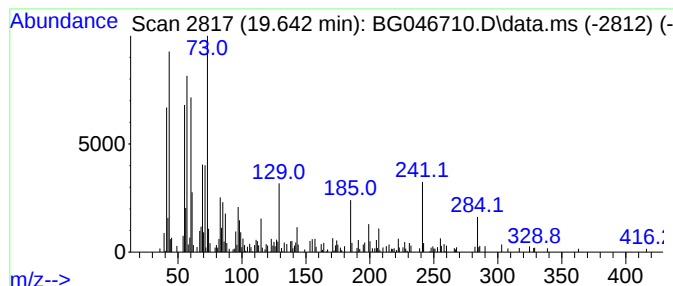
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.642	2.70 ng	182735	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	97
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
5			Dodecanoic acid	200	C12H24O2	000143-07-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
Operator : CG/JU
Sample : L4132-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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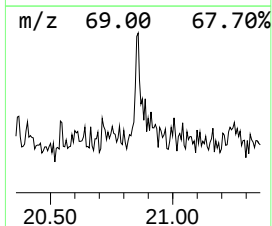
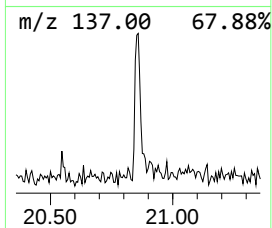
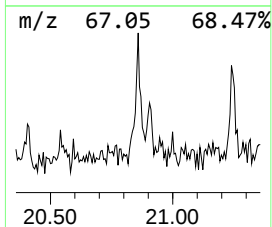
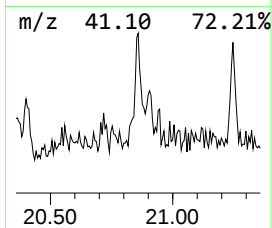
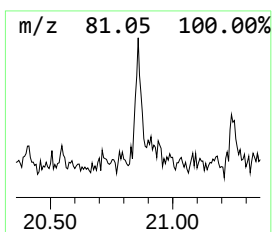
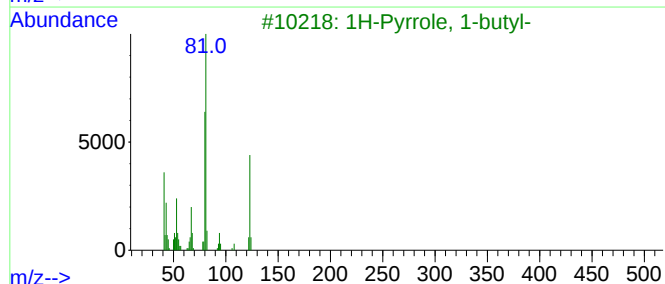
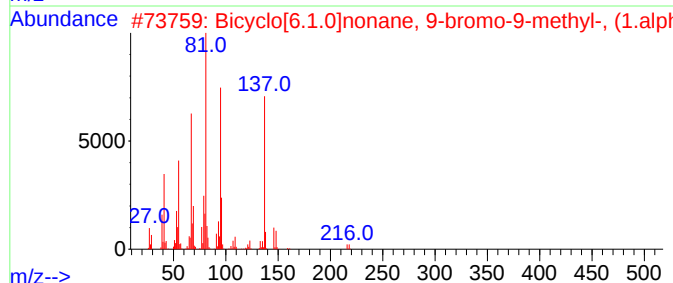
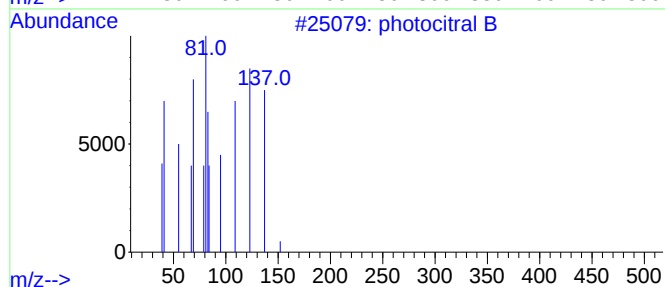
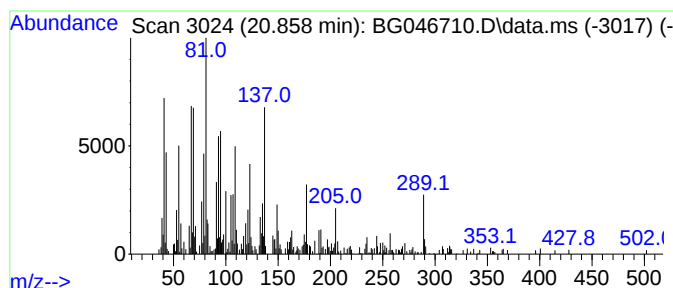
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown20.858 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.858	4.11 ng	278235	Chrysene-d12	21.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		photocitral B	152	C10H16O	006040-45-5	43
2		Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	38
3		1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	38
4		Naphthalene, 2-ethyldecahydro-	166	C12H22	001618-23-1	38
