

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
 Data File : BG050526.D
 Acq On : 9 Oct 2021 2:33
 Operator : CG/JU
 Sample : M4113-09
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-5

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.797	384	393	402	rBV	899093	1496460	54.91%	6.435%
2	6.925	580	585	591	rBV	27701	45741	1.68%	0.197%
3	7.401	657	666	677	rBV	893945	1623578	59.57%	6.982%
4	8.259	804	812	822	rBV	261220	456704	16.76%	1.964%
5	9.428	1002	1011	1021	rBV	568930	1049684	38.51%	4.514%
6	10.827	1241	1249	1258	rBV	95009	166255	6.10%	0.715%
7	11.085	1284	1293	1307	rVB	364951	677754	24.87%	2.915%
8	13.241	1655	1660	1668	rBV3	19045	37753	1.39%	0.162%
9	13.500	1693	1704	1712	rVB	1357389	2150966	78.92%	9.250%
10	13.753	1736	1747	1757	rBV6	35050	70943	2.60%	0.305%
11	14.199	1816	1823	1829	rVB	295850	450774	16.54%	1.939%
12	14.281	1830	1837	1842	rBV2	39374	60049	2.20%	0.258%
13	14.704	1903	1909	1913	rBV3	18888	28309	1.04%	0.122%
14	14.828	1921	1930	1933	rBV	88240	141410	5.19%	0.608%
15	14.875	1933	1938	1944	rVV	561732	905455	33.22%	3.894%
16	14.928	1944	1947	1959	rVB6	25517	59773	2.19%	0.257%
17	15.110	1973	1978	1985	rBV2	40257	68044	2.50%	0.293%
18	15.180	1985	1990	1997	rVB3	23941	46378	1.70%	0.199%
19	15.862	2099	2106	2111	rBV3	55759	86002	3.16%	0.370%
20	16.355	2177	2190	2197	rBV	951760	1578291	57.91%	6.787%
21	16.555	2219	2224	2234	rVB7	14290	30924	1.13%	0.133%
22	17.619	2396	2405	2410	rBV	680431	1058887	38.85%	4.554%
23	17.660	2410	2412	2419	rVB	100269	140924	5.17%	0.606%
24	18.259	2510	2514	2520	rVB	25915	34702	1.27%	0.149%
25	18.477	2546	2551	2558	rVV2	121628	182984	6.71%	0.787%
26	18.535	2558	2561	2570	rVB2	23060	44878	1.65%	0.193%
27	18.688	2581	2587	2591	rBV4	18852	40192	1.47%	0.173%
28	19.023	2640	2644	2648	rVB4	21556	28587	1.05%	0.123%
29	19.475	2717	2721	2726	rVB2	36692	51658	1.90%	0.222%
30	19.657	2746	2752	2761	rVV	194105	340200	12.48%	1.463%
31	19.992	2801	2809	2810	rBV4	36419	68751	2.52%	0.296%
32	20.016	2810	2813	2820	rVB	148753	216332	7.94%	0.930%
33	20.210	2840	2846	2852	rVB	2025476	2725508	100.00%	11.721%
34	20.339	2862	2868	2869	rBV6	23663	33268	1.22%	0.143%
35	20.462	2885	2889	2892	rBV6	24395	42667	1.57%	0.183%
36	20.504	2892	2896	2907	rVB4	62684	119012	4.37%	0.512%

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37	20.791	2941	2945	2949	rBV2	31620	48003	1.76%	0.206%
38	20.891	2959	2962	2971	rVB5	23500	40183	1.47%	0.173%
39	21.167	3005	3009	3016	rVB4	45808	82517	3.03%	0.355%
40	21.285	3025	3029	3033	rBV2	19889	35462	1.30%	0.153%
41	21.350	3034	3040	3049	rVB	1203416	1717465	63.01%	7.386%
42	21.520	3064	3069	3075	rBV2	203998	313346	11.50%	1.348%
43	21.920	3128	3137	3143	rBV2	579334	1153376	42.32%	4.960%
44	21.967	3143	3145	3152	rVB	63216	88802	3.26%	0.382%
45	22.102	3164	3168	3170	rBV2	20781	29851	1.10%	0.128%
46	22.354	3207	3211	3216	rVB6	35955	55410	2.03%	0.238%
47	22.760	3271	3280	3293	rBV	210704	526508	19.32%	2.264%
48	23.465	3398	3400	3406	rVB3	20556	29395	1.08%	0.126%
49	23.847	3460	3465	3472	rVB8	40805	84314	3.09%	0.363%
50	24.240	3526	3532	3538	rBV2	38804	108845	3.99%	0.468%
51	24.328	3540	3547	3554	rVV2	184981	451714	16.57%	1.943%
52	24.399	3554	3559	3573	rVB4	78227	215844	7.92%	0.928%
53	25.339	3708	3719	3729	rBV2	339499	1047055	38.42%	4.503%
54	26.555	3917	3926	3940	rVB2	137452	430348	15.79%	1.851%
55	29.787	4469	4476	4477	rBV5	38261	70168	2.57%	0.302%
56	31.021	4675	4686	4705	rVB9	71859	365002	13.39%	1.570%

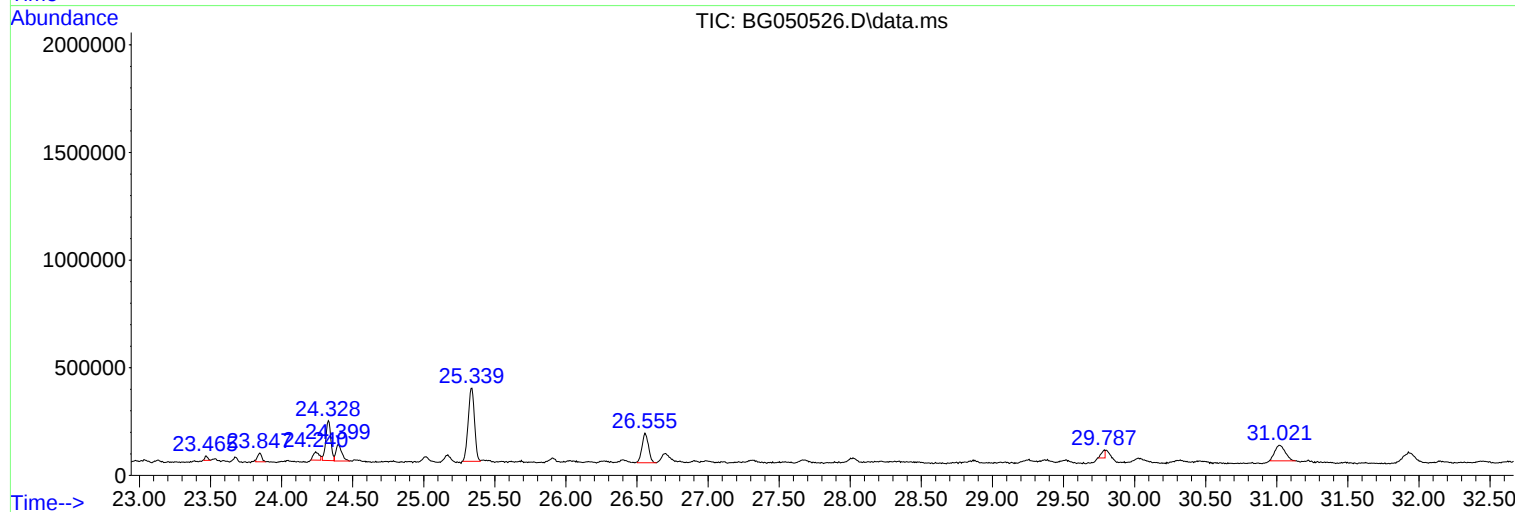
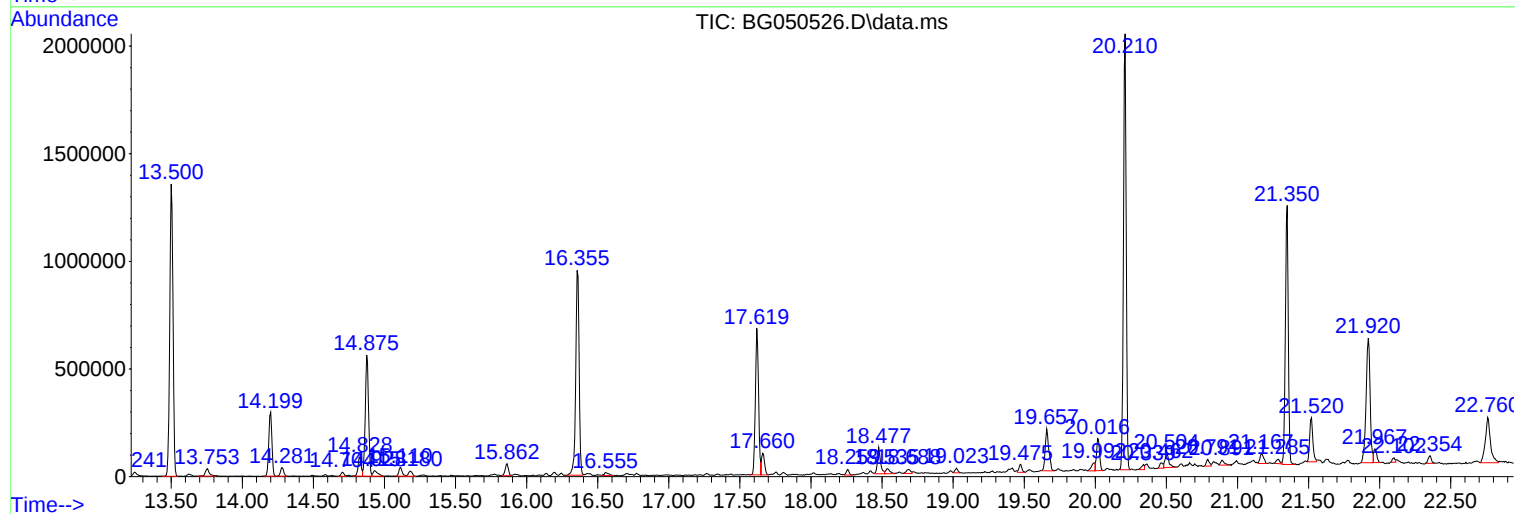
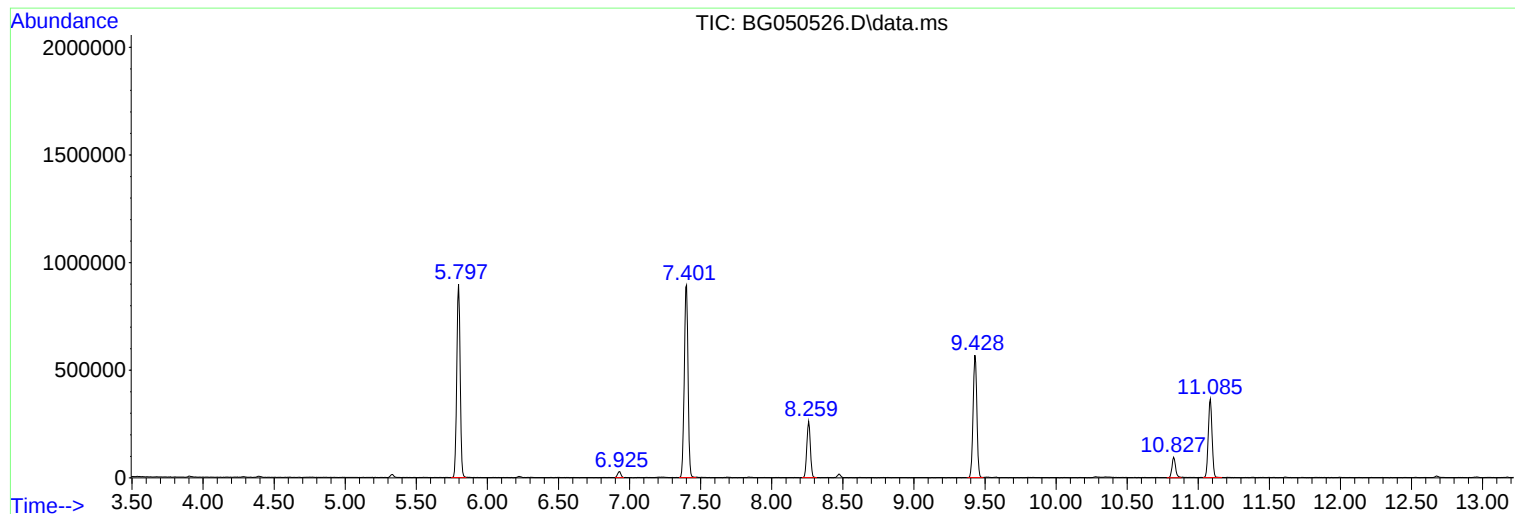
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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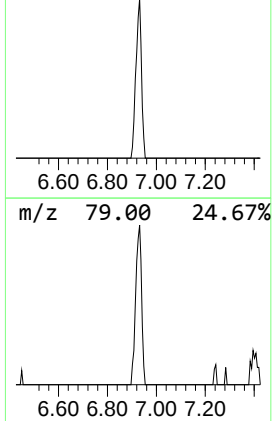
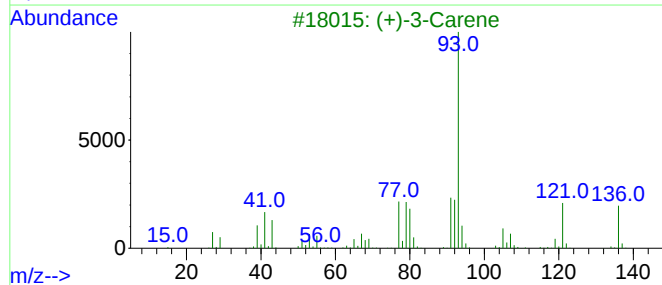
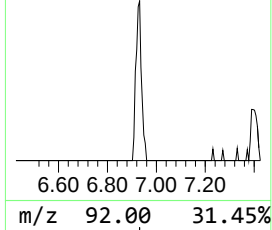
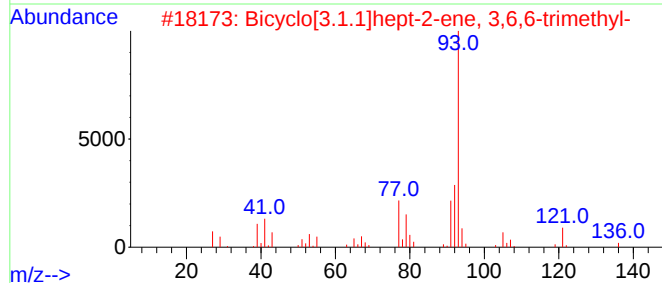
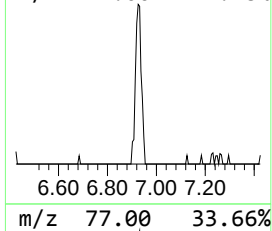
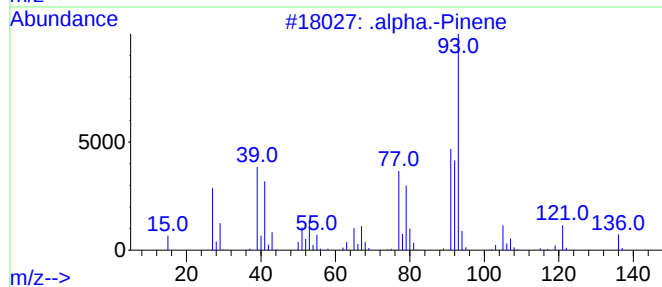
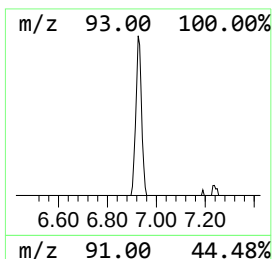
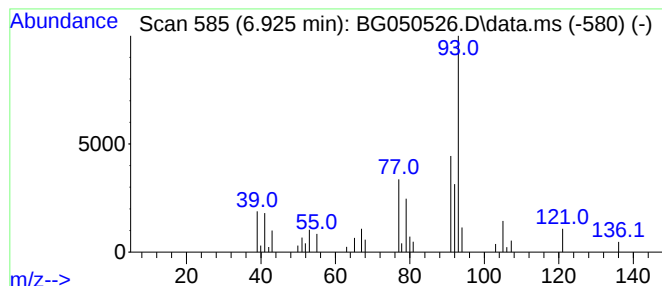
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 .alpha.-Pinene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.925	2.00 ng	45741	1,4-Dichlorobenzene-d4	8.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	95
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...			136	C10H16	004889-83-2	91
3	(+)-3-Carene			136	C10H16	000498-15-7	91
4	3-Carene			136	C10H16	013466-78-9	90
5	(1R)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-70-8	83