5		2,2,4-Trimethyl-3-(3,8,12,16-tet...	428	C30H52O	1000194-01-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
Operator : CG/JU
Sample : L4132-04
Misc :
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Instrument :
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ClientSampleId :
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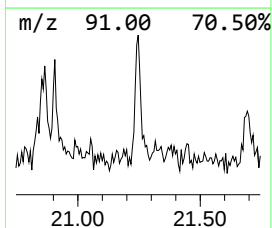
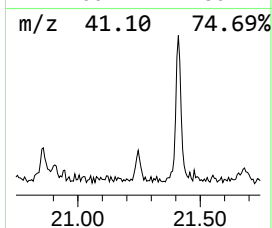
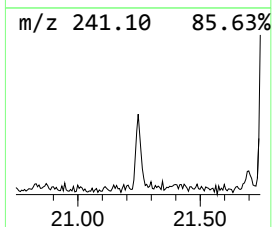
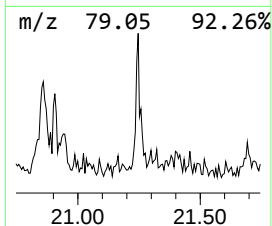
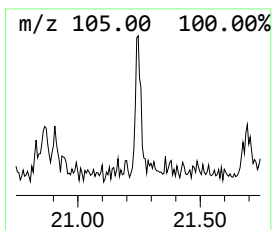
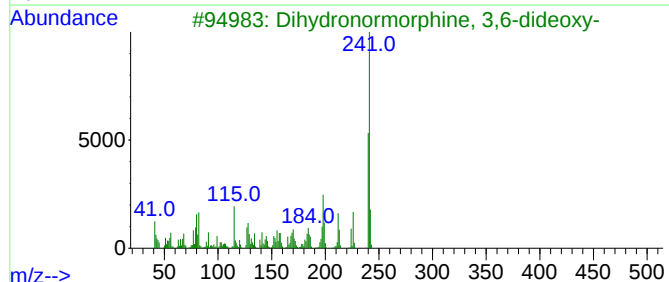
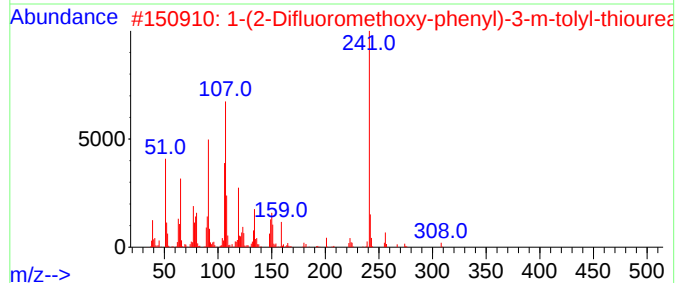
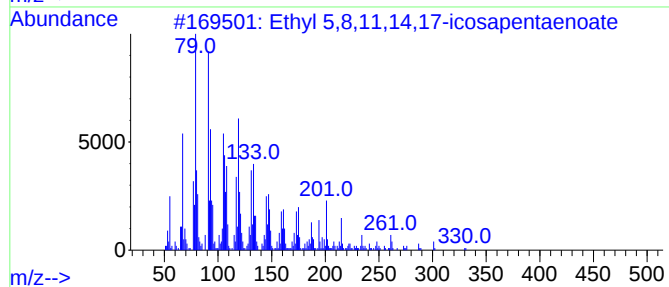
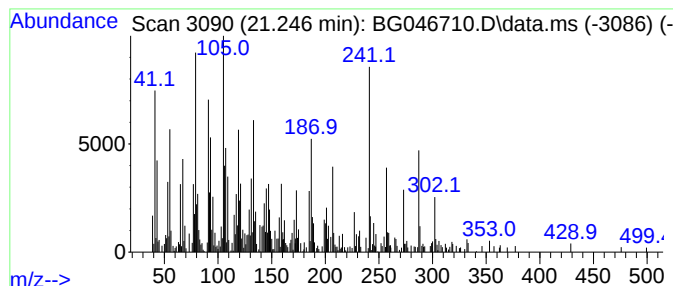
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown21.246 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.246	3.92 ng	265221	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 5,8,11,14,17-icosapentaenoate	330	C22H34O2	084494-70-2	40
2			1-(2-Difluoromethoxy-phenyl)-3-m...	308	C15H14F2N2OS	1000300-87-1	25
3			Dihydronormorphine, 3,6-dideoxy-	241	C16H19NO	1000129-30-2	25
4			3-Phenylpropionic acid, 2,7-dime...	284	C19H24O2	1000299-17-7	22
5			3-Hydroxypyridine, pentafluoropr...	241	C8H4F5NO2	1000376-22-0	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