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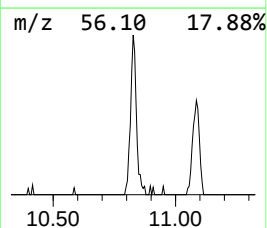
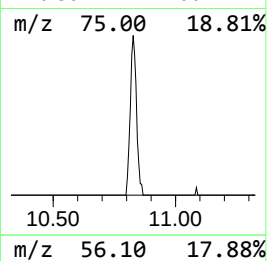
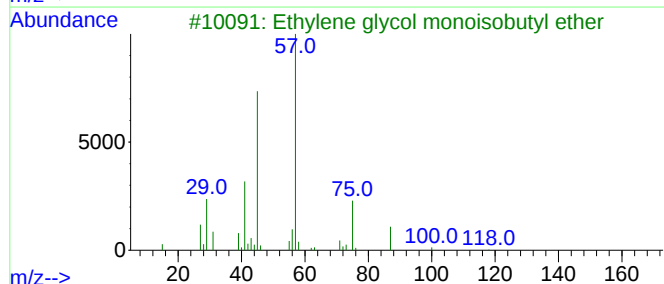
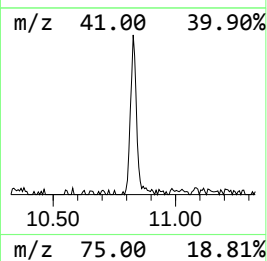
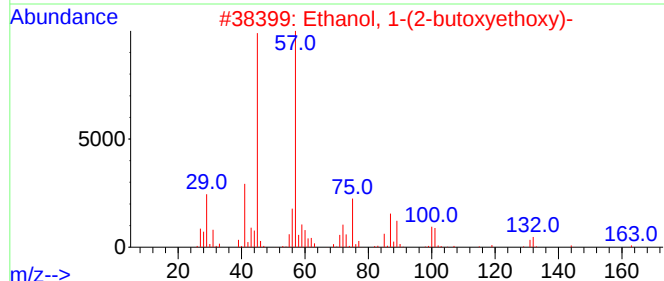
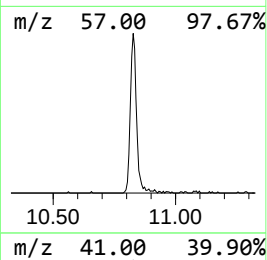
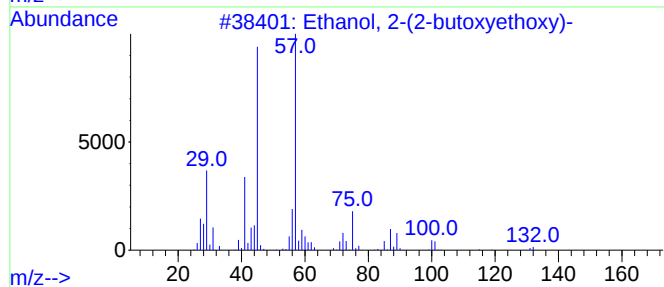
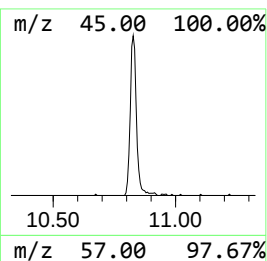
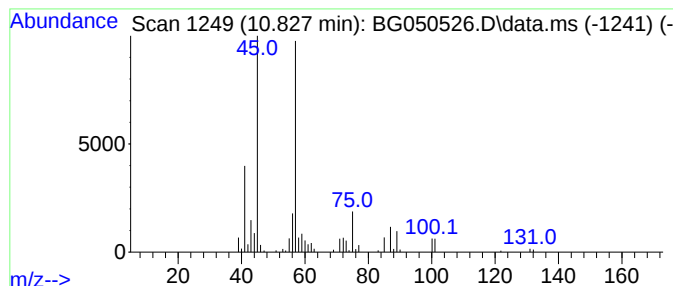
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.827	4.91 ng	166255	Naphthalene-d8	11.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53



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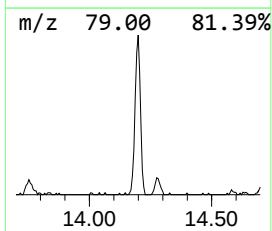
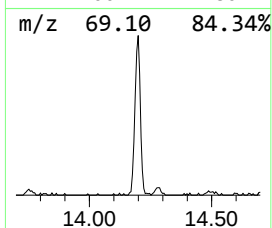
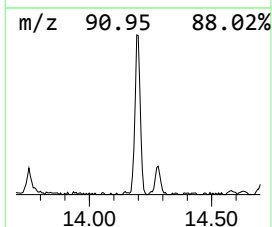
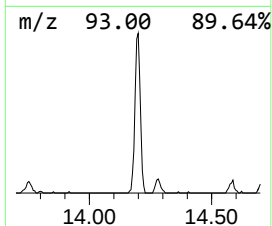
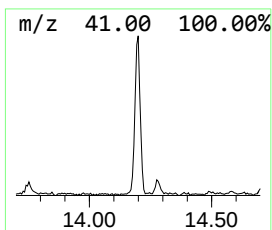
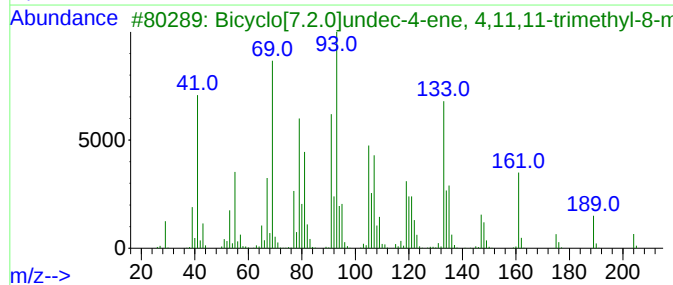
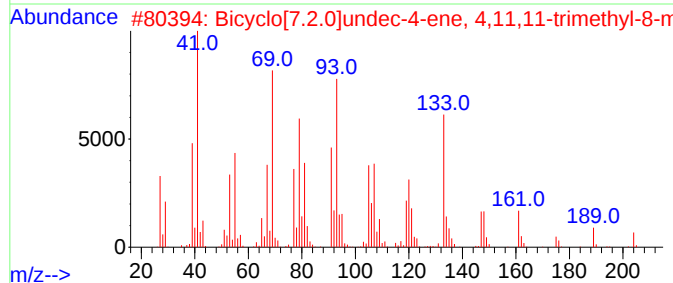
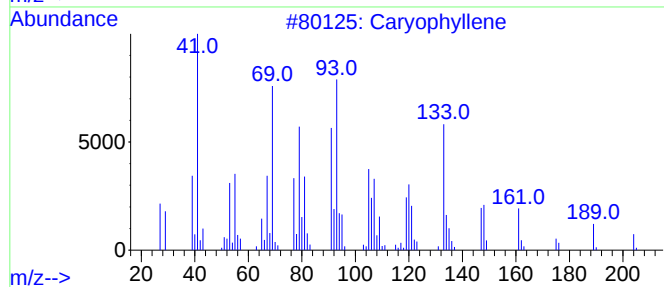
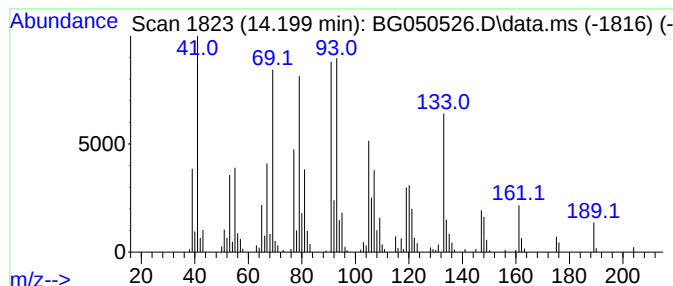
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Caryophyllene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.199	9.96 ng	450774	Acenaphthene-d10	14.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	95
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	94
3			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	70
4			Spiro[2.4]heptane, 1,5-dimethyl-...	136	C10H16	062238-24-8	38
5			Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	38



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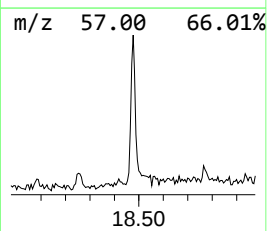
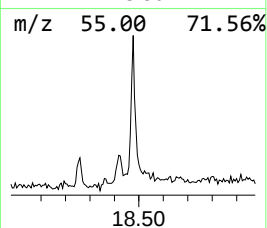
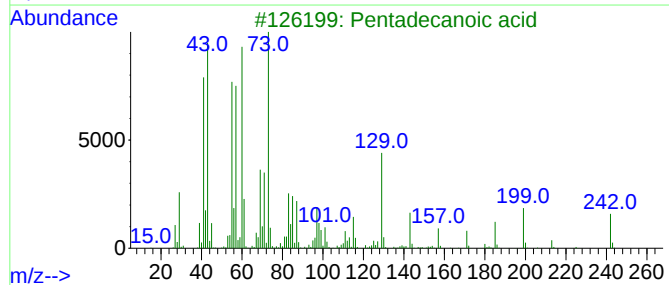
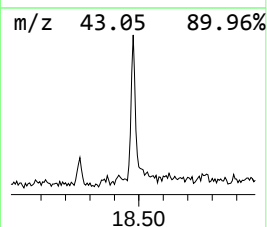
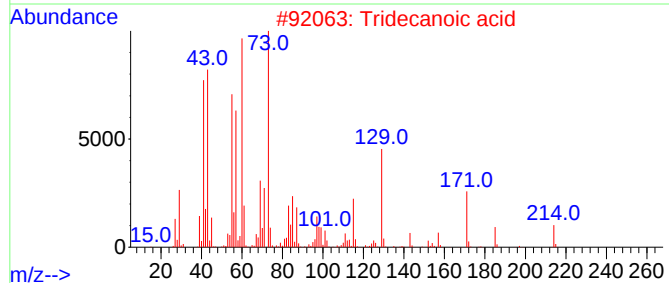
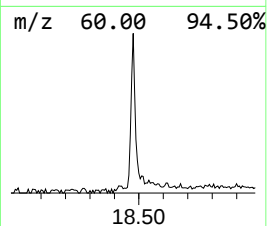
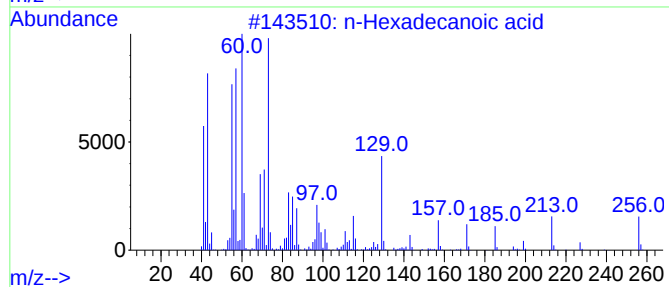
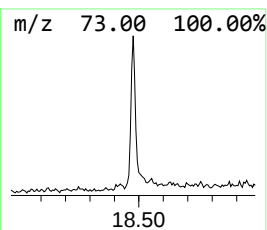
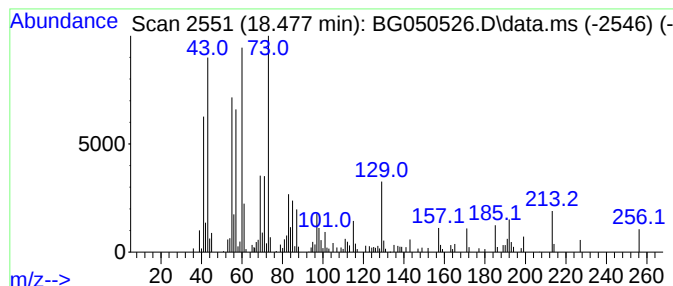
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.477	3.46 ng	182984	Phenanthrene-d10	17.619

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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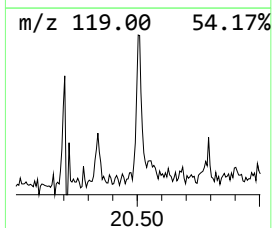
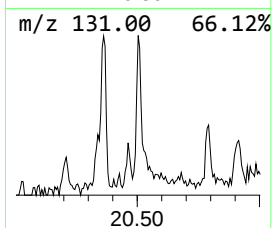
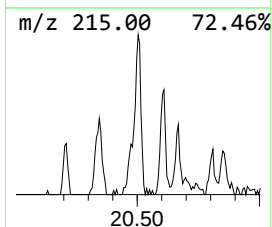
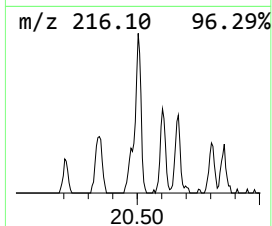
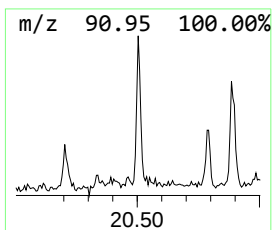
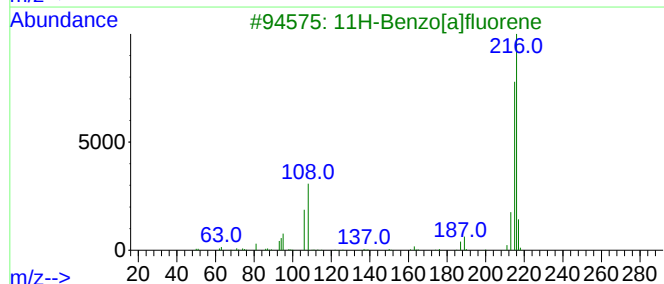
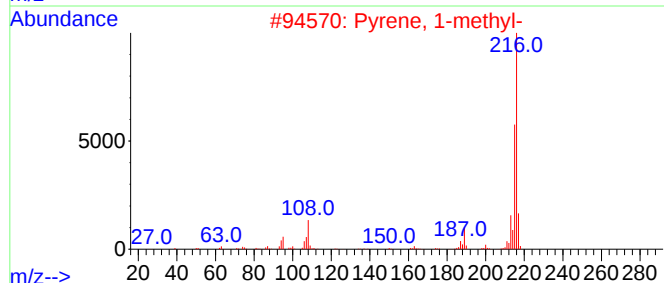
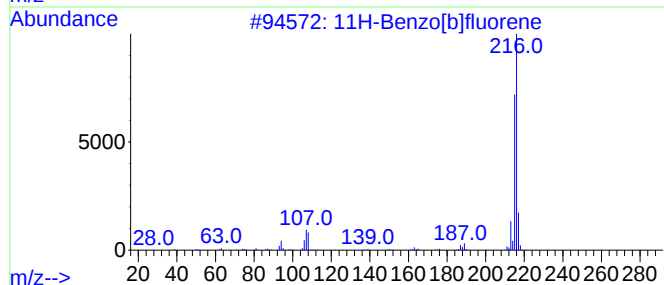
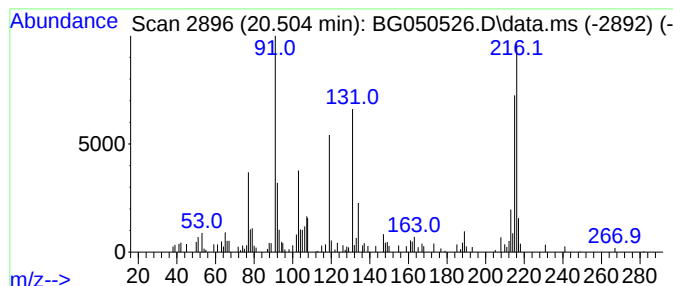
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.503	2.06 ng	119012	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	50
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	41
5			3-Trifluoromethylcinnamic acid	216	C10H7F3O2	000779-89-5	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
Operator : CG/JU
Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-5