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Sample : L4132-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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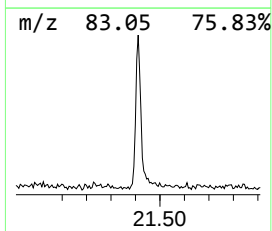
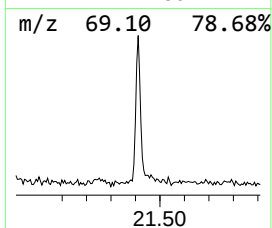
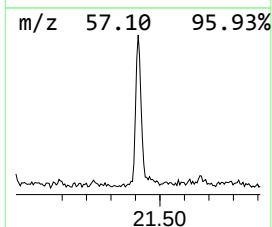
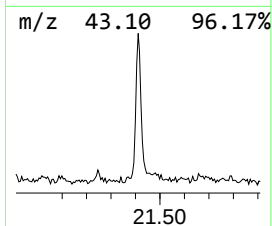
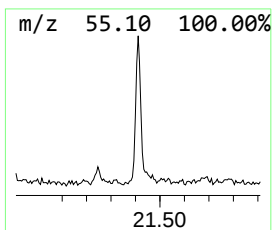
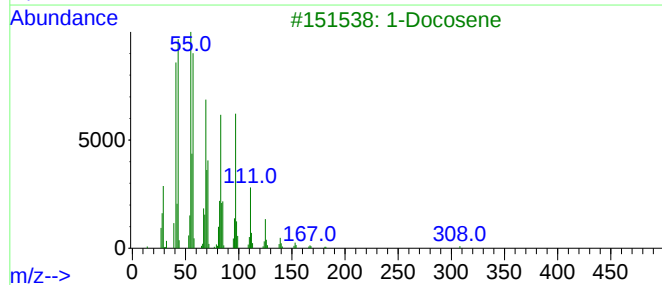
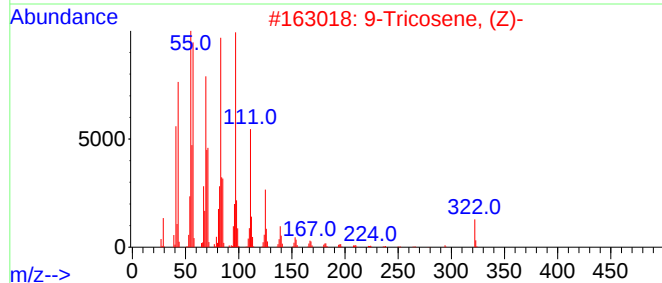
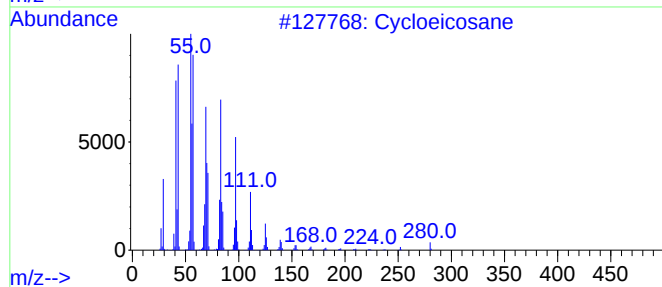
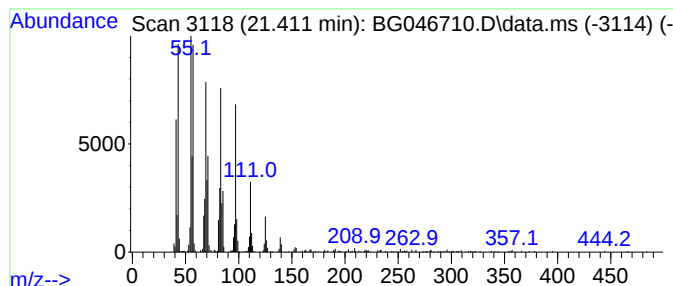
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.411	9.47 ng	640737	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	98
2			9-Tricosene, (Z)-	322	C23H46	027519-02-4	96
3			1-Docosene	308	C22H44	001599-67-3	93
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046710.D
Acq On : 25 Sep 2020 20:30
Operator : CG/JU
Sample : L4132-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-20413

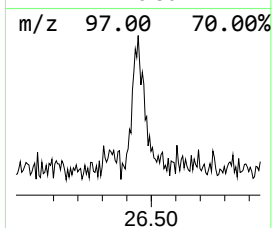
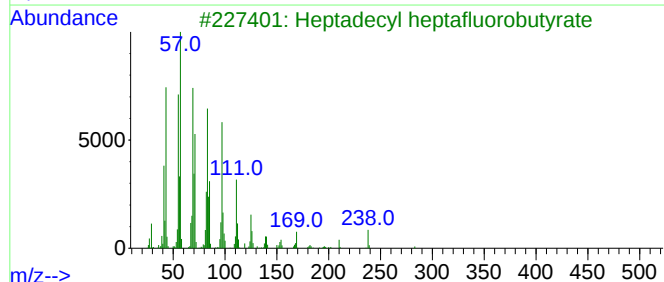
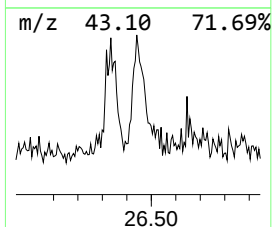
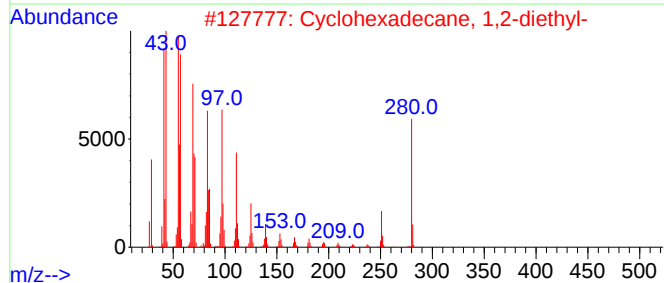
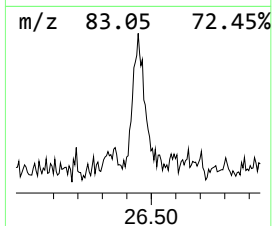
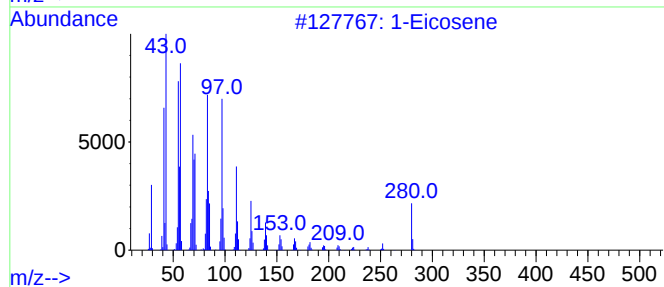
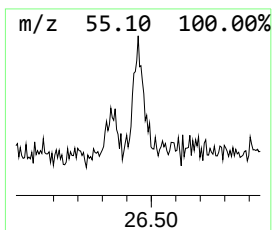
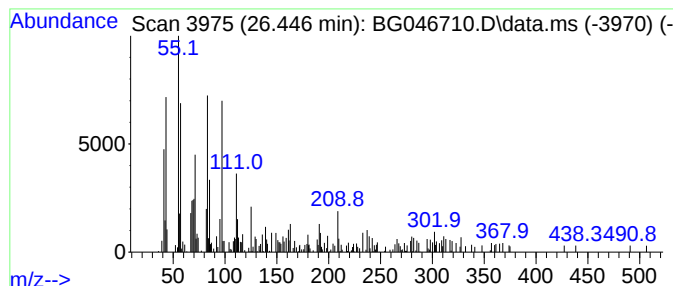