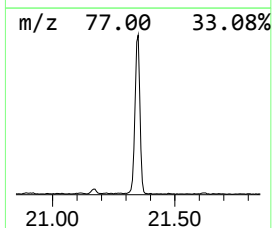
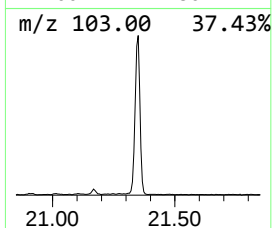
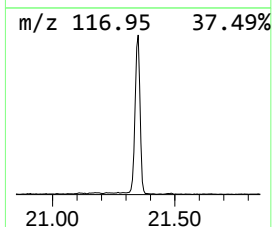
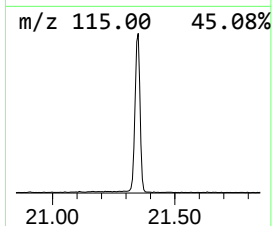
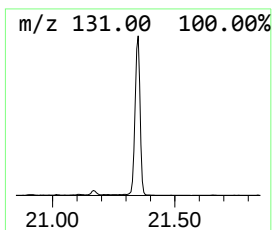
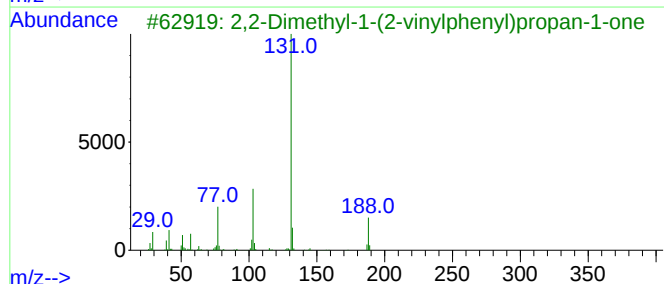
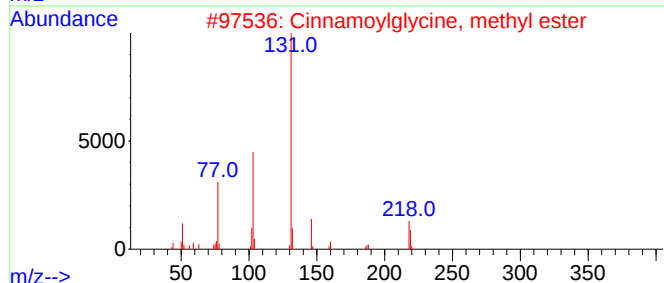
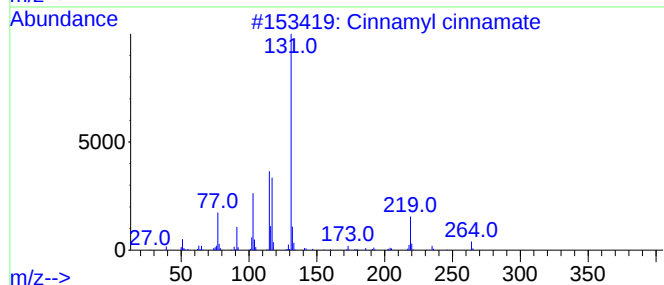
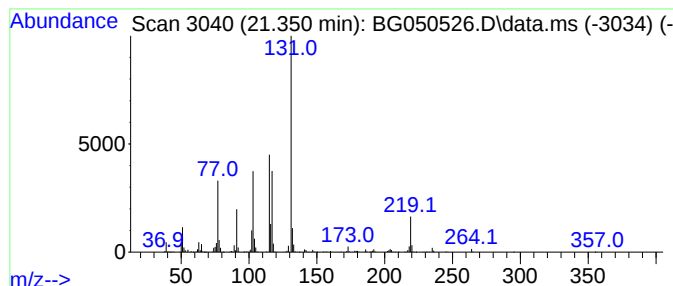
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.350	29.78 ng	1717470	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	49
3			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
4			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
5			N-(4-Fluorophenyl)-3-phenyl-2-pr...	255	C16H14FNO	1621516-09-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
Operator : CG/JU
Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-5

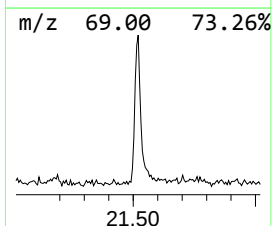
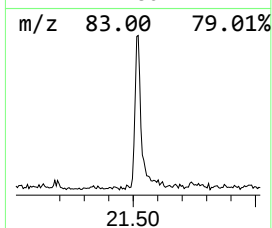
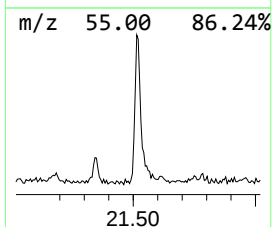
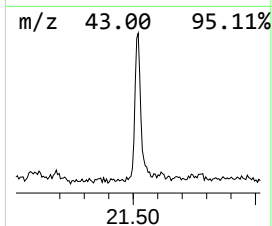
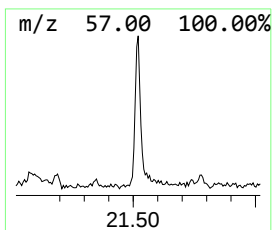
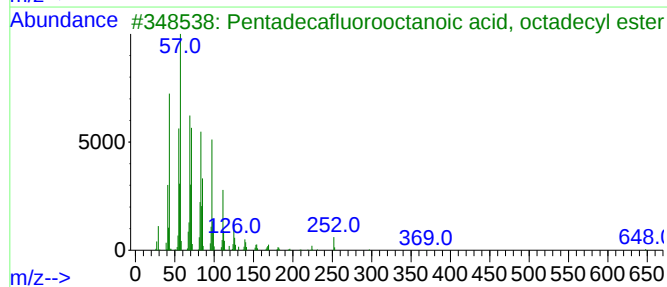
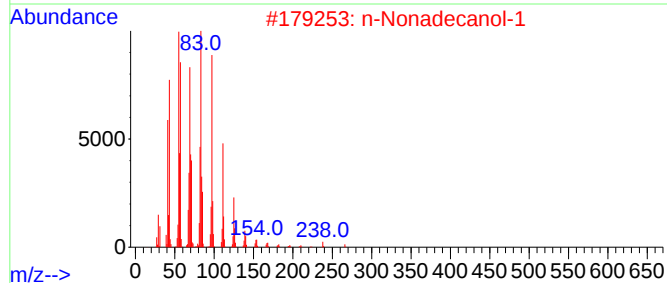
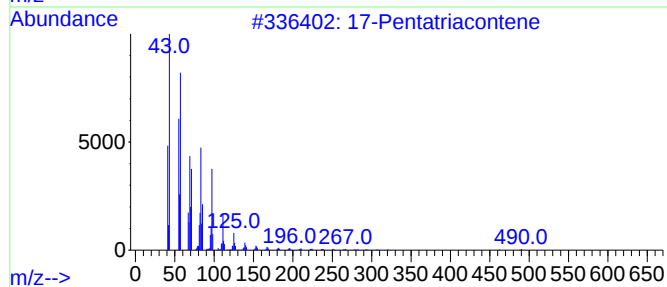
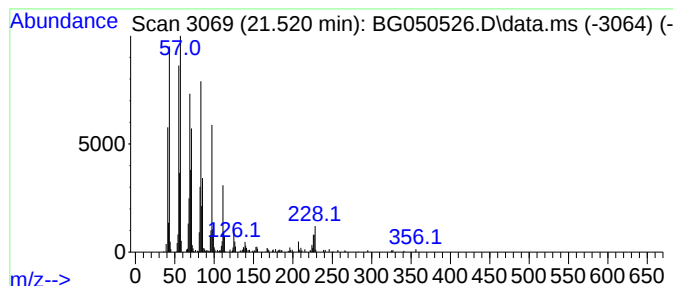
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.520	5.43 ng	313346	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4			1-Hexadecanol	242	C16H34O	036653-82-4	87
5			Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
Operator : CG/JU
Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