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1-Eicosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.446	3.73 ng	224237	Perylene-d12	25.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene			280	C20H40	003452-07-1	90
2	Cyclohexadecane, 1,2-diethyl-			280	C20H40	1000155-85-3	83
3	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	83
4	1-Hexadecanesulfonyl chloride			324	C16H33ClO2S	038775-38-1	83
5	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
 Data File : BG046710.D
 Acq On : 25 Sep 2020 20:30
 Operator : CG/JU
 Sample : L4132-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHRT-20413

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane	3.203	12.1	ng	334510	1	8.120	554534	20.0
unknown3.291	3.291	3.0	ng	82512	1	8.120	554534	20.0
unknown5.224	5.224	2.5	ng	70315	1	8.120	554534	20.0
trans-.beta.-Oc...	6.816	2.5	ng	70690	1	8.120	554534	20.0
Ethanol, 2-(2-e...	7.703	4.0	ng	111424	1	8.120	554534	20.0
Bicyclo[7.2.0]u...	14.078	2.1	ng	107000	3	14.742	1026300	20.0
n-Hexadecanoic ...	18.373	9.2	ng	543848	4	17.486	1177210	20.0
Pentadecanoic acid	19.642	2.7	ng	182735	5	21.763	1352620	20.0
unknown20.858	20.858	4.1	ng	278235	5	21.763	1352620	20.0
unknown21.246	21.246	3.9	ng	265221	5	21.763	1352620	20.0
Cycloeicosane	21.411	9.5	ng	640737	5	21.763	1352620	20.0
1-Eicosene	26.446	3.7	ng	224237	6	25.048	1202000	20.0