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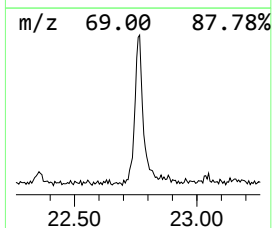
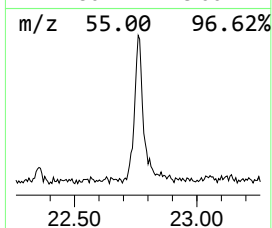
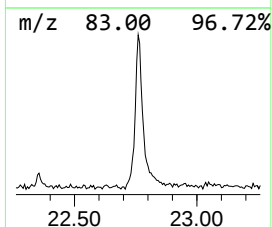
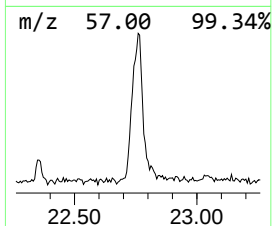
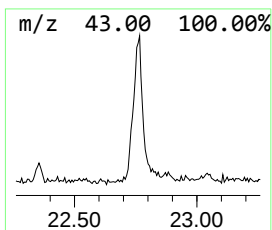
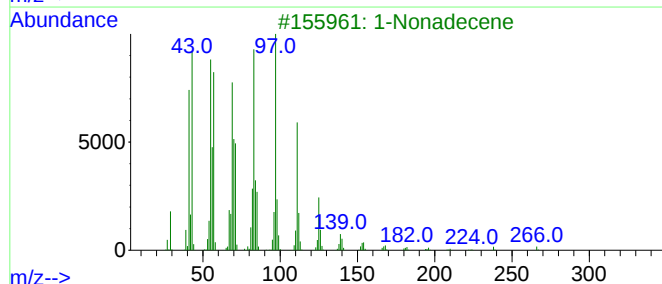
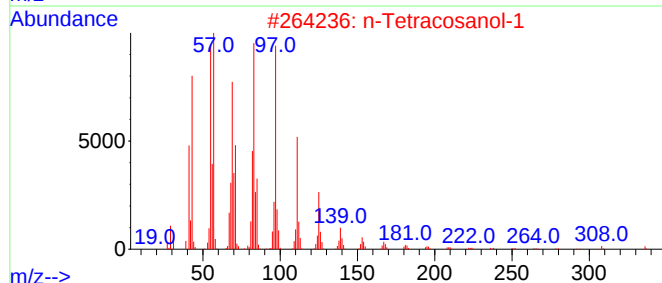
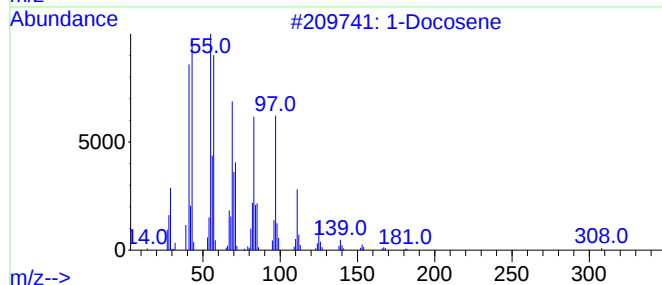
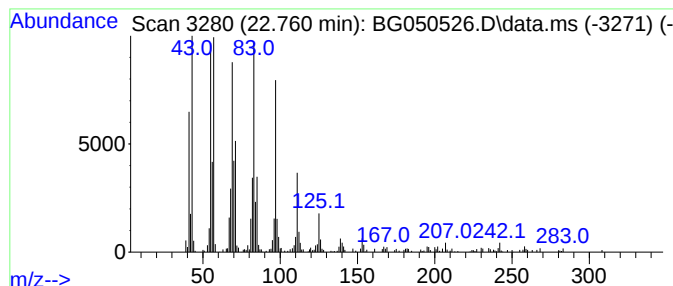
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.760	9.13 ng	526508	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	99
2	n-Tetracosanol-1			354	C24H50O	000506-51-4	94
3	1-Nonadecene			266	C19H38	018435-45-5	92
4	1-Tetracosene			336	C24H48	010192-32-2	91
5	1-Hexacosanol			382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
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Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-5

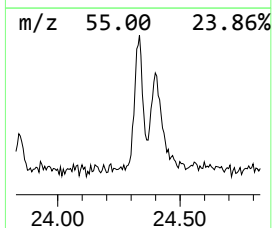
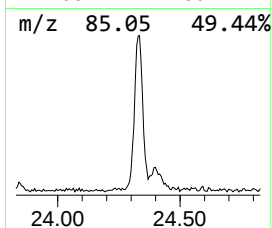
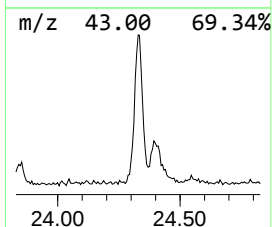
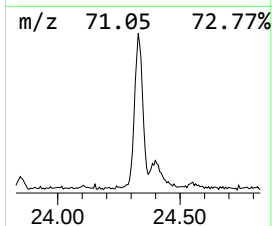
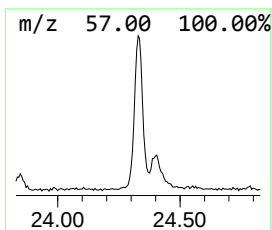
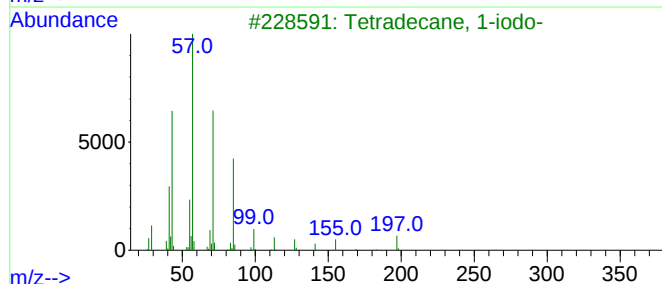
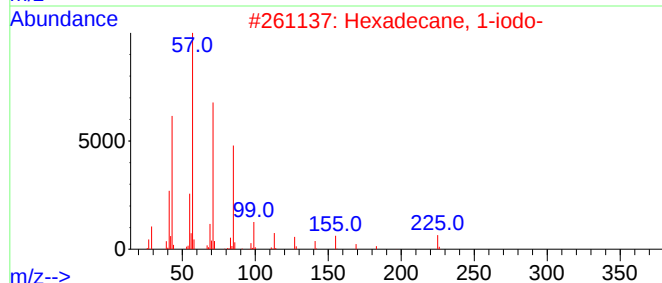
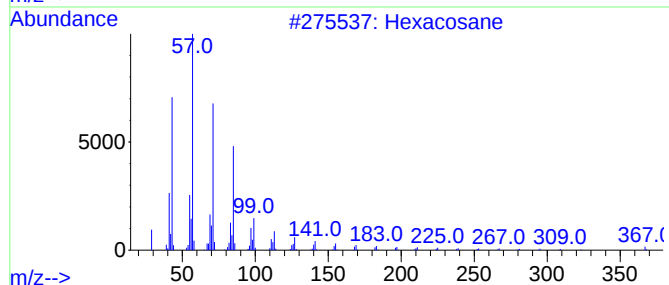
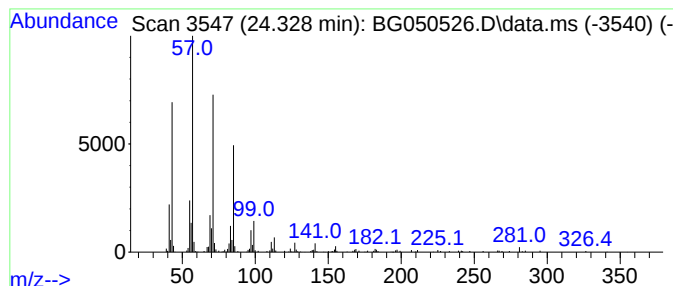
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.328	8.63 ng	451714	Perylene-d12	25.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5			Decane, 5-propyl-	184	C13H28	017312-62-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
Operator : CG/JU
Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-5

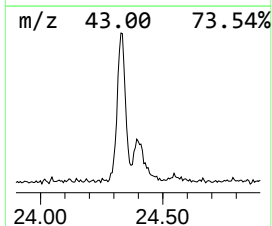
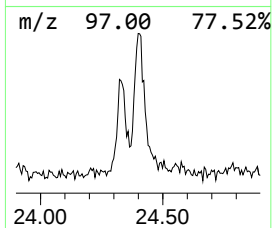
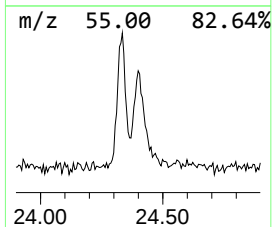
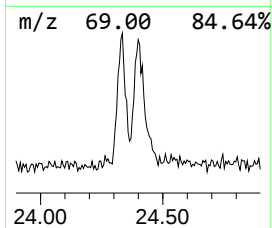
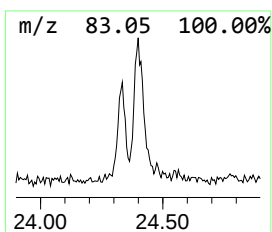
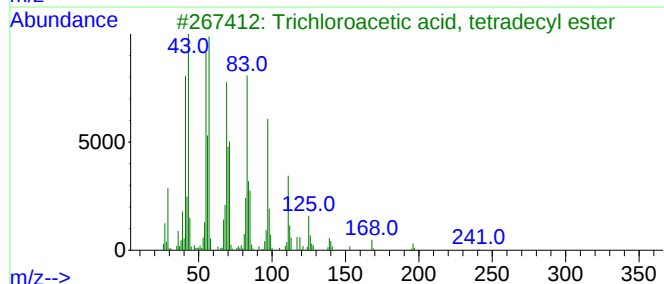
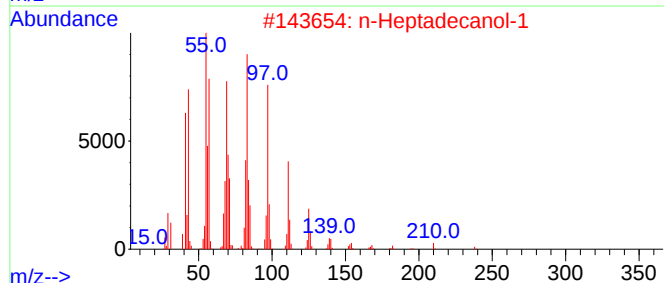
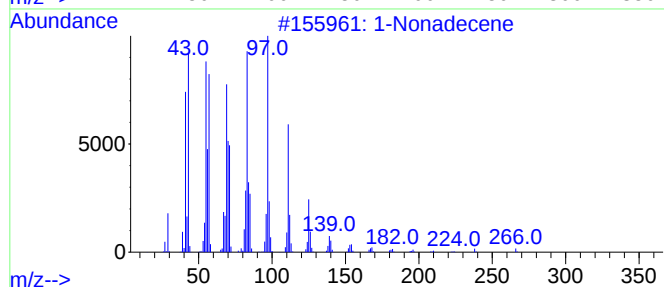
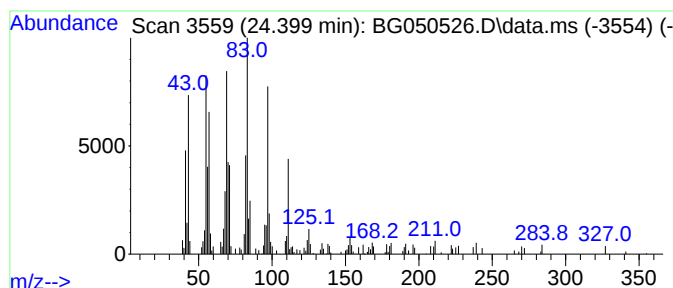
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.399	4.12 ng	215844	Perylene-d12	25.333

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	91
2	n-Heptadecanol-1		256	C17H36O	001454-85-9	91
3	Trichloroacetic acid, tetradecyl...		358	C16H29Cl3O2	074339-52-9	90
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	90
5	1-Octadecanol		270	C18H38O	000112-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
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Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
TP-5

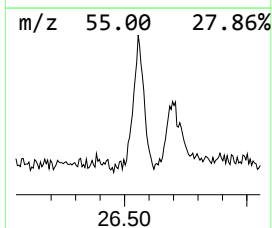
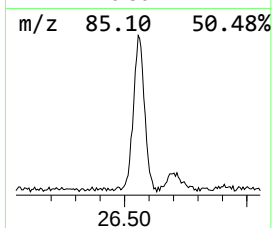
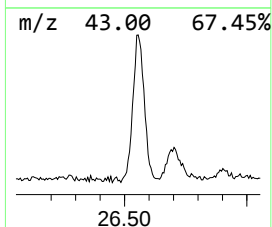
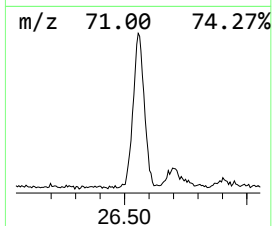
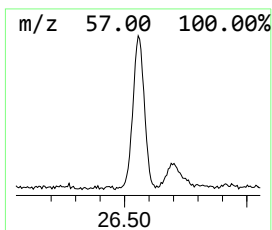
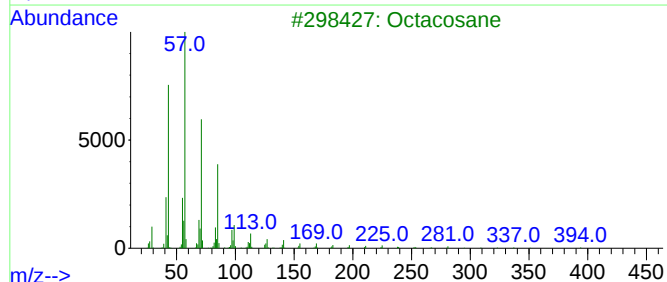
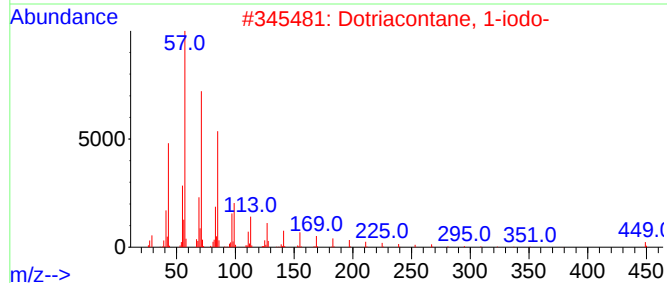
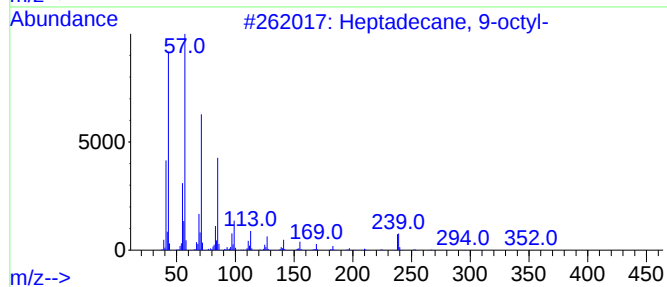
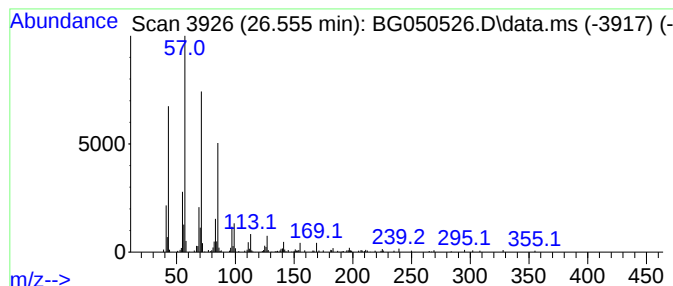
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.555	8.22 ng	430348	Perylene-d12	25.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane	240	C17H36	000629-78-7	90
5			Docosane	310	C22H46	000629-97-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
Operator : CG/JU
Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
TP-5

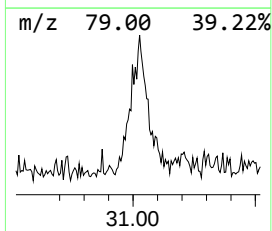
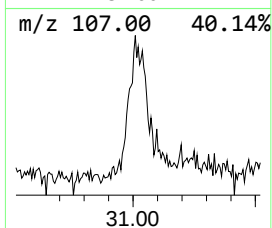
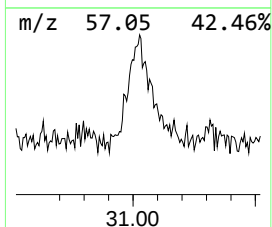
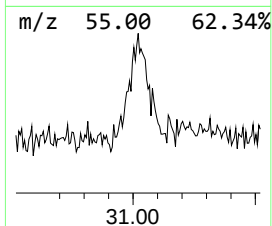
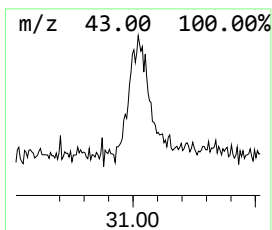
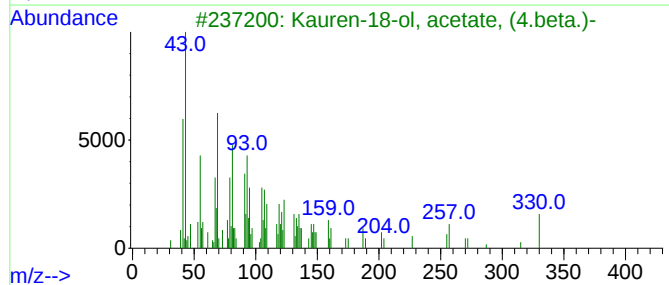
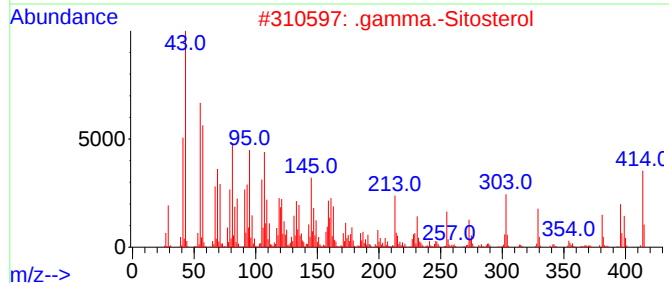
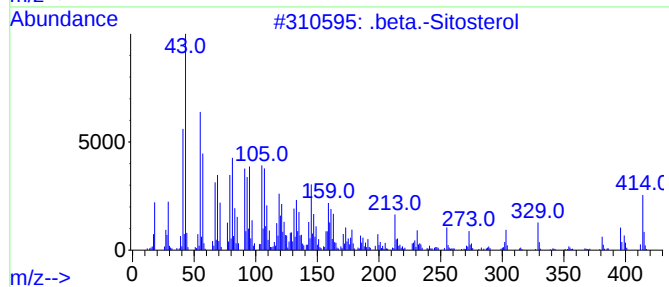
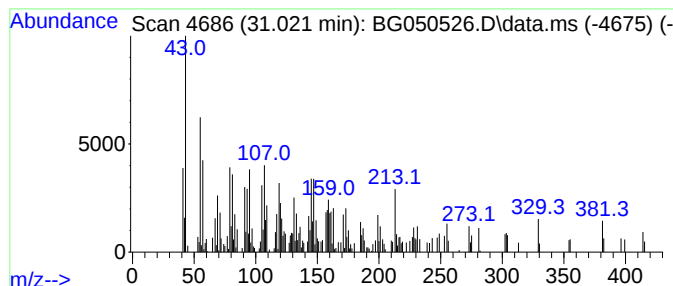
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.021	6.97 ng	365002	Perylene-d12	25.333

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	97
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	89
3		Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	41
4		5-Cholene, 3,24-dihydroxy-	360	C24H40O2	1000251-69-2	32
5		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050526.D
Acq On : 9 Oct 2021 2:33
Operator : CG/JU
Sample : M4113-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
.alpha.-Pinene	6.925	2.0	ng	45741	1	8.259	456704	20.0
Ethanol, 2-(2-b...	10.827	4.9	ng	166255	2	11.085	677754	20.0
Caryophyllene	14.199	10.0	ng	450774	3	14.875	905455	20.0
n-Hexadecanoic ...	18.477	3.5	ng	182984	4	17.619	1058890	20.0
11H-Benzo[b]flu...	20.503	2.1	ng	119012	5	21.919	1153380	20.0
Cinnamyl cinnamate	21.350	29.8	ng	1717470	5	21.919	1153380	20.0
17-Pentatriacon...	21.520	5.4	ng	313346	5	21.919	1153380	20.0
1-Docosene	22.760	9.1	ng	526508	5	21.919	1153380	20.0
Hexacosane	24.328	8.6	ng	451714	6	25.333	1047060	20.0
1-Nonadecene	24.399	4.1	ng	215844	6	25.333	1047060	20.0
Heptadecane, 9-...	26.555	8.2	ng	430348	6	25.333	1047060	20.0
.beta.-Sitosterol	31.021	7.0	ng	365002	6	25.333	1047060	20.